

# Thermophysical Properties

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ADVANCED COMPUTER SIMULATION TECHNOLOGY is a powerful tool used to understand the critical aspects of heat transfer and fluid transport phenomena and their relationships to metallurgical structures and defect formation in metal casting processes. Computational models are enabling the design and production of more economical and higher-quality castings. In order to produce accurate and reliable simulation of the complex solidification processes, accurate, self-consistent, and realistic thermophysical properties input data are necessary. Unfortunately, reliable data for many alloys of industrial interest are very limited.

Sand, ceramic, and metal molds are extensively used to cast most metals. During the solidification process, the predominant resistance to heat flow is within the mold/metal interface and the mold itself; thus, the primary interest is not the mold thermal history but rather the rate at which the heat is extracted from the solidifying metal. Therefore, heat transfer is the governing phenomenon in any casting process. Heat transfer is fundamentally described by the heat-transfer coefficient, the temperature gradient, the geometry of the system, and the thermophysical properties of both metal and mold material.

Table 1 shows the required thermophysical properties that must be available for input before reliable numerical simulations of a casting process can be performed, as well as their influence in the prediction of defects. Current commercial software requires that the thermal conductivity, specific heat capacity, latent heat, solidus and liquidus temperatures, and density must be known for heat-transfer operations. Viscosity, density, wetting angle, and surface tension of the molten alloy are required for fluid flow operations. In addition to the metal properties, mold materials properties are also needed to conduct an effective simulation.

## Sources and Availability of Reliable Data

The thermophysical property data found in the literature for engineering and design calculations

of casting processes must not be used indiscriminately without knowing their source and reliability. Prior to using a given set of data, it is very important to critically evaluate and analyze the available thermophysical property data, to give judgment on their reliability and accuracy.

There are several main sources of thermophysical property data that provide the most authoritative and comprehensive compilations of critically and systematically evaluated data that are presently available. The challenge of finding data is discussed in Ref 2. The data have been published and can be found in the following resources:

- The Center for Information and Numerical Data Analysis and Synthesis (CINDAS) generated and recommended reference values for diverse materials (Ref 3–12).
- Smithells' *Metals Reference Book* provides an extensive compilation of thermochemical data for metals, alloys, and compounds of metallurgical importance (Ref 13).
- *Summary of Thermal Properties for Casting Alloys and Mold Materials* by R.D. Pehlke and co-workers (Ref 14).
- The ASM International Materials Properties Database Committee publishes a comprehensive thermal properties database of most commercially available metals (Ref 15).
- *Recommended Values of Thermophysical Properties for Selected Commercial Alloys* by K.C. Mills. Experimental determination, estimation, and validation of the thermophysical properties in the solid and liquid states (Ref 16)

Computer models based on first principles of thermodynamics and kinetics of phase transformations have been developed to calculate thermophysical properties for various materials in the solid and liquid states (Ref 17–22). However, their use is still limited due to the lack of thermodynamic data and accurate measurements of thermophysical properties for materials of industrial interest. Also, sensitivity studies (Ref 23) are necessary to truly evaluate the reliability of calculated thermophysical property data from these models in actual casting processes.

## Limitations and Warning on the Use of Data

The thermophysical properties data presented in this article are provided to assist in the materials properties selection for the simulation of casting processes. Great effort has been exercised in the compilation and analysis of the data, and careful attention has been taken to faithfully duplicate the data and their sources found in the literature. The thermophysical properties data provided here shall bear the warning "not for design purposes." It is the full responsibility of the reader to further investigate the sources of information and follow all necessary engineering steps to make sure the validity and quality of the data meet the requirements of the intended application.

## Methods to Determine Thermophysical Properties

Experimental determinations of reliable thermophysical properties are difficult. In the solid state, the properties recorded in the technical literature are often widely diverging, conflicting, and subject to large uncertainties. This problem is particularly acute for materials in the mushy and liquid state. Also, accurate, consistent, and reliable thermophysical property measurements are experimentally difficult. Convection effects in molten samples and their interactions and reactivity with their containers and environment often exacerbate the difficulties.

