

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

†S. I. ABU-EISHAH, Y. HADDAD, A. SOLIEMAN, and A. BAJBOUJ‡

†*Department of Chemical & Petroleum Engineering, UAEU, Al-Ain, UAE*
siam20022001@yahoo.com

‡*Chemical Engineering Department, Jordan University of Science & Technology, Irbid 22110, Jordan*

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 $C_p = aT^b e^{cT} e^{dT}$ 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 thermo-physical 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 thermo-physical 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

$$C_p = aT + bT^3 + c/T^2 \quad (1)$$

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

$$C_p = aT^b e^{cT} e^{dT} \quad (2)$$

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

$$C_p = aT^b [A + BT + CT^2 + \dots + D/T + E/T^2 + \dots] \quad (3)$$

which can be rewritten as

$$C_p = A'T^b + B'T^{b+1} + C'T^{b+2} + \dots + D'/T^{b-1} + E'/T^{b-2} + \dots \quad (4)$$