and the ether was evaporated at approximately 40°C. The gas chromatography in this case was performed on a 6-ft Porapak Q column and thermal conductivity detector. In this way the solubility of water in diethyl ether was determined to be 1.28% (w/w) at 23°C. A value of 1.31% w/w is calculated from the data of Hill *(4)*, who employed a volumetric procedure. This is within the ±3% range assumed for the precision of the sampling technique.

According to other data reported by Hill *(4)*, the solubility of diethyl ether in water at 25°C is 60 mg/ml. Therefore, liquid-liquid extraction with diethyl ether as the organic phase and water at 25°C or ammonia at −74°C as the polar phase provides essentially the same conditions with regard to the solubility of the organic phase in the polar phase.

Literature Cited

(1) Francis, A. W., *Ind. Eng. Chem.*, **36**, 764 (1944).
(2) Franklin, E. C., Krause, C. A., *Amer. Chem. J.*, **20**, 820 (1898).
(3) Hala, J., Tuck, D. G., *J. Chem. Soc.*, **(A) 1970**, 3242.
(4) Hill, A. E., *J. Amer. Chem. Soc.*, **45**, 1143 (1923).
(5) Ishida, K., *Bull. Chem. Soc. Japan*, **31**, 143 (1958).
(6) McAuliffe, C., *J. Phys. Chem.*, **70**, 1267 (1966).
(7) Phipps, A. M., Hume, D. N., *Anal. Chem.*, **39**, 1755 (1967).
(8) Phipps, A. M., Hume, D. N., *J. Chem. Ed.*, **45**, 664 (1968).
(9) Phipps, A. M., McDermott, J. X., *Anal. Chem.*, **43**, 530 (1971).

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Effect of Pressure and Temperature on the Liquid Densities of Pure Hydrocarbons

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Two different approaches were taken to improve the methods of predicting the effect of pressure and temperature on the liquid densities of pure compounds. First, the Rackett equation for obtaining the saturated liquid density was introduced into two correlations previously given in the literature. Second, a set of generalized polynomials was developed to predict the correlating parameter of the Lu chart which is frequently used to evaluate the density variation with temperature and pressure. These correlations were evaluated for a set of 2590 data points for 32 compounds, mainly hydrocarbons. The regression of the Lu chart is shown to be quite accurate and the most general of the methods. A modification of the Chueh-Prausnitz approach is the most accurate when the specific constant of the Rackett equation is available.

At pressures higher than the vapor pressure, liquid densities increase with increasing pressure, provided, of course, the temperature remains constant. A number of correlations have been presented in the literature to predict this change in the liquid densities.

In a 1966 review of such correlations *(16)*, the methods of Watson *(35)*, Lu *(21)*, Lydersen et al. *(23)*, and Ritter et al. *(26)* were evaluated. The methods are all graphical in nature, and, while they may be convenient for obtaining a few predicted values, they are tedious for obtaining a large number of values and are not easily adaptable for use in computer programs. In the above review the following average percent errors in the predicted liquid densities were found for a data set consisting of approximately 150 points: Watson (2.06), Lu (1.57), Lydersen et al. (3.51), Ritter et al. (2.76). The Lu chart thus emerged from this study as the most accurate and was also commended for its general applicability.

Of these methods therefore only the method of Lu was considered in the present study. For this purpose a set of polynomial equations was developed to substitute for the graph normally used in the Lu procedure.

In addition, two newer methods, those of Yen and Woods *(36)* and of Chueh and Prausnitz *(4)*, were considered. Both of these methods require a saturated liquid density value at the temperature of interest. In addition to examining these methods as originally presented, an evaluation was made of the effect of introducing into them the modified Rackett equation *(31)* for predicting the saturated liquid density.

Approximately 2600 experimental data points for 32 compounds, mainly hydrocarbons, were used for these evaluations. The literature sources of these data are indicated in Table I.

Analytical Form of Lu Chart

The graphical method of Lu *(21)* is based on the approach recommended by Watson *(35)*:

$$\rho_1 = \left(K_1/K_R\right)\rho_R \qquad (1)$$

where ρ_1 and ρ_R are the desired density and the density at some reference condition, respectively, and K_1 and K_R are the corresponding values of the correlating parameter. Watson defined K as an empirical factor depending on T_r and P_r, while Lu defined it as $(Z_c^{0.77}/V_r)$. In both cases, the K factors are given in graphical form as a function of the reduced temperature and reduced pressure. The Lu chart covers a reduced temperature range of 0.5 to 1.0 and reduced pressures from saturation to 30.0.