The measurements are difficult because of high temperatures and the reactivity of some alloys. Strategies adopted to minimize these effects are:

- Perform the experiments quickly using transient methods
- Choose crucible materials that contact the sample to minimize reactions
- Eliminate container levitation
- Measure properties in microgravity
- Control the composition of the atmosphere

Mills et al. (Ref 24) describe the necessity to exercise care when analyzing the experimental results. The following cases are discussed:

**Table 1 Thermophysical property data required for metal casting**

Casting process component	Transport phenomena for casting	Thermophysical data required	Computer modeling for process, part design, and defect prediction
Furnace metal	S	Heat transfer	Effective design for: • Riser • Chill • Insulation Solidification direction Solidification shrinkage Porosity Hot spots
	O	• Conduction • Convection • Radiation	
	L	• Metal/mold • Metal/core • Metal/chill • Mold/chill • Mold/environment Emissivity—Metal/mold/furnace wall Temperature-dependent parameters	
	I	• Density • Heat capacity • Conductivity Latent heat of fusion Liquidus and solidus	
Mold core chill	D	Mass transfer (fluid flow)	Effective design for: • Ingate • Runner • Vents Pouring parameters • Temperature • Pouring rate Mold filling time Cold shut Missruns
	I	Temperature dependent • Viscosity • Surface tension • Density	
	F		
Insulation	I	Microstructural evolution	Microsegregation Macrosegregation Grain size Grain orientation Phase morphology Mechanical properties
	C	Phase diagram Phase chemical composition Capillarity effect (Gibbs-Thompson coefficient) Nucleation and growth parameters Solid fraction vs. temperature Diffusivity	
	A	• Solubility	
	T	Stress analysis	Casting design for: • Dimension and distortion Internal stresses Hot tears and hot cracks
	I	Temperature-dependent parameters • Coefficient of thermal expansion • Stress/strain	
	O		
	N		

Source: Ref 1

**Table 2 Thermophysical and mechanical properties needed for casting process simulation and common measurement techniques**

Thermophysical property	Measurement technique
Thermal conductivity	Comparative stationary (solid), indirect (liquid)
Heat capacity	Differential scanning calorimetry, pulse heating; drop calorimetry
Density	Archimedian balance, push-rod dilatometry; levitation
Thermal diffusivity	Laser flash
Heat of fusion	Differential scanning calorimetry, pulse heating
Transformation temperatures	Differential scanning calorimetry, thermal analysis
Fraction solid	Differential scanning calorimetry, thermal analysis
Electrical resistivity	Pulse heating, four-point probing
Hemispherical emissivity	Pulse heating
Viscosity	Levitation, viscometer
Surface tension	Levitation, sessile drop
Young's modulus, Poisson's ratio	Tensile test, sound speed measurements
Thermal expansion	Push-rod dilatometry
Yield strength	Tensile test

Source: Ref 26

- The specific heat capacity ( $C_p$ ) peaks recorded by differential scanning calorimetry (DSC) for fusion (or solidification) are only apparent  $C_p$  values, since they contain enthalpy contributions.
- Use of these apparent  $C_p$  values for the conversion of thermal diffusivities to conductivities can lead to massive overestimation of thermal conductivities for temperatures in the transition range.
- There is a temperature lag between the sample and reference pans in differential thermal analysis (DTA)-type DSC instruments, which causes some uncertainty in the temperature scale for fraction solid/temperature relations. The temperature difference between the sample and reference pans results in heating/cooling rate-dependent variations in transition temperatures (see also Ref 25 for a detailed critique).

- Thermal diffusivity measurements for the mushy region are prone to error because some of the energy supplied may be used for further melting of the alloy.
- Oxide films on the surface of the molten alloy can affect measurements of physical properties; wettability of the metal on the crucible and/or rotor can affect viscosity measurements and nonwetting, leading to low values for the viscosity.

Table 2 lists some common techniques used for the measurement of relevant thermophysical properties.

Numerous methods exist for the measurement of thermophysical properties of metallic materials and are cited in the literature (Ref 16, 27–47). However, only a few of them have been standardized, and most of them are limited to the solid-state properties. The current ASTM International standards and selected CEN and ISO standards include:

- *Specific heat capacity*: Differential scanning calorimetry, ASTM E 1269, E 967, E 968, E 2253, E 793, and D 2766 (Ref 48–53). Ceramics, EN 821–3 drop and DSC (Ref 54)
- *Thermal expansion*: Dilatometry, ASTM E 228; interferometry, ASTM E 289; and thermomechanical analysis, ASTM E 831 (Ref 55–57). Ceramics, EN 821–1 and ISO 17562, both dilatometry (Ref 58, 59)
- *Thermal conductivity*: Modulated-temperature scanning calorimetry, ASTM E 1952; thermal diffusivity of solids by the laser flash method, ASTM E 1461; and the steady-state heat flow, ASTM C 518 (Ref 60–62). Ceramics, EN 821–2 and ISO 18755, both laser flash (Ref 63, 64)
- *Thermal emittance*: Radiometric techniques, ASTM E 307 and E 408 (Ref 65, 66)

Best practices for the measurement of alloy freezing and melting temperatures by DTA and DSC measurements are found in Boettinger et al. (Ref 25).

