A NEW CORRELATION FOR THE SPECIFIC HEAT OF METALS, METAL OXIDES AND METAL FLUORIDES AS A FUNCTION OF TEMPERATURE

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Abstract

The objective of this work is to find a suitable correlation that best fits the specific heat of metals, metal oxides and metal fluorides as a function of temperature. It was found that a multilinear regression model of the form $C_P = aT^b e^{cT} e^{d/T}$ has the lowest deviation from experimental data compared to other correlations including a 4th to 6th-order polynomial regression model. The coefficient of determination, R^2, was very close to unity in most cases and the average of the absolute relative errors, AARE, was less than 5% for the specific heat of most of the systems studied. The overall AARE was about 1.8% for metals and 3% for metal oxides and metal fluorides, which is within the experimental error.

Key Words: correlations; metals; metal fluorides; metal oxides; specific heat.

I. Introduction

Materials are diverse in our life and have many uses. Many applications of metals, ceramics, fluxing materials and composites are based upon their unique thermophysical properties. Specific heat, thermal conductivity and thermal expansion are the properties that are often critical in the practical utilization of solids as materials of construction (Abu-Eishah, 2001a). These properties depend upon the state, chemical composition, and physical structure of that material. They also depend on temperature and to a lesser extent on pressure, to which the material is subjected. In the design of rocket-engine thrust chambers, for example, considerable attention must be given to the effect of temperature on the thermophysical properties of its structure. The primary concern of engineers is to match the material properties to service requirements of the component, knowing the conditions of load and environment under which the component must operate. Engineers must then select an appropriate material, using tabulated test data, as the primary guide (Abu-Eishah, 2001b).

Specific heat is the property that is indicative of materials ability to absorb heat from external surroundings. The specific heat of a material is largely determined by the effect of temperature on the vibration and rotational energies of the atoms within the material, the change in energy level of electrons in the structure of the material, and changes in atomic positions during formation of lattice defects (vacancies and interstitials), order-disorder transitions, magnetic orientation or polymorphic transformations (Richerson, 1992).

In a previous work, Abu-Eishah (2001a) proposed a multilinear correlation to fit the thermal conductivity of metals as a function of temperature and found it among the best. In this study it is intended to check the suitability of such a multilinear correlation to fit the specific heat of metals, metal oxides and metal fluorides as a function of temperature.

II. Proposed Fitting Equations

The theories of the specific heat of metallic and non-metallic solids are covered in detail by Touloukian and Ho (1972a,b). The theoretical equation that represents the specific heat, in general, is given in Touloukian and Ho (1972a) as

$$C_P = aT + bT^3 + c/T^2 \qquad (1)$$

The terms on the right-hand side of Eq. (1) belong to the electronic, lattice combination, and nuclear combination parts of the specific heat. Up to the knowledge of the authors, Eq. (1) was not used as is to fit the specific heat experimental data. Perry and Green (1997) give C_P for pure compounds (metallic and non-metallic solids) as a linear equation of the form ($C_P = a + bT$) for some compounds and by a nonlinear equation of the form ($C_P = a + bT + c/T^2$) for others. The temperature range (starting at 273 K), the values of the coefficients a, b and c, and the uncertainty (%) of these correlations are also given in Perry and Green (1997) and summarized in Appendix. In this work, a wider and more comprehensive temperature ranges were covered compared to those used in Perry and Green (1997).

The multilinear fitting equation proposed in this study has the form

$$C_P = aT^b e^{cT} e^{d/T} \qquad (2)$$

If the exponential terms in Eq. (2) are expanded by a Taylor's series, then we get

$$C_P = aT^b[A + BT + CT^2 + \ldots + D/T + E/T^2 + \ldots] \qquad (3)$$

which can be rewritten as

$$C_P = A'T^b + B'T^{b+1} + C'T^{b+2} + \ldots + D'/T^{b-1} + E'/T^{b-2} + \ldots \qquad (4)$$

where, $A' = aA$, $B' = aB$, etc. By comparing Eqs. (1) and (4), all terms in Eq. (1) are almost there in Eq. (4), but Eq. (4) has extra merits; it is more than just a polynomial, a power or an exponential function, it is a combination of all of these functions. It can have positive and negative exponents, with integer and non-integer values. Also, while Eq. (1) may predict negative specific heat at low temperatures, the parameter a in Eq. (2) is always nonnegative, which is needed for presenting always positive thermophysical data such as specific heat. Taking the logarithm of both sides of Eq. (2) gives

$$\ln C_P = \ln a + b \ln T + cT + d/T \tag{5}$$

T in Kelvin and a, b, c and d are fitting constants. That is, Eq. (5) can be rewritten as

$$Y = a_1 X_1 + a_2 X_2 + a_3 X_3 + a_4 X_4 \tag{6}$$

where $a_1 = \ln a$, $a_2 = b$, $a_3 = c$, $a_4 = d$, and $Y = \ln C_P$, $X_1 = 1.0$, $X_2 = \ln T$, $X_3 = T$, and $X_4 = 1/T$. That is, all terms in Eq. (6) are linear in X_i, i = 1, 2, 3, and 4; from which the multilinear name of the proposed model is derived. In addition to the multilinear regression, and for comparison purposes, an nth-order polynomial model of the form

$$C_P = B_0 + B_1 T + B_2 T^2 + B_3 T^3 + \ldots + B_n T^n \tag{7}$$

is used in this study. Here B_0, B_1, B_2 … B_n are the polynomial fitting parameters.