Ewbank and Harden *(9)* revised a portion of the Lu chart. They expanded the scale in the range of reduced pressures less than 3.0 and reduced temperatures less than 0.76.

In the present study the correlating parameter of the Lu chart, as revised by Ewbank and Harden, has been represented by a set of generalized polynomials in T_r and P_r. A regression analysis of the Lu coefficient as a function of reduced temperature was made for each of the

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Table I. Comparison of the Correlations for the Effect of Pressure and Temperature on the Liquid Density

		Average % deviation[a]							
Compound	No. of data points	Regression of Lu chart	Original method of Yen and Woods	Modified[b] method of Yen and Woods	Original method of Chueh and Prausnitz	Modified[b] method of Chueh and Prausnitz	Temperature range of data, °F	Pressure range of data, psia	Data sources
Ethane	4	2.17	5.81	2.16	2.62	0.14	70	700 → 2,500	*(30)*
Propane	185	1.02	3.87	1.66	2.06	1.17	86 → 200	200 → 10,000	*(7, 20, 28)*
n-Butane	342	0.83	0.95	1.09	0.96	0.64	70 → 280	60 → 10,000	*(20, 28, 29)*
2-Methylpropane	183	0.64	4.70	0.70	3.06	0.29	100 → 250	80 → 5,000	*(14, 28)*
n-Pentane	477	0.79	4.34	1.46	2.21	0.80	100 → 370	20 → 10,000	*(20, 28)*
2-Methylbutane	6	2.45	5.39	5.20	2.29	2.83	212 → 347	152 → 3,110	*(18)*
2,2-Dimethylpropane	78	2.61	2.08	2.40[c]	1.28	2.24[c]	100 → 280	100 → 8,000	*(15)*
n-Hexane	105	1.18	1.44	1.39	1.49	1.04	−58 → 437	15 → 10,000	*(19, 24, 32)*
2-Methylpentane	46	0.98	1.42	1.61[c]	0.49	0.35[c]	212 → 392	82 → 4,583	*(19)*
3-Methylpentane	74	1.53	3.20	2.81[c]	2.87	3.24[c]	122 → 437	82 → 4,583	*(6)*
2,2-Dimethylbutane	69	0.74	1.01	1.30[c]	0.46	0.68[c]	212 → 392	147 → 4,410	*(12)*
n-Heptane	59	0.90	1.77	0.95	1.52	0.64	40 → 482	15 → 10,000	*(8, 25)*
n-Octane	78	1.23	2.78	1.66	0.51	0.60	212 → 527	73 → 4,410	*(11)*
2,2,4-Trimethylpentane	72	0.91	2.15	1.61	1.45	0.65	212 → 482	73 → 4,410	*(13)*
2,2,3,3-Tetramethylbutane	53	3.12	3.99	3.18	4.22	2.41	230 → 464	147 → 4,410	*(10)*
n-Nonane	66	1.40	2.25	1.89	2.00	0.71	86 → 572	200 → 10,000	*(3, 8)*
n-Decane	140	1.12	1.36	1.40	3.37	0.42	100 → 460	200 → 8,000	*(20)*
n-Undecane	42	2.09	2.47	4.09[c]	5.26	5.38[c]	86 → 572	739 → 21,770	*(8)*
n-Dodecane	18	0.49	2.39	1.98	3.81	0.41	100 → 275	15 → 10,000	*(1)*
n-Tridecane	42	1.91	4.22	8.11[c]	8.91	6.31[c]	86 → 572	739 → 14,518	*(8)*
n-Pentadecane	18	0.45	1.65	8.56[c]	9.33	9.94[c]	100 → 275	15 → 10,000	*(1)*
n-Heptadecane	30	2.85	4.64	16.02[c]	14.05	13.39[c]	122 → 572	739 → 7,267	*(8)*
n-Octadecane	15	0.46	5.50	30.90[c]	9.62	32.24[c]	140 → 275	15 → 10,000	*(1)*
n-Eicosane	25	3.41	8.79	30.24[c]	17.89	26.86[c]	212 → 572	739 → 7,267	*(8)*
Propene	12	1.07	0.87	0.74	0.83	0.54	40 → 160	200 → 10,000	*(27)*
1-Butene	12	1.51	2.00	1.38	1.92	1.02	100 → 280	200 → 10,000	*(27)*
1-Pentene	51	0.87	12.80	1.64	3.83	1.04	176 → 347	82 → 4,584	*(5)*
Propyne	9	1.56	4.83	1.91	2.58	0.35	122 → 212	200 → 3,829	*(34)*
1,2-Dimethylbenzene	201	0.80	1.25	1.05	1.85	1.14	77 → 662	19 → 7,369	*(17)*
1,3-Dimethylbenzene	60	0.69	2.23	1.48	1.86	0.43	68 → 527	15 → 5,880	*(33)*
Hydrogen Sulfide	12	1.39	3.02	3.54	0.81	1.23	40 → 160	200 → 10,000	*(27)*
Carbon dioxide	6	1.57	2.08	2.12	0.77	0.65	40	600 → 10,000	*(27)*
Overall	2590	1.09	2.95	2.29	2.52	1.75			