Standardized methods to determine the thermal properties of liquid metals are practically nonexistent. Several methods, such as the oscillating viscometer (Ref 67); the levitated drop apparatus to measure surface tension, density, and viscosity (Ref 34, 67–69); and the laser flash to measure thermal diffusivity and specific heat capacity (Ref 37–43), are successfully being used. Reference 33 provides a comprehensive critical survey of the microstructural characteristics of liquid metals, which determine properties of viscosity, surface tension, density, specific heat capacity, thermal conductivity, electrical resistivity, diffusion, and velocity of sound transmission. The experimental techniques used to obtain these data are also reviewed, with correlations and reference data.

In this article, the methods to measure thermophysical properties are not discussed further; instead, available thermophysical properties for pure metals and some commercial alloys are presented.

## Specific Heat Capacity and Enthalpy of Transformation

Specific heat capacity of a material is the amount of thermal energy needed to change the temperature of a unit mass ( $m$ ) of a substance by one degree Kelvin. The specific heat capacity is an extensive property of matter that depends on the amount of species in the system and is sensitive to phase changes. Specific heat capacity can be defined for a constant volume ( $C_v$ ) or for a constant pressure ( $C_p$ ). The specific heat capacity in SI units is expressed in  $\text{J/kg} \cdot \text{K}$ . Also, the specific heat term is often used interchangeably with heat capacity. While this is not precisely correct, it is not a cause of misunderstanding.

The total amount of thermal energy or enthalpy,  $\Delta H$ , associated with the specific heat capacity and a temperature change ( $T_1$  to  $T_2$ ) is given by:

$$\Delta H = \int_{T_1}^{T_2} C_p dT \quad (\text{Eq 1})$$

A good approximation to estimate the specific heat capacity as a function of temperature is given by:

$$C_p = a + bT + cT^{-2} + \dots \quad (\text{Eq 2})$$

where  $C_p$  is the molar heat capacity;  $a$ ,  $b$ , and  $c$ , are constants; and  $T$  is the temperature in degrees Kelvin. Table 3 shows the specific heat capacity of solids as a function of temperature, the specific heat capacity of liquids at the melting point ( $T_m$ ), and the enthalpy of fusion for most common elements found in cast metals.

Changes in specific heat capacity and most thermophysical properties with changing temperature in liquid metals may be gradual and continuous, rather than showing the abrupt effects of phase transitions that take place in the mushy and solid state. Thus, a reasonable estimate of the specific heat capacity for a liquid alloy ( $C_{pL}$ ) can be calculated from the elemental heat capacities of the components in the alloy by using the commonly known Kopp-Neuman rule of mixtures (Ref 72, 73):

$$C_{pL} = \sum_{i=1}^n Y_i (C_p)_{L_i} \text{ in cal}/(\text{mol} \cdot \text{K}) \quad (\text{Eq 3})$$

where  $Y_i$  is the atomic fraction of element  $i$  in the alloy. The small changes in the specific heat capacity of the liquid with temperature allows for a reasonable estimate ( $\pm 3\%$ ) using Eq 3. Equation 3 can be expressed in SI units by multiplying  $C_{pL}$  by 4.184 J/cal and dividing by the atomic mass of the element  $i$  in kg/mol.