Although the polynomial regression method is well known and easy to implement on digital computers, its main disadvantages are more fitting parameters are needed to get higher accuracy, and it might give impractical (or unrealistic negative) values for the predicted property. Polynomials are based on power laws and diverge greatly at or near the end points of the data region. They are thus poor candidates for fitting "smooth" curves. In addition, polynomials force a certain number of inflection points that may not be in the "real" behavior of the physical property.

No body can claim any physical significance of the parameters of the proposed model, at least for the time being, but this model, which is a combination of power and exponential series, is characterized by (a) smaller number of fitting parameters and (b) a more realistic representation of the experimental data (no negative values, for example). The main disadvantage of this method is that it does not properly fit sharp changes in the physical properties.

III. Results and Discussion

The experimental data for the specific heat of metals, metal oxides and metal fluorides were taken from Touloukian and Ho (1972a,b). Information about the purity, composition, and specifications concerning the samples used originally for experimental analysis as well as the reported error (last column of Appendix) are available in Touloukian and Ho (1972a). Throughout the analysis of results, the following basic definitions have been used:

$$\text{Absolute Error, AE} = |C_{P\text{exp}} - C_{P\text{cal}}|$$

Absolute Relative Error,

$$\text{ARE} = |C_{P\text{exp}} - C_{P\text{cal}}|/C_{P\text{exp}}$$

Average of Absolute Errors,

$$\text{AAE} = \sum (\text{Absolute Errors})/M$$

Average of Absolute Relative Errors,

$$\text{AARE} = \sum (\text{Absolute Relative Errors})/M$$

M is the number of data points in a given set of data. The coefficient of determination, R^2, is defined in terms of the symbols used in Eq. (6) as

$$R^2 = \frac{\sum_i \left(Y_{\text{exp},i}\, Y_{\text{cal},i}\right) - \left(\sum_i Y_{\text{cal},i}\right)\left(\sum_i Y_{\text{exp},i}\right)/M}{\sum_i \left(Y_{\text{exp},i}\right)^2 - \left(\sum_i Y_{\text{exp},i}\right)^2 / M} \tag{8}$$

and the standard error of estimate, *SSE*, is defined as

$$SEE = \sqrt{\sum_i^M \left(Y_{\text{exp},i} - Y_{\text{cal},i}\right)^2 /(M\text{-}2)} \tag{9}$$

where $Y_{\text{cal},i} = \sum_j a_j X_{ji}$, and i = 1, 2, …, M and j = 1, 2, … 4.

The experimental data used for metals, metal oxides and metal fluorides were taken from Touloukian and Ho (1972a,b) on the basis of very similar purity and composition of the chosen samples (curves). It should be mentioned first that, up to the knowledge of the authors, there is no single equation that fits all the temperature range of the specific heat of the studied systems. Equation (1) is just a proposed theoretical formula, but not used to fit the experimental specific heat data of the studied systems.

For all the metal samples used, any impurity in the sample is less than 0.2% each, and the total impurity in any sample is less than 0.5% (Touloukian and Ho, 1972a,b). Table 1 shows the calculated fitting parameters for the specific heat of metals, the coefficient of determination, R^2, and the average of the absolute relative error, AARE. R^2 values are very close to unity, the values of AARE are less than 5%, and the overall AARE is about 1.8%, which is within the experimental error. The standard error of estimate, *SEE*, defined by Eq. (9) is shown on the last column of Table 1. The values of *SEE* are generally low, and vary in accordance with the AARE values. A comparison between the calculated and experimental data for the specific heat of metals is shown in Figs. 1 to 3, where the match is thought to be sufficient.

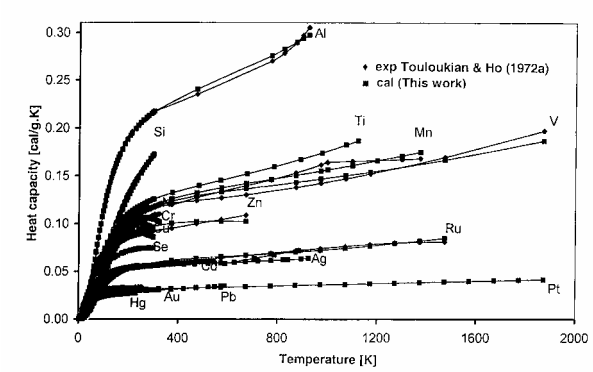

Fig. 1: 1st set of calculated heat capacity of metals as a function of temperature using proposed multilinear regression model vs. experimental data (Touloukian and Ho, 1972a).

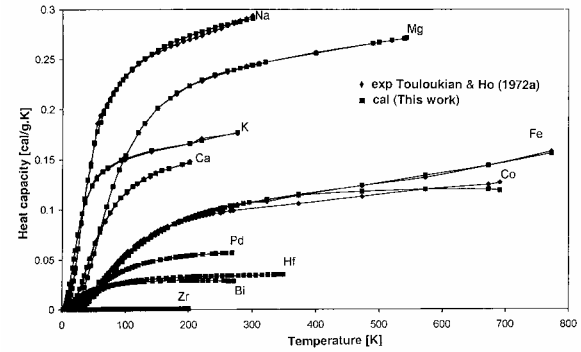

Fig. 2: 2nd set of calculated heat capacity of metals as a function of temperature using proposed multilinear regression model vs. experimental data (Touloukian and Ho, 1972a).