[a] $(100/N)\ \Sigma\ |\text{calculated value} - \text{experimental value}/\text{experimental value}|$. [b] Rackett eq. (Eq. 10) used to predict required saturated liquid density. [c] No Z_{RA} available, Z_c used.

reduced pressures. The coefficients for these equations were then regressed against the values of reduced pressure. Equations 2 and 3 give the form of the final equations:

$$K = A_0 + A_1T_r + A_2T_r^2 + A_3T_r^3 \qquad (2)$$

where A_i is given by

$$A_i = B_{0,i} + B_{1,i}P_r + B_{2,i}P_r^2 + B_{3,i}P_r^3 + B_{4,i}P_r^4 \qquad (3)$$

Various degrees of polynomials were investigated and the best fit of the data was obtained using the equations in the form as given above. The values of $B_{j,i}$ coefficients are given in Table II.

In the evaluation of these equations for the 32 compounds a reference density is required for use in Equation 1. For all compounds which are liquids at 60°F and 1 atm, the liquid density values were taken from the "Tech. Data Book—Petrol. Refining" *(2)*. For the others, the liquid density at 60°F and the equilibrium vapor pressure were used. All critical values were taken from *(2)*. The results of this correlation are given in Table I.

Alternative Analytical Methods

Yen and Woods *(36)* defined the density of a compressed liquid in reduced quantities as

$$\rho_r - \rho_{rs} = (\Delta\rho_r)_{27} + \delta_{Z_c} \qquad (4)$$

Here $(\rho_r - \rho_{rs})$ is the isothermal pressure effect on the reduced density based on the saturated reduced density, ρ_{rs}, and $(\Delta\rho_r)_{27}$ represents the reduced density increase for compounds with a Z_c of 0.27 when the pressure is increased from the equilibrium vapor pressure to the pressure of interest. The term $\delta_{Z(c)}$, which equals zero for compounds having a Z_c of 0.27, further corrects

Table II. Coefficients for Generalized Equations to Predict K Values of Lu Chart

i	$B_{0,i}$	$B_{1,i}$	$B_{2,i}$	$B_{3,i}$	$B_{4,i}$
0	1.6368	−0.04615	2.1138 (10^{-3})	−0.7845 (10^{-5})	−0.6923 (10^{-6})
1	−1.9693	0.21874	−8.0028 (10^{-3})	−8.2823 (10^{-5})	5.2604 (10^{-6})
2	2.4638	−0.36461	12.8763 (10^{-3})	14.8059 (10^{-5})	−8.6895 (10^{-6})
3	−1.5841	0.25136	−11.3805 (10^{-3})	9.5672 (10^{-5})	2.1812 (10^{-6})

the isothermal pressure effect on density for compounds with other Z_c values. It was recommended that the reduced saturated liquid density be calculated by the following equation:

$$\rho_{rs} = 1 + A(1 - T_r)^{1/3} + B(1 - T_r)^{2/3} + D(1 - T_r)^{4/3} \quad (5)$$