Major changes in the specific heat capacity with heating or cooling rates are observed in the solid-liquid range (mushy region). Macro- and microsegregation, as well as the presence of eutectics, peritectics, and other phase transformations that occur during solidification, cannot be easily described by Eq 1. Instead, the

**Table 3 Specific heat capacity values and enthalpy of fusion for pure metals**

Element	$C_p = a + bT + cT^{-2} + \dots$ (a), J/K · mol	Temperature range, K	$T_m$ (b), K	$C_{pL}$ , J/g · K	$\Delta H_f$ , J/g	Reference
Al <sub>(s)</sub>	$4.94 + 2.96 \times 10^{-3}T$	298–932	933	1.18	397	16, 70
Al <sub>(l)</sub>	7.0	932–1273				
C <sub>(graphite)</sub>	$4.1 + 1.02 \times 10^{-3}T - 2.10 \times 10^{-5}T^{-2}$	298–2300	4073	...	...	70
Co <sub>(β)</sub>	$3.3 + 5.86 \times 10^{-3}T$	715–1400	1768	0.59	275	13, 16, 70
Co <sub>(γ)</sub>	9.60	1400– $T_m$				
Co <sub>(l)</sub>	9.65	$T_m$ –1900				
Cr <sub>(s)</sub>	$5.84 + 2.35 \times 10^{-3}T - 0.88 \times 10^{-5}T^{-2}$	298– $T_m$	2130	0.78	401.95	13
Cr <sub>(l)</sub>	9.4	$T_m$				
Cu <sub>(s)</sub>	$5.41 + 1.4 \times 10^{-3}T$	298– $T_m$	1356	0.495	208.7	13, 16
Cu <sub>(l)</sub>	7.50	$T_m$ –1600				
Fe <sub>(α, δ)</sub>	$8.873 + 1.474 \times 10^{-3}T - 56.92T^{-1/2}$	298– $T_m$	1809	0.762	247	13, 16, 71
Fe <sub>(γ)</sub>	$5.85 + 2.02 \times 10^{-3}T$	1187–1664				
Fe <sub>(l)</sub>	$9.74 + 0.4 \times 10^{-3}T$	$T_m$ –2000				
Hf <sub>(s)</sub>	$5.61 + 1.82 \times 10^{-3}T$	298–1346	2500	...	134.85	13
Li <sub>(s)</sub>	$3.33 + 8.21 \times 10^{-3}T$	273– $T_m$	454	...	422.1	13, 70
Li <sub>(l)</sub>	$5.85 + 1.31 \times 10^{-3}T + 2.07 \times 10^{-5}T^{-2} - 467 \times 10^{-6}T^{-2}$	$T_m$ –580				
Mg <sub>(s)</sub>	$5.33 + 2.45 \times 10^{-3}T - 0.103 \times 10^{-5}T^{-2}$	298– $T_m$	922	1.32	349	13, 16
Mg <sub>(l)</sub>	7.68	$T_m$ –1100				
Mn <sub>(α)</sub>	$5.70 + 3.38 \times 10^{-3}T - 0.375 \times 10^{-5}T^{-2}$	298–1000	1517	0.838	267.5	13
Mn <sub>(β)</sub>	$8.33 + 0.66 \times 10^{-3}T$	1108–1317				
Mn <sub>(γ)</sub>	$6.03 + 3.56 \times 10^{-3}T - 0.443 \times 10^{-5}T^{-2}$	1374–1410				
Mn <sub>(δ)</sub>	11.10	1410–1450				
Mn <sub>(l)</sub>	11.0	$T_m$ – $T_{bp}(c)$				
Mo <sub>(s)</sub>	$5.77 + 0.28 \times 10^{-3}T + 2.26 \times 10^{-6}T^2$	298–2500	2893	0.57	371	13
Nb <sub>(s)</sub>	$5.66 + 0.96 \times 10^{-3}T$	298–1900	2740	0.334	315.4	13
Ni <sub>(α)</sub>	$7.80 - 0.47 \times 10^{-3}T - 1.335 \times 10^{-5}T^{-2}$	298–630	1726	0.63	292.4	13, 16, 70
Ni <sub>(β)</sub>	$7.10 + 1.0 \times 10^{-3}T - 2.23 \times 10^{-5}T^{-2}$	630– $T_m$				
Ni <sub>(l)</sub>	9.20	$T_m$ –2200				
Pb <sub>(s)</sub>	$5.63 + 2.33 \times 10^{-3}T$	298– $T_m$	600	0.142	23.2	13
Pb <sub>(l)</sub>	$7.75 - 0.74 \times 10^{-3}T$	$T_m$ –1300				
Si <sub>(s)</sub>	$5.72 + 0.59 \times 10^{-3}T - 0.99 \times 10^{-5}T^{-2}$	298–1200	1685	0.968	1877	13, 16
Si <sub>(l)</sub>	6.498	$T_m$ –1873				
Ta	$6.65 - 0.52 \times 10^{-3}T - 0.45 \times 10^{-5}T^{-2} + 0.47 \times 10^{-6}T^2$	298–2300	3288	...	136.5	13, 16
Ti <sub>(α)</sub>	$5.28 + 2.4 \times 10^{-3}T$	298–1155	1940	0.965	295	13, 16
Ti <sub>(β)</sub>	$4.74 + 1.90 \times 10^{-3}T$	1155–1350				
Ti <sub>(l)</sub>	11.042	$T_m$ –2073				
V <sub>(s)</sub>	$4.90 + 2.58 \times 10^{-3}T + 0.2 \times 10^{-5}T^{-2}$	298–1900	2175	...	328.6	13
W <sub>(s)</sub>	$5.74 + 0.76 \times 10^{-3}T$	298–2000	3673	...	176.8	...
Y <sub>(α)</sub>	$5.72 + 1.805 \times 10^{-3}T + 0.08 \times 10^{-5}T^{-2}$	298–1758	1803	0.394	128.6	13
Y <sub>(β)</sub>	8.37	1758– $T_m$				
Y <sub>(l)</sub>	9.51	$T_m$ –1950				
Zn <sub>(s)</sub>	$5.35 + 2.4 \times 10^{-3}T$	298– $T_m$	692.5	0.481	112	13, 16
Zn <sub>(l)</sub>	7.5	$T_m$ – $T_{bp}$				
Zr <sub>(α)</sub>	$5.25 + 2.78 \times 10^{-3}T - 0.91 \times 10^{-5}T^{-2}$	298–1135	2125	...	211.6	13
Zr <sub>(β)</sub>	$5.55 + 1.11 \times 10^{-3}T$	1135– $T_m$	...	...	...	...