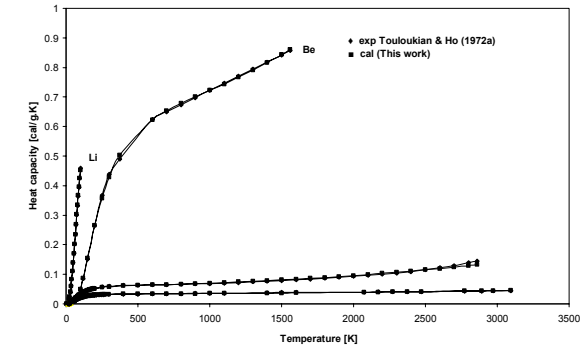

Fig. 3: 3rd set of calculated heat capacity of metals as a function of temperature using proposed multilinear regression model vs. experimental data (Touloukian and Ho, 1972a).

In order to get the best fit, the data points for *some* metals (see Table 1) were divided here into two sets; low temperature range and high temperature range. On the other hand, when the full range of temperature for those metals were considered, the AARE jumps to above 10% and reaches 31%, see Table 2.

In order to compare the proposed model in Eq. (3) or (5) with that given in Perry's Handbook (1997), one needs to consider the temperature range used for both equations. The temperature range used for Perry's Handbook equation starts from 273 K and above, while that for Eq. (5) may start at as low as a few degrees K. Thus the comparison might not be valid for many of the studied systems. Anyway, the proposed model in Eq. (5) fits the specific heat of aluminum and molybdenum, for example, better than Perry's Handbook equation for the temperature range shown in Fig. 4.

It should be mentioned, as shown in the last column of Appendix, that the reported error for the studied metals is ranging from 0.1 to ≤5%, and some samples have no reported error (Touloukian and Ho, 1972a). To make things shorter, no summary tables are included here for the polynomial regression results of the specific heat of the studied metals.

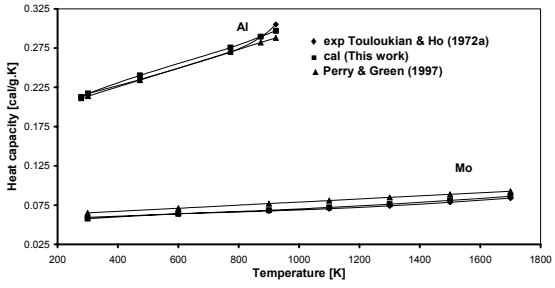

Fig. 4: Calculated specific heat vs. temperature for Al and Mo using ($C_P = a + bT + c/T^2$) proposed in Perry and Green (1997) and Eq. (5) proposed in this work.

Table 3 shows a comparison between the fittings of a 4th-order polynomial model and the multilinear regression model for the specific heat of metal oxides and metal fluorides. The reported error for these metal oxides and metal fluorides ranges from 0.1 to 5%, except for uranium oxides (U_3O_8) where it reaches 15% (Touloukian and Ho, 1972b), and some samples have no reported error. Again as shown in Table 3, although the polynomial model has $R^2 > 0.98$, the corresponding AARE for the specific heat of some metal oxides is so high (190% for Li_2O, 102% for MgO, 120% for SiO_2 quartz glass, and 77% for SiO_2 quartz crystal). This is because of the prediction of negative values for the specific heat of those metal oxides. For other metal oxides, R^2 may be as low as 0.23 (for U_3O_8) while AARE = 4.6%, $R^2 = 0.86$ (for Cr_2O_3) and AARE = 7.7%, or $R^2 = 0.9985$ (for SiO_2 cristobalite) and AARE = 12.4%.

The corresponding values of R^2 and AARE for the multilinear method are much better (see Table 3) with no non-realistic prediction of the specific heat. The maximum AARE is less than 5% and reaches only 14.5% for Li_2O, 16.7% for MgO, and 8.8% for SiO_2 quartz glass. Again for U_3O_8, although R^2 is low (0.146) due to the uncertainty of the original data (15%) in Touloukian and Ho (1972b), the value of AARE is very

similar to the polynomial model prediction and equals only 4.5%.

For the studied metal fluorides, Table 3 shows that the polynomial model predictions are very close to those of the multilinear model except for KF where AARE reaches 25% (because of the negative values prediction) while the corresponding value for KF using the multilinear model is only about 4.1%. Otherwise, the maximum error in the 4th-order polynomial model predictions reaches 7.2% for CaF_2. In brief, the multilinear model has an overall AARE of only 3% for all the systems shown in Table 3, which is again within the reported experimental error.

Lastly, the calculated fitting parameters for the specific heat as a function of temperature are shown in Tables 4 and 5 for metal oxides and metal fluorides using the polynomial and multilinear regression methods, respectively.

IV. Conclusions

In this work, a multilinear regression model of the form $C_P = aT^b e^{cT} e^{d/T}$ was used to fit the specific heat of several metals, metal oxides, and metal fluorides as a function of temperature. The coefficient of determination, R^2, was very close to unity for most of the systems studied. The average of the absolute relative errors, AARE, did not exceed 5% for the systems studied, except for Li_2O and MgO where it reaches 14.5% and 16.7%, respectively. The overall AARE was about 1.8% for metals, and 3.0% for metal oxides and metal fluorides, which is within the experimental error.

On the other hand, the polynomial fitting correlation, gave very close, and sometimes better, predictions for the specific heat of metals, metal oxides, and metal fluorides where the coefficient of determination, R^2, was very close to unity in most cases and the average of the absolute relative errors, AARE, was less than 7.7% except for thorium (8.5%), and Li_2O (190%), MgO (102%), SiO_2 quartz glass (120%), SiO_2 quartz crystal (77%), and potassium fluoride (25%). The polynomial method failed here because of the unrealistic negative values predicted for the specific heat of those systems.