The A, B, and D in this equation have been correlated as polynomial functions of Z_c. The value of $(\Delta\rho_r)_{27}$ is calculated from

$$(\Delta\rho_r)_{27} = E + F \ln \Delta P_r + Ge^{H\Delta P_r} \quad (6)$$

Here ΔP_r is the reduced pressure increase from the vapor pressure to the pressure of interest and E, F, G, and H are given by complicated functions of T_r. Similarly, $\delta_{Z(c)}$ is given as a function of ΔP_r:

$$\delta_{Z_c} = I + J \ln \Delta P_r + Ke^{L\Delta P_r} \quad (7)$$

where I, J, K, and L are defined functions of T_r and Z_c. The critical density must be known or estimated. Needless to say, these calculations are extremely tedious and intended exclusively for computer applications.

Chueh and Prausnitz *(4)* have presented a generalized correlation for compressibilities of normal liquids in the following form:

$$\log \rho = \log \rho_s + \frac{1}{9} \log [1.0 + 9\beta_s(P - P_s)] \quad (8)$$

where β_s is the compressibility at saturation given as a function of T_r and ω. The equation of Lyckman et al. *(22)* is the recommended method for calculating the saturated liquid density, ρ_s. This equation has the form:

$$\rho_c/\rho_s = V_r = V_r^{(0)} + \omega V_r^{(1)} + \omega^2 V_r^{(2)} \quad (9)$$

The $V_r^{(i)}$'s are generalized functions of T_r and ω is the acentric factor. Again, the critical density must be known or estimated.

The accuracy of the correlations for the density of liquids under pressure depends strongly on the value of the saturated liquid density used. In an earlier paper *(31)* the Rackett equation was shown to be simple and accurate for the prediction of the saturated liquid densities over the entire temperature range from the triple point to the critical point. This equation has been given as

$$\frac{1}{\rho_s} = \left(RT_c/MP_c\right) Z_{RA}{}^{[1.0 + (1.0 - T_r)^{2/7}]} \quad (10)$$

where Z_{RA} is a specific constant for each compound; or, with some loss in accuracy, Z_c can be used if no Z_{RA} is available. The methods of Yen and Woods and Chueh and Prausnitz were therefore evaluated using the modified Rackett equation to obtain the saturated liquid densities—that is, Equation 10 was used in the correlations in place of Equations 5 and 9. All critical data were obtained from *(2)* in these calculations. The results are given in Table I.

Results and Conclusions

Examination of the results presented in Table I shows that the use of the Rackett equation to predict the required saturated liquid densities improves the accuracy of the methods of Yen and Woods and of Chueh and Prausnitz. In these modified methods, if no Z_{RA} was available for a compound *(31)* the Z_c value from *(2)* was used in place of Z_{RA}. For the higher molecular weight compounds the critical properties are only estimates and the values of Z_c are not reliable. Thus, it is not surprising that the errors are large when the Rackett equation was used for the compounds listed between *n*-tridecane and *n*-eicosane. The improvement obtained by use of the Rackett equation is much more pronounced if only those compounds having a Z_{RA} value are considered. This modification of the data set eliminates 439 points.

Thus, the average percent deviation for the remaining 2151 data points by the method of Yen and Woods goes from 2.98 to 1.39 by introduction of the Rackett equation, while by the method of Chueh and Prausnitz the improvement is from 2.04 to 0.80%. On this basis it is clear that the Rackett equation should be used in these correlations if a Z_{RA} value is available. For this smaller data set the Chueh-Prausnitz method using the Rackett equation gave an average percent bias of −0.15 and an average percent root mean square deviation of 1.53. The regression of the Lu chart for this same set of data gave the following results: average percent deviation, 0.96; average percent bias, 0.10; average percent root mean square deviation, 1.42. In both methods the largest errors generally occurred in the region where the reduced temperature was greater than 0.95.

The outstanding feature of the data presented in Table I is the performance of the Lu chart as represented by the generalized polynomials, Equations 2 and 3. This method gives the best over-all performance for the 32 compounds, exhibiting no serious deviations for any one of them. In addition, it is quite general, relatively simple to apply, and easily programmed on a computer. Its only possible disadvantage is the requirement for a reference density at some known temperature and pressure. One such value is practically always available, however.