(a)  $C_p$  in SI units (J/kg · K) when multiplied by 4.184 J/cal and divided by the corresponding element atomic mass (kg/mol). (b)  $T_m$  = melting point. (c)  $T_{bp}$  = boiling point

behavior in the solid or mushy state is more complex, since the phase transformations are dependent on the heating and cooling rates and on the chemistry of the alloy system. The dynamic characteristics of a given casting process require the input of all liquid-to-solid changes to understand the behavior of the solidifying metal. Therefore, in casting processes, determination of the specific heat capacity must be conducted on cooling for the solidifying metal and on heating for the mold and core materials, since the latter absorb most of the superheat and latent heat of solidification.

## Enthalpy of Melting, Solidus, and Liquidus Temperatures

The enthalpy or latent heat of melting ( $\Delta H_f$ ) is the heat that is required during solid-to-liquid

transformations, and the latent heat of solidification is the heat released during liquid-to-solid transformations. The latent heats of melting and solidification in a multicomponent alloy system occur over a temperature range. The temperature at which the alloy starts to melt is called the solidus temperature, and the temperature at which the melting is completed is called the liquidus temperature.

In actual melting and casting processes, equilibrium conditions do not exist, since melting and solidification processes are ruled by the rate of phase transformations and by the heat and mass transfer phenomena. On melting, high heating rates may displace the solidus and liquidus temperatures to higher values, while on cooling and prior to the nucleation of the solid phase, the molten alloy is usually undercooled. High undercooling generally decreases the liquidus and solidus temperatures. Also, the

degree of undercooling directly affects the kinetics of the liquid-solid phase transformation and the type of second phases that evolve during solidification. A more detailed discussion of nonequilibrium structures can be found in Ref 74. In actual casting processes, depending on the process and degree of inhomogeneity and impurities in a cast material, the liquidus and solidus temperatures can differ by several or even tens of degrees from equilibrium. The latent heat, solidus, liquidus, and other phase transformation temperatures are determined using the same techniques as for heat capacity and are described elsewhere in the literature (Ref 27).

The enthalpy of fusion and the solidus and liquidus temperatures for various alloys of commercial interest are shown in Table 4. The heat capacity, along with the thermal conductivity and density, for some commonly used sand molds is shown in Table 11.