Nomenclature

AARE	Average of absolute relative errors
a_1, a_2, a_3, a_4	Constants in Eq. (6)
a, b, c, d	Multilinear equation coefficients, Eqs. (1), (2)
$A, B \ldots E$	Constants in Eq. (3)
$B_0, B_1 \ldots B_n$	Polynomial coefficients, Eq. (7)
C_P	Specific heat at constant pressure, $kJ.kg^{-1}.K^{-1}$
M	Number of data points in a given set of data
R^2	Coefficient of determination, Eq. (8)
SEE	Standard error of estimate, Eq. (9)
T	Temperature, K

Subscripts

cal	Calculated
exp	Experimental

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Table 1: Multilinear Regression Parameters and R^2 and AARE for the Specific Heat of Metals (cal.g^{-1}.K^{-1} = 4.186 kJ.kg^{-1}.K^{-1}). Experimental Data from Touloukian and Ho (1972a)

Metal, curve #	*M*	Temperature range (K)	*a*	*b*	*c*	*d*	R^2	AARE (%)	SEE
Aluminum, 3	8	15.3 - 46	7.88E-13	6.93201	-0.07139	46.4363	0.9999	0.9103	0.0173
Aluminum, 3, 4	48	46 - 923	6.273517	-0.5469	0.000925	-156.932	0.9997	0.7134	0.0102
Antimony, 2	22	13.2 - 69.8	0.010036	0.476018	-0.00402	-36.7579	0.9997	1.1564	0.0165
Antimony, 1	4	587 - 885	1.082056	-0.46742	0.000855	-262.136	1.0	0.0169	0.0160
Barium, 1	18	1.5 - 20	1.28E-7	4.945923	-0.17307	4.62518	0.9998	2.4422	0.0309
Beryllium, 1	7	5 - 100	1.1084E-7	2.493536	0.014295	8.22423	1.0	0.8215	0.0139
Beryllium, 1, 2	18	100 - 1560	1.71E+2	-0.82579	0.000682	-445.695	0.9997	1.0226	0.0167
Bismuth, 1, 3	81	11.8 - 270.6	0.016594	0.190338	-0.00163	-23.9523	0.9990	1.6907	0.0300
Cadmium, 1, 2	60	12 - 543.2	0.126794	-0.14431	4.58E-4	-39.5176	0.9993	1.3247	0.0175
Calcium, 1, 2	22	4 - 27.6	8.89E-8	3.352949	-0.01459	4.7751	0.9995	2.4858	0.0353
Calcium, 1	21	27.6 - 200.8	1.546848	-0.39784	0.000872	-84.0207	0.9995	0.8335	0.0142
Chromium, 4, 5	62	17.8 - 324.1	1.13E-5	2.060219	-0.00825	-43.2655	0.9990	4.8561	0.0610
Cobalt, 2, 3	60	22.4 - 41.2	0.109352	0.08064	-4.19E-4	-104.197	0.9980	4.3783	0.0602
Copper, 9, 11	43	16 - 300	0.002842	0.901841	-0.00511	-60.9522	0.9982	4.7985	0.0599
Gold, 1	41	15.8 - 309	0.124058	-0.22521	2.21E-4	-55.5703	0.9996	0.9267	0.0130
Hafnium, 1	20	7 - 23.9	3.76E-9	4.730106	-0.06139	7.273762	0.9997	1.6533	0.0235
Hafnium, 1	52	23.9 - 348	0.670925	-0.53884	0.001274	-83.8955	0.9999	0.3299	0.0056
Iron, 16	11	16.9 - 57.8	6.12E-13	6.306475	-0.04336	62.73629	0.9998	0.8338	0.0174
Iron, 1, 2	34	57.8 - 773	10.06843	-0.76423	0.001506	-190.421	0.9992	0.7616	0.0179
Lead, 1, 3	48	14.2 - 588	0.156391	-0.32702	0.001089	-31.14	0.9992	0.808	0.0116
Lithium, 1, 5	43	22 - 300	0.0049744	1.20667	-0.00538	-54.3917	0.9984	3.0902	0.0411
Magnesium, 4	13	12.0 - 70	3.73E-10	5.456967	-0.05739	18.08019	0.9999	1.3112	0.0216
Magnesium, 3, 4	26	70 - 543.2	10.1548	-0.63256	0.001139	-138.874	1.0	0.1421	0.0032
Manganese, 9	22	14.4 - 107.7	5.45E-9	4.182151	-0.03174	21.80552	0.9999	1.4219	0.0148
Manganese, 2, 9, 13	41	107.7 - 1374	0.648	-0.25057	4.25E-4	-115.934	0.9943	1.1121	0.0187
Mercury, 6, 8	44	2 - 255.8	0.003972	0.526935	-0.0032	-7.94946	0.9986	4.0359	0.0484
Molybdenum, 7, 11	57	23.2 - 2860	0.759856	-0.40103	0.000522	-133.789	0.9968	3.9578	0.0549
Nickel, 10	35	14.7 - 294.0	3.92E-5	1.798192	-0.00787	-29.5527	0.9977	4.9788	0.0614
Palladium, 4	16	13.7 - 50.1	2.40E-11	5.881118	-0.06726	41.56738	0.9996	1.314	0.0217
Palladium, 4	39	50.1 - 268.4	0.158762	-0.1061	-4.19E-4	-85.0623	0.9997	0.3604	0.0055
Platinum, 1	18	273.1 - 1873	0.030764	0.002236	1.58E-4	-9.87843	0.9992	0.0972	0.0290
Potassium, 4	11	2 - 16	1.378E-6	4.887671	-0.21684	3.618142	0.9994	3.2743	0.0526
Potassium, 4, 6	16	16 - 276.5	977.3141	-0.36814	0.001756	-34.4841	0.9996	0.6944	0.0104
Rhodium, 1	14	14.3 - 28.8	3.97E-18	9.916627	-0.09819	99.66928	0.9989	1.371	0.0215
Rhodium, 1, 2	67	28.8 -1473.2	0.912441	-0.43157	0.000585	-134.053	0.9995	1.6727	0.0221
Selenium, 1	46	15 - 300.3	0.009596	0.476722	-0.00195	-26.2792	0.9997	1.0816	0.0132
Silicon, 2, 4	95	17.2 – 300.5	0.012832	0.549836	-0.00083	-87.3243	0.9993	3.2389	0.0492
Silver, 10	6	3 - 20	2.29E-7	3.032626	0.028334	2.150185	1.0	0.0488	0.0050
Silver, 2, 3, 10	56	20 - 925.3	0.475069	-0.35933	0.000571	-77.0249	0.9997	0.6157	0.0106
Sodium, 1, 9	22	1.5 - 45	8.13E-7	4.006211	-0.072065	3.553549	0.9999	1.713	0.0219
Sodium, 1, 5, 6	37	45 - 300	0.49701	-0.09132	3.7087E-4	-37.4533	0.9865	1.4081	0.0224
Strontium, 1	18	1.5 - 21	3.02E-7	3.884739	-0.05646	4.158019	0.9998	2.5528	0.0324
Thorium, 3	57	20 - 1273.2	0.121968	-0.26375	0.000658	-48.3007	0.9988	1.0699	0.0137
Titanium, 14, 16	43	1.2 - 32.2	1.72E-5	0.788464	0.107547	-0.03959	0.9997	1.7017	0.0260
Titanium, 6, 7, 14, 20	39	32.2 - 1123	1.559395	-0.40482	0.000743	-129.994	0.9996	0.9722	0.0153
Tungsten, 11	11	13.1 - 36.9	0.044961	-1.86986	0.143424	-36.2539	0.9955	3.9854	0.0732
Tungsten, 5, 6, 7,. 8, 11	62	36.9 - 3093	0.316659	-0.34182	2.76E-4	-119.669	0.9975	2.6189	0.0320
Vanadium, 3, 4	44	25 - 1873.2	1.104239	-0.33365	4.32E-4	-140.02	0.9978	3.4583	0.0520
Zinc, 9	15	4.6 - 12.5	1.79E+12	-17.3817	1.271913	-84.368	0.9983	4.319	0.0632
Zinc, 2, 3, 9, 10	41	12.5 - 673	0.109501	0.023389	-2.05E-4	-56.3477	0.9984	4.4065	0.0607
Zirconium, 1	37	20 - 200	0.060019	0.160028	-0.00227	-71.5492	0.9996	1.2478	0.0156
Overall AARE								1.8104	