In summary, the method of Chueh and Prausnitz, as modified by the introduction of the Rackett equation, generally predicts the best values for those compounds having a defined Z_{RA}. If a Z_c value must be used in the Rackett equation in place of Z_{RA}, however, large errors may result, as shown in Table I. Thus for a case where generality, as well as accuracy, is important, the polynomials representing the Lu chart are recommended. On the other hand, for a particular calculation involving a compound for which a Z_{RA} is available the modified Chueh-Prausnitz procedure may be more accurate.

Nomenclature

K = correlating parameter of Lu chart
M = molecular weight
P_c = critical pressure, atm
P_r = reduced pressure, P/P_c
R = universal gas constant, 82.06 atm cm^3/g mole K
T_c = critical temperature, K
T_r = reduced temperature, T/T_c
V = volume, cm^3/g

V_c = critical volume, cm^3/g
V_r = reduced volume, V/V_c
Z_c = critical compressibility factor
Z_{RA} = constant of modified Rackett equation
β_s = liquid compressibility at saturation
ρ = liquid density, g/cm^3
ρ_c = critical density, g/cm^3
ρ_r = reduced density, ρ/ρ_c
ρ_s = saturated liquid density, g/cm^3
ρ_{rs} = reduced saturation liquid density, ρ_s/ρ_c
ω = acentric factor

Literature Cited

(1) American Petroleum Institute, "Properties of Hydrocarbons of High Molecular Weight Synthesized by Research Project 42, 1940-66," Am. Petrol. Inst., Washington, D.C., 1966.
(2) American Petroleum Institute, "Technical Data Book—Petroleum Refining," 2nd ed., Am. Petrol. Inst., Washington, D.C., 1971.
(3) Carmichael, L. T., Sage, B. H., Lacey, W. N., *Ind. Eng. Chem.*, **45**, 2697 (1953).
(4) Chueh, P. L., Prausnitz, J. M., *AIChEJ*, **15**, 471 (1969).
(5) Day, H. O., Felsing, W. A., *J. Amer. Chem. Soc.*, **73**, 4839 (1951).
(6) Day, H. O., Felsing, W. A., *ibid.*, **74**, 1951 (1952).
(7) Deschner, W. W., Brown, G. G., *Ind. Eng. Chem.*, **32**, 836 (1940).
(8) Doolittle, A. K., *J. Chem. Eng. Data*, **9**, 275 (1964).
(9) Ewbank, W. J. Harden, D. G., *ibid.*, **12**, 363 (1967).
(10) Felsing, W. A., Cuellar, A. M., Newton, W. M., *J. Amer. Chem. Soc.*, **69**, 1972 (1947).
(11) Felsing, W. A., Watson, G. M., *ibid.*, **64**, 1822 (1942).
(12) Felsing, W. A., Watson, G. M., *ibid.*, **65**, 1889 (1943).
(13) Felsing, W. A., Watson, G. M., *ibid.*, **65**, 780 (1943).
(14) Gonzales, M. H., Lee, A. L., *J. Chem. Eng. Data*, 11, 357 (1966).
(15) Gonzales, M. H., Lee, A. L., *ibid.*, **13**, 66 (1968).
(16) Holmes, A. S., Thompson, W. H., Braun, W. G., Fenske, M. R., "Documentation of the Basis for Selection of the Constants of Chapter 6, 'Density,' in 'Technical Data Book—Petroleum Refining'," Doc. Rept. No. 6-66, Am. Petrol. Inst., Washington, D.C., 1966.
(17) Imanov, Sh. Yu., Akhundov, T. S., *Zh. Fiz. Khim.*, **43** [6] 1568 (1969).
(18) Isaac, R., Li, K., Canjar, L. N., *Ind. Eng. Chem.*, **46**, 199 (1954).
(19) Kelso, E. A., Felsing, W. A., *J. Amer. Chem. Soc.*, **62**, 3132 (1940).
(20) Lee, A. L., "Viscosity of Light Hydrocarbons," Monograph of API Research Project No. 65, Am. Petrol. Inst., Washington, D.C., 1965.
(21) Lu, B. C.-Y., *Chem. Eng.*, **66** [9], 137 (1959).
(22) Lyckman, E. W., Eckert, C. A., Prausnitz, J. M., *Chem. Eng. Sci.*, **20**, 703 (1965).
(23) Lydersen, A. L., Greenkorn, R. A., Hougen, O. A., "Generalized Thermodynamic Properties of Pure Fluids," Univ. Wisconsin Eng. Expt. Sta. Res. Rept. No. 4, 1955.
(24) Mopsik, F. I., *J. Res. Nat. Bur. Stand.*, **A 4**, 287 (1967).
(25) Newton, R. H., *Ind. Eng. Chem.*, **27**, 302 (1935).
(26) Ritter, R. B., Lenoir, J. M., Schweppe, J. L., *Petrol. Refiner*, **37** (11) 225 (1958).
(27) Sage, B. H., Lacey, W. N., "Some Properties of the Lighter Hydrocarbons, Hydrogen Sulfide, and Carbon Dioxide," Monograph of API Research Project 27, Am. Petrol. Inst., Washington, D.C., 1959.
(28) Sage, B. H., Lacey, W. N., "Thermodynamic Properties of the Lighter Paraffin Hydrocarbons and Nitrogen," Monograph of API Research Project Number 37, Am. Petrol. Inst., Washington, D.C., 1950.
(29) Sage, B. H., Webster, D. C., Lacey, W. N., *Ind. Eng. Chem.*, **29**, 658 (1937).
(30) Sage, B. H., Webster, D. C., Lacey, W. N., *ibid.*, **29**, 1188 (1937).
(31) Spencer, C. F., Danner, R. P., *J. Chem. Eng. Data*, **17**, 236 (1972).
(32) Stewart, D. E., Sage, B. H., Lacey, W. N., *Ind. Eng. Chem.*, **46**, 2529 (1954).
(33) Tairov, A. D., Akhundov, T. S., Mamedov, A. M., *Izv. Vysshikh Uchebn. Zavedenii Neft. i Gaz*, **9**, 71 (1966).
(34) Vohra, S. P., Kang, T. L., Kobe, K. A., McKetta, J. J., *J. Chem. Eng. Data*, **7**, 150 (1962).
(35) Watson, K. M., *Ind. Eng. Chem.*, **35**, 398 (1943).
(36) Yen, L. C., Woods, S. S., *AIChEJ*, **12**, 95 (1966).