## Coefficient of Thermal Expansion

The coefficient of linear thermal expansion ( $\alpha$ ) is a material property that indicates the extent to which the material expands or contracts with temperature changes. At a constant pressure, the true coefficient of volumetric thermal expansion ( $\alpha_V$ , or commonly  $\beta$ ) is defined by the changes that occur by a differential temperature change ( $dT$ ). This is usually expressed by the relationship:

$$\alpha_V = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_P \quad (\text{Eq 4})$$

where  $V$  is the volume at a temperature,  $T$ , at a constant pressure,  $P$ .

The corresponding definition for the linear coefficient of expansion can be represented by the relationship:

$$\alpha_l = \frac{1}{l} \left( \frac{\partial l}{\partial T} \right)_P \quad (\text{Eq 5})$$

Usually, the coefficient of thermal expansion is not measured directly but is calculated by the derivative of the equation that represents the expansion. Also, the instantaneous coefficient of linear thermal expansion is frequently defined as the fractional increase of length per unit rise in temperature. Further analyses and the theory of thermal expansion can be found in the literature (Ref 6).

The temperature dependence of the coefficient of thermal expansion for solids is very complex, but it has been shown that it varies inversely with the melting point ( $T_m$ ) of the material and is expressed by:

$$\alpha = \gamma_G / 100T_m \quad (\text{Eq 6})$$

where  $\gamma_G$  is the Grüneisen parameter and, for most solid materials, is close to 1. Semiempirical analyses (Ref 6) of the thermal expansion of crystalline materials, such as close-packed

metals, have shown that the mean coefficient of linear thermal expansion ( $\alpha_m$ ) can also be related to their melting temperature by the relationship:

$$(L_m - L_0)/L_0 = T_m \alpha_m \approx 0.0222 \quad (\text{Eq 7})$$

where  $L_m$  is the length at  $T_m$ .

It has been found that most metals with melting points above 900 K linearly expand approximately 2% on heating from 298 K to  $T_m$  (Ref 6). Many metals exhibit a thermal expansion  $\alpha_m \approx 10^{-4} \text{ K}^{-1}$  in the liquid phase just above the liquidus temperature. Table 5 shows the linear expansion ( $\Delta L/L_0$ ) and the coefficient of linear thermal expansion ( $\alpha$ ) for some pure metals at temperatures closer to their melting points (Ref 6). Unfortunately, few data at the solidus and/or liquidus are available for alloys of commercial interest. Data have been determined in the liquid by levitation, and recent developments with piston dilatometry enable measurements across the liquid/solid region. Using this technique, Blumm and Henderson (Ref 75) and Morrell and Queded (Ref 76) have performed measurements on nickel, aluminum, and cast irons, and typical data for alloys are included in Tables 14 to 17.

## Density

Density ( $\rho$ ) is defined as the mass per unit volume of a material. The reciprocal of the density ( $1/\rho$ ) is the specific volume. Room temperature and liquid density for pure metals and some materials of commercial interest are available in the literature (Ref 13, 15, 16, 28, 77).

Accurate density values are highly desirable since it is a variable in the calculation of thermal conductivity, surface tension, and viscosity. Further, the evaluation of fluid flow phenomena in a solidifying metal is dominated by the changes of density. Density of liquid metals is also useful to calculate volume changes during melting, solidification, and alloying. As a general rule, the average density change of non-close-packed metals on fusion is approximately 3% while the average volume change of a close-packed metal does not exceed 5% (Ref 71). Bismuth, gallium, antimony, germanium, silicon, cerium, and plutonium are the exceptions to the general rule, since these elements contract on melting.

Density of solid alloys as a function of temperature can be calculated from thermal expansion data using the following relationship:

$$\rho_T = \rho_{RT} / (1 + \Delta L_{\text{exp}})^3 \quad (\text{Eq 8})$$

where  $\Delta L_{\text{exp}}$  is the linear expansion ( $\Delta L_{\text{exp}} = (L_T - L_0)/L_0 = \alpha T$ ) at a temperature,  $T$ .

Alternatively, the density of a heterogeneous phase mixture ( $\rho_m$ ) containing a number,  $n$ , of phases can be roughly estimated using the empirical relationship:

$$\rho_m = \frac{1}{\sum_{i=1}^n (X_p / \rho_p)} \quad (\text{Eq 9})$$

where  $X_p$  and  $\rho_p$  are the fraction and density of the phase, respectively, at a given temperature.