Table 2: Multilinear Regression Parameters and R^2, SEE, and AARE for the Specific Heat of Some Metals with Full- Range Data (cal.g^{-1}.K^{-1} = 4.186 kJ.kg^{-1}.K^{-1}).

Metal, curve #	*M*	Temp. range (K)	*a*	*b*	*c*	*d*	R^2	AARE (%)	SEE
Beryllium, 1,2	24	5 - 1560	0.1146E-6	2.8022	4.8988	-0.00338	0.9873	31.364	0.3727
Calcium, 1,2	42	4 - 200.8	0.2445E-5	2.8491	-0.2863	-0.02182	0.9969	10.506	0.1317
Hafnium, 1	72	7 - 348	8.1408E-4	0.9622	-33.270	-0.00560	0.9938	11.450	0.1397
Iron, 1,2,16	44	16.9 - 773	16.4400E-4	0.8942	-64.905	-0.00197	0.9897	11.699	0.1523
Magnesium, 3,4	38	12 - 543.2	107.8839E-4	0.7299	-59.375	-0.00251	0.9946	10.492	0.1355
Sodium, 1,5,6,9	54	1.5 - 300	0.7099E-4	2.1106	-3.0338	-0.01367	0.9879	23.887	0.2829

Table 3: R^2 and AARE for the Specific Heat of Metal Oxides and Metal Fluorides for Polynomial and Multi-linear Fittings. Experimental Data from Touloukian and Ho (1972b)