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Prediction of Bubble-Point Density of Mixtures

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Methods for predicting the density of mixtures at their bubble points have been extensively evaluated. Two analytical methods for pure compounds recently reported by the authors—the modified Rackett equation and the generalized polynomials representing the Lu chart—have been extended to mixtures. On the basis of a comparison of the experimental densities of a series of binary systems with those predicted by these methods and the equations of others, a modification of the Rackett equation is recommended for its accuracy and versatility. For mixtures containing only hydrocarbons, the average percent error in the predicted bubble-point densities was less than 2. The method of Harmens was essentially equivalent in accuracy for the systems studied. Results for systems containing a nonhydrocarbon suggest that larger errors should be expected for such systems.

The authors have recently reported that a modified version of the Rackett equation and an analytical form of the Lu chart are accurate methods of predicting the liquid density of pure compounds (*22*, *31*). To be of real practical value, these methods must be shown to be applicable to mixtures.

Available Correlations

A number of investigators have developed equations for predicting the bubble-point density of mixtures. Ritter et al. (*27*) have presented a nomograph for calculating the specific gravity of paraffinic hydrocarbon mixtures at their bubble points. This procedure requires only the average molecular weight of the mixture, but is limited to molecular weights less than 100. It has the disadvantage of being available only in a graphical form, and thus is not readily applied to a large number of data points or in a computer program.

Harmens (*5*, *6*) has developed a correlation in the following form:

$$\frac{1}{V_{bp}} = \rho_{bp} = C \cdot F(T_r) \qquad (1)$$

C is a constant which has been specified for a number of compounds in the range of C_1 to C_7. When no specific C value is available, a value can be predicted by Equation 2.

$$C = \rho_c\,[0.43875 - 0.625\,Z_c] \qquad (2)$$

$F(T_r)$ was originally given in tabular form. In the present evaluation, a regression analysis was used to transform this tabular function into the following analytical form:

$$F(T_r) = 15.81 - 17.71\,T_r + 22.67\,T_r^2 + 15.07\,T_r^3 \qquad (3)$$

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