The density of pure liquid metals as a function of temperature can be reasonably estimated from the following empirical equation (Ref 28):

$$\rho_L = a - b(T - T_m) \quad (\text{Eq 10})$$

where  $\rho_L$  is in  $\text{g/cm}^3$ ,  $a$  (the density at the liquidus temperature,  $\rho_m$ ) and  $b$  are dimensionless constants, and  $T$  is the temperature above the melting point ( $T_m$ ). Both temperatures are in degrees Kelvin.

Table 6 shows the density at the melting point and the values for the parameters  $a$  and  $b$  for estimation of the liquid density as a function of temperature for various elements. Table 6 also shows the viscosity and activation energy for viscous flow for some pure metals.

## Surface Tension

Knowledge of the surface tension phenomena of metals is essential in the understanding of solidification during casting. In solidification phenomena, the transformation of liquid into solid requires the creation of curved solid/liquid interfaces that lead to capillarity, microscopic heat flow, and solute diffusion effects. The interplay of the heat flow and solute diffusion effects determines the solidification morphologies. Solute diffusion effects have the tendency to minimize the scale of the morphology, while the capillarity effects tend to maximize the scale. A compromise between these two tendencies has a profound effect on the crystal morphologies with respect to nucleation, interface instability, and dendritic and eutectic growth (Ref 80). The surface energy has an important role because of the creation of the solid/liquid interface area. Also, during solidification, a decrease in the equilibrium melting point produces a positive undercooling and is associated to the solid/liquid interface curvature, which is usually convex toward the liquid phase. This curvature effect is often called the Gibbs-Thomson effect ( $\Gamma = \gamma_{sl}/\Delta S_f$ ), which is a function of the solid/liquid interfacial energy ( $\gamma_{sl}$ ) and the volume entropy of fusion ( $\Delta S_f$ ).

The Gibbs-Thompson effect is of the order of  $10^{-7}$  mK for most metals. This indicates that the effect of the surface energy becomes important only when a given morphology such as nuclei, interface perturbations, dendrites, and eutectic phases have a radius less than 10  $\mu\text{m}$  (Ref 80). Unfortunately, data on the surface energy or surface tension ( $\text{J/m}^2$ ) for most metals and their alloys are very limited or not available. Surface tension of liquid metals can be measured using various contact and noncontact techniques (Ref 33–36, 68, 69).

Semitheoretical models have been developed to calculate the surface tension of pure metals.

Table 4 Specific heat capacity data, latent heat of fusion, and solidus and liquidus temperatures for some alloys of commercial interest