Metal oxide or fluoride, curve #	*M*	Temperature range (K)	Polynomial Fitting R^2	Polynomial Fitting AARE (%)	Multilinear Fitting R^2	Multilinear Fitting AARE (%)
Al_2O_3, 3, 9, 10, 13, 15	103	298.2 - 1922	0.9714	1.4445	0.9727	1.322
BaO, 1, 2	30	56.1 - 1262	0.9737	4.194	0.9989	0.7897
B_2O_3, 1, 2	42	52.9 - 1800	0.9979	3.266	0.9992	1.3538
CaO, 1, 2	19	87.2 - 1176	0.9982	1.751	1.0000	0.2041
Cr_2O_3, 2, 3	33	298.1 - 1800	0.8598	7.673	0.9585	5.0156
Cu_2O, 1	21	75.9 - 291	0.9997	0.192	0.9998	0.2611
CuO, 4	55	218.6 - 297.2	0.9986	7.721	0.9995	2.3158
Fe_2O_3, 1, 2, series 2, 3, 4	50	89.8 - 1051	0.9944	2.077	0.9979	2.1045
Fe_3O_4 magnetite, 1, 2 ,3	43	90 - 1800	0.9680	6.885	0.9850	4.3075
PbO, 1,2,6	44	298 - 1200	0.9096	3.838	0.9490	3.8511
PbO_2, 1	17	69.9 - 298.1	0.9996	0.524	0.9996	0.5430
Pb_2O_3, 1	25	53.4 - 296.6	1.0000	0.061	1.0000	0.1201
Pb_3O_4, 1	16	71.5 - 292.6	0.9970	0.642	0.9988	0.7122
Li_2O, 1, 2	43	20.7 - 1050	0.9935	190.036 [a]	0.9864	14.5350
MgO, 2, 6, 11	72	20.3 - 1811.5	0.9843	102.309 [a]	0.9701	16.7029
NiO, 1, 2	41	68.1 - 1100	0.9907	1.881	0.9961	2.2171
Ag_2O, 1, series 1	29	13.5 - 301.7	0.9951	2.594	0.9992	1.0543
SiO_2 quartz glass, 1, 2, 3	74	63.2 - 344	0.9907	120.142 [a]	0.9863	8.7823
SiO_2 quartz crystal, 1, 2, 3	72	10 - 949.5	0.9858	76.764 [a]	0.9978	3.8936
SiO_2 cristobalite, 1, 2	37	10 - 297.3	0.9985	12.435	0.9990	2.2118
SiO_2 tridymite, 1	18	54.2 - 294.9	1.0000	0.360	1.0000	0.3584
Na_2O, 1	11	298 - 1170	1.0000	0.006	1.0000	0.0371
TiO, 1	25	52.6 - 296.3	1.0000	0.432	1.0000	0.2207
U_3O_8, 1	12	526 - 1365	0.2315	4.558	0.1455	4.5370
V_2O_5, 1	17	81.8 - 297.9	0.9995	0.406	0.9995	0.5067
ZnO, 1	14	298 - 1500	0.9729	1.597	0.9732	1.7867
ZrO_2, 1, 3	43	54.3 - 1850	0.9929	3.926	0.9987	1.8966
AlF_3, 1	31	53.7 - 298.1	1.0000	0.3597	1.0000	0.1188
CaF_2, 1, 2	46	53.5 - 1691	0.9877	7.2389	0.9984	1.8793
MgF_2, 1, 2	45	54.2 - 1536	0.9974	2.7581	0.9989	1.9832
KF, 1, 2	57	16 - 530	0.9980	25.013	0.9988	4.0632
SiF_4, 1	85	16.8 - 194	0.9884	3.8833	0.9944	3.0947
Na_2AlF_6, 1	30	53.2- 298.1	1.0000	0.1613	1.0000	0.2284
NaF, 1	30	54 - 299	0.9998	0.7546	1.0000	0.3244
Overall AARE						3.02

[a] Predicts negative values at low temperatures

Table 4: Multilinear Regression Parameters for the Specific Heat of Metal Oxides and Metal Fluorides (cal.mol^{-1}.K^{-1} = 4.186 kJ.kg^{-1}.K^{-1}). Experimental Data from Touloukian and Ho (1972b)

Metal oxide or fluoride, curve #	*M*	Temperature range (K)	*a*	*b*	*c* x 10^4	*d*
Al_2O_3, 3, 9, 10, 13, 15	103	298.2-1922	2.073E2	-0.6188	4.1142	-390.6075
BaO, 1, 2	30	56.1-1262	0.1974	-0.1368	2.1642	-76.9538
B_2O_3, 1, 2	42	52.9-1800	5.8967E-3	0.6959	-4.8152	-67.8232
CaO, 1, 2	19	87.2-1176	2.7497	-0.3727	2.8363	-200.9362
Cr_2O_3, 2, 3	33	298.1-1800	1.1309E2	-0.9644	6.4820	-338.2318
Cu_2O, 1	21	75.9-291	1.6862E-3	0.7861	-14.4850	19.5208
CuO, 4	55	218.6-297.2	3.7963E-4	1.2354	-35.9380	-43.3101
Fe_2O_3, 1, 2, series 2, 3, 4	50	89.8-1051	2.1225	-0.4105	12.9220	-200.6348
Fe_3O_4 magnetite, 1, 2 ,3	43	90-1800	3.8325E-2	0.3397	-4.6591	-109.7939
PbO, 1,2,6	44	298-1200	1.6125E-2	0.2378	-2.3513	-45.9577
PbO_2, 1	17	69.9-298.1	3.3201E-4	1.0520	-23.8050	-5.5235
Pb_2O_3, 1	25	53.4-296.6	6.1450E-4	0.9048	-21.6440	-2.1592
Pb_3O_4, 1	16	71.5-292.6	7.4880E-6	1.7891	-53.0790	59.2901
Li_2O, 1, 2	43	20.7-1050	3.7982E-5	1.8422	-30.5430	-57.2851
MgO, 2, 6, 11	72	20.3-1811.5	5.5852E-3	0.7296	-8.2860	-106.5475
NiO, 1, 2	41	68.1-1100	3.1474E-2	0.3919	-8.8320	-134.1595
Ag_2O, 1, series 1	29	13.5-301.7	7.5694E-2	-0.0788	15.0520	-26.6037
SiO_2 quartz glass, 1, 2, 3	74	63.2-344	4.7397E-4	1.1784	-23.2810	-23.6759
SiO_2 quartz crystal, 1, 2, 3	72	10-949.5	8.6600E-4	1.0184	-12.1030	-32.8107
SiO_2 cristobalite, 1, 2	37	10-297.3	1.0946E-3	0.9804	-12.7940	-31.5748
SiO_2 tridymite, 1	18	54.2-294.9	2.1330E-4	1.3249	-26.2200	-12.2849
Na_2O, 1	11	298-1170	5.5064E-2	0.2492	1.9919	45.4078
TiO, 1	25	52.6-296.3	2.1416E-3	0.9632	-30.3320	-102.8743
U_3O_8, 1	12	526-1365	7.3916E7	-3.0700	17.7490	-1291.428
V_2O_5, 1	14	298-1500	11.2972	-0.5590	3.4779	-334.6547
ZnO, 1	17	81.8-297.9	7.0827E-5	1.4848	-36.3880	13.2479
ZrO_2, 1, 3	43	54.3-1850	6.6324E-2	0.1765	-2.6752	-134.2145
AlF_3, 1	31	53.7-298.1	4.2630E-3	0.8560	-22.1400	-90.8506
CaF_2, 1, 2	46	53.5-1691	6.4554	-0.5305	7.1890	-190.3078
MgF_2, 1, 2	45	54.2-1536	0.4280	-0.0132	-0.5549	-154.9709
KF, 1, 2	57	16-530	0.1052	0.2199	-0.2810	-75.2920
SiF_4, 1	85	16.8-194	44.2601	-1.4240	139.996	-66.2493
Na_2AlF_6, 1	30	53.2- 298.1	1.250E-2	0.6581	-18.895	-63.2492
NaF, 1	30	54 - 299	3.0922	-0.3291	-0.8845	-164.9017

Table 5: 4th-order Polynomial Parameters for the Specific Heat of Metal Oxides (cal.mol^{-1}.K^{-1}). Experimental Data from Touloukian and Ho (1972b)

Metal oxide or fluoride, curve #	M	Temperature range (K)	B_0	B_1 x 10^3	B_2 x 10^6	B_3 x 10^8	B_4 x 10^{12}
Al_2O_3, 3, 9, 10, 13, 15	103	298.2 - 1922	-0.01750200	9.3560000	-0.11.7017	0.666911	-1.373790
BaO, 1, 2	30	56.1 - 1262	0.0152132	0.405667	-0.904660	0.086103	-0.287213
B_2O_3, 1, 2	42	52.9 - 1800	-0.0173182	0.966979	-0.738521	0.024433	-0.030627
CaO, 1, 2	19	87.2 - 1176	-0.0556158	1.523520	-3.159770	0.284068	-0.918467
Cr_2O_3, 2, 3	33	298.1 - 1800	-0.0444342	1.283920	-2.216370	0.152412	-0.359542
Cu_2O, 1	21	75.9 - 291	0.0227417	0.636609	-2.713580	0.814030	-10.7179
CuO, 4	55	218.6-297.2	-0.0068636	0.356188	3.380890	-1.491230	15.1664
Fe_2O_3, 1, 2 series 2, 3, 4	50	89.8 - 1051	-0.0491753	1.201850	-2.431610	0.262594	-0.97793
Fe_3O_4 magnetite, 1, 2 ,3	43	90 - 1800	-0.0085369	0.766576	-0.772193	0.026587	-0.01972
PbO, 1,2,6	44	298 - 1200	0.0041579	0.303059	-0.640608	0.058638	-0.18883
PbO_2, 1	17	69.9 - 298.1	-0.0026294	0.405671	-0.610033	-0.052753	1.82672
Pb_2O_3, 1	25	53.4 - 296.6	0.0011597	0.385949	-0.925394	0.070690	0.3764
Pb_3O_4, 1	16	71.5 - 292.6	0.0078551	0.228815	0.179537	-0.260003	3.44112
Li_2O, 1, 2	43	20.7 - 1050	-0.1073740	2.467450	-2.539430	0.039665	0.47371
MgO, 2, 6, 11	72	20.3-1811.5	-0.0596987	1.487170	-2.357940	0.158893	-0.36891
NiO, 1, 2	41	68.1 - 1100	-0.0395455	0.993474	-1.460380	0.074618	-0.07007
Ag_2O, 1, series 1	29	13.5 - 301.7	-0.0017737	1.072670	-8.675710	3.328730	-45.7915
SiO_2 quartz glass, 1, 2, 3	74	63.2 - 344	-0.0077884	0.638979	2.106020	-1.117030	13.4036
SiO_2 quartz crystal, 1, 2, 3	72	10 - 949.5	-0.0287849	1.159530	-2.358630	0.295669	-1.48266
SiO_2 cristobalite, 1, 2	37	10 - 297.3	-0.0071976	0.588701	1.896610	-0.841823	7.9682
SiO_2 tridymite, 1	18	54.2 - 294.9	-0.0105527	0.660987	1.863810	-1.073850	14.0293
Na_2O, 1	11	298 - 1170	0.2335830	0.160888	-0.003525	0.000347	-0.001218
TiO, 1	25	52.6 - 296.3	-0.0157912	0.256453	6.404290	-3.017900	40.468
U_3O_8, 1	12	526 - 1365	0.0755914	-0.111168	0.360777	-0.038155	0.130551
V_2O_5, 1	17	81.8 - 297.9	0.0183166	-0.022039	5.890930	-2.646580	36.0638
ZnO, 1	14	298 - 1500	-0.0323629	1.099810	-1.771770	0.128239	-0.338095
ZrO_2, 1, 3	43	54.3 - 1850	-0.0188867	0.667700	-0.978581	0.060906	-0.135324
AlF_3, 1	31	53.7 - 298.1	-0.2961556	7.416	48.9597	-26.1089	353.377
CaF_2, 1, 2	46	53.5 - 1691	-0.3457438	14.361	-25.1225	1.80710	-4.36021
MgF_2, 1, 2	45	54.2 - 1536	-0.5877450	17.032	-29.7725	2.21345	-5.80136
KF, 1, 2	57	16 - 530	-0.4628922	25.596	-100.552	17.7044	-113.581
SiF_4, 1	85	16.8 - 194	-0.1962403	29.1423	-149.508	-19.6063	3170.44
Na_2AlF_6, 1	30	53.2- 298.1	-0.4975770	20.0439	-34.0111	-4.22496	142.283
NaF, 1	30	54 - 299	-1.1780267	33.5888	-94.3394	4.37473	134.410

Appendix: Heat Capacity Coefficients for Metals, Metal Oxides and Metal Fluorides for $C_P = a + bT + c/T^2$ (cal.mol^{-1}.K^{-1}) and Uncertainty (Perry and Green, 1997), and Reported Error as given by Touloukian and Ho (1972a,b).

Metal, metal oxide or metal fluoride	Temperature range (K)	a	b x 10^3	c x 10^{-5}	Uncertainty (%)	Reported error (%) as given in Refs. 4 & 5
Aluminum	273-931	4.8	3.22		1	< 3-5
Antimony	273-903	5.51	1.78		2	< 0.2
Beryllium	273-1173	4.698	1.555	-1.210	1	< 2
Bismuth	273-544	5.38	2.60		3	NA
Cadmium	273-594	5.46	2.466		1	0.1-0.4
Calcium	273-673	5.31	3.33		2	2-3
Chromium	273-1823	4.84	2.95		5	NA, 0.13
Cobalt	273-1763	5.12	3.33		5	NA
Copper	273-1357	5.44	1.462		1	1-2
Gold	273-1336	5.61	1.44		2	NA
Iron α	273-1041	4.13	6.38		3	0.3-2
β	1041-1179	6.12	3.36		3	
γ	1079-1674	8.4	--		5	
δ	1674-1803	10.0	--		5	
Lead	273-600	5.77	2.02		2	<5
Magnesium	273-923	6.2	1.33	-0.678	1	0.1, NA
Manganese α	273-1108	3.76	7.47		5	NA
β	1108-1317	5.06	3.95		5	
γ	1317-1493	4.80	4.22		5	
Mercury, liquid	273-630	6.61	--		1	NA, 0.1-3
Molybdenum	273-1773	5.69	1.88	-0.503	5	4, NA
Nickel α	273-626	4.26	6.40		2	NA
β	626-1725	6.99	0.905		5	
Palladium	273-1822	5.41	1.84		2	NA
Platinum	273-1873	5.92	1.16		1	NA
Potassium	273-336	5.24	5.55		5	NA
Rhodium	273-1877	5.4	2.19		2	NA
Silicon	273-1174	5.74	0.617	-1.010	2	0.5
Silver	273-1234	5.60	1.50		1	NA, ±5
Sodium	273-371	5.01	5.36		1.5	<2
Thorium	273-373	6.40			NA	2
Titanium	273-713	8.91	1.14	-4.330	3	NA
Tungsten	273-2073	5.65	8.66		1	<0.5-1.2
Vanadium	273-1993	5.57	0.97		NA	<0.2
Zinc	273-692	5.25	2.70		1	NA
Al_2O_3	273-1973	22.08	8.971	-5.225	3	± 0.4-5
B_2O_3	273-513	5.14	32.0		3	---
CaO	273-1173	10.0	4.84	-1.080	2	NA
Cr_2O_3	273-2263	26.0	4.00		NA	1
CuO	273-810	10. 87	3.576	-1.506	2	NA
Fe_2O_3	273-1097	24.72	16.04	-4.234	2	NA
Fe_3O_4	273-1065	41.17	18.82	-9.795	2	≤ 0.5
PbO	273-544	10.33	3.18		2	NA
PbO_2	273- ?[a]	12.70	7.80		NA	NA
MgO	273-2073	10.86	1.197	-2.087	2	0.4-3
NiO	273-1273	11.30	2.15		NA	NA
SiO_2 quartz α	273-848	10.87	8.712	-2.412	1	<5
SiO_2 quartz β	848-1873	10.95	5.50		3.5	NA
SiO_2 cristobalite α	273-523	3.65	20.4		2.5	NA
SiO_2 cristobalite β	523-1973	17.09	0.454	-8.972	2	NA
TiO	273-713	11.81	7.54	-0.419	3	NA
U_3O_8	273-314	59.8	--		NA	≤ 15
ZnO	273-1573	11.40	1.45	-1.824	1	NA
ZrO_2	273-1673	11.62	0.01046	-1.777	NA	0.2-0.3
AlF_3	288-326	19.3			NA	NA
CaF_2	273-1651	14.7	3.80		NA	0.1-0.3
KF	273-1129	10.8	2.84		NA	0.2-1
NaF	273-1261	10.4	2.89		NA	NA

[a] As in source reference, NA = Not Available

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