Material	Nominal composition, wt%	Specific heat capacity, J/g · K	Temperature range, K	$C_p$ at 25 °C	$C_p$ at $T_L$	$\Delta H_f$ , J/g	$T_S$ , K	$T_L$ , K	Reference
<b>Aluminum alloys</b>									
A319 (LM4; Al-5Si-3Cu)	Al-3Cu-5Si-1Zn-0.35Ni-0.4Mn-0.1Mg	$C_p = 0.7473 + 2 \times 10^{-4}T + 5 \times 10^{-7}T^2$	298–780	0.87	1.17	393	798	898	16
A356 (LM25; Al-7Si-0.5Mg)	Al-7Si-0.5Fe-0.4Mg-0.3Mn-0.2Cu-0.1Ni-0.2Ti	$C_p = 0.7284 + 5 \times 10^{-4}T - 8 \times 10^{-7}T^2$	298–840 Trans. $T$ 653	0.88	1.16	425	840	887	16
2003	Al-4.5Cu	$C_p = 0.749 + 4.44 \times 10^{-4}T$	$T < 775$	0.882	1.059	...	775	911	14
3004	Al-0.2Cu-1Mg-1Mn-0.43Fe-0.14Si-0.25Zn	$C_p = 1.287 - 2.5 \times 10^{-4}T$ $C_p = 0.7989 + 3 \times 10^{-4}T - 9 \times 10^{-8}T^2$	775–991 298–873	0.90	1.22	383	890	929	16
2024-T4	Al-4.4Cu-1.5Mg-0.6Mn-0.5Fe-0.5Si-0.25Zn-0.1Cr-0.15Ti	$C_p = 0.7688 + 3 \times 10^{-4}T - 2 \times 10^{-7}T^2$	298–811	0.87	1.14	297	811	905	16
6061-T6	Al-0.3Cu-1Mg-0.15Mn-0.7Fe-0.6Si-0.25Zn-0.04Cr-0.15Ti	$C_p = 0.7067 + 6 \times 10^{-4}T - 1 \times 10^{-7}T^2$	298–873	0.87	1.17	380	873	915	16
7075-T6	Al-1.6Cu-2.5Mg-0.3Mn-0.5Fe-0.4Si-5.6Zn-0.2Cr-0.2Ti	$C_p = 0.7148 + 5 \times 10^{-4}T + 4 \times 10^{-10}T^2$	298–805	0.86	1.13	358	805	901	16
<b>Copper alloys</b>									
Cu-Al (Al-bronze)	Cu-9.7Al-4.6Fe-0.64Mn-4.6Ni	$C_p = 0.353 + 3 \times 10^{-4}T - 1 \times 10^{-7}T^2$	298–1313	0.442	0.582	240	1313	1350	16
Brass	70Cu-30Zn	$C_p = 0.582$ $C_p = 0.355 + 1.36 \times 10^{-4}T$ $C_p = 1.32 + 6.75 \times 10^{-4}T$ $C_p = 0.49$	1313–1773 298–1188 1188–1228 $1228 \leq T$	0.396	0.49	164.8	1188	1228	14
Brass	60Cu-40Zn	$C_p = 0.354 + 1.11 \times 10^{-4}T$ $C_p = -0.689 + 1.0 \times 10^{-3}T$ $C_p = 0.489$	$T \leq 1173$ 1173–1178 $1178 \leq T$	0.387	0.489	160.1	1173	1178	14
Copper-nickel	70Cu-30Ni-Fe-Mn	$C_p = 0.37 + 1.13 \times 10^{-4}T$ $C_p = 0.348 + 1.28 \times 10^{-4}T$ $C_p = 0.543$	$T \leq 1443$ 1443–1513 $1513 \leq T$	0.404	0.543	...	1443	1513	14
<b>Iron and steel alloys</b>									
Carbon steel AISI 1008	Fe-0.08C-0.31Mn-0.08Si-0.45Cr-0.03P-0.05S	$C_p = 0.593 + 4.8 \times 10^{-5}T$	1273–1550	0.469	...	...	1768	1808	14
Carbon steel AISI 1026	Fe-0.23C-0.63Mn-0.11Si-0.07Ni-0.03P-0.03S	$C_p = 0.354 + 2.1 \times 10^{-4}T$	1379–1550	0.469	...	...	1768	1798	14
1% Cr	Fe-0.3C-0.69Mn-0.2Si-1.1Cr-0.7Ni-0.012Mo-0.039P-0.036S	$C_p = 0.436 + 1.22 \times 10^{-3}T$	1173–1683	0.477	0.856	251	1693	1793	14
304 stainless steel	Fe-0.08C-19Cr-0.3Cu-2Mn-9.5Ni	$C_p = 0.443 + 2 \times 10^{-4}T - 8 \times 10^{-10}T^2$	298–1727	0.49	0.80	290	1673	1727	14, 16
316 stainless steel	Fe-0.08C-17Cr-0.3Cu-2Mn-2.5Mo-12Ni-1Si	$C_p = 0.412 + 2 \times 10^{-4}T - 2 \times 10^{-8}T^2$	298–1658	0.45	0.79	260	1658	1723	14, 16
420 stainless steel	Fe-0.3C-13Cr-0.12Cu-0.5Mn-0.06Mo-0.5Ni-0.4Si	$C_p = 1.92 - 1.587 \times 10^{-2}T$ $C_p = 0.569$	1150–1173 $T > 1173$	0.477	...	304	1727	1783	14
Ductile iron	Fe-3.61C-2.91Si-0.08Cr-0.12Cu-0.65Mn-0.02Mo-0.13Ni $\leq$ 0.002Mg	$C_p = 0.80$	1373	0.48	0.83	220	1413	1451	16
Gray cast iron	Fe-3.72C-1.89Si-0.95Cr-0.66Mn-0.59Mo-0.19Ni $\leq$ 0.002Mg	$C_p = 0.66$	1353	0.49	0.95	240	1353	1463	16
<b>Magnesium alloys</b>									
AZ31B	Mg-3Al-1Zn-0.5Mn	$C_p = 1.88 - 5.22 \times 10^{-4}T$ $C_p = 0.979 + 4.73 \times 10^{-4}T$	$839 \leq T \leq 905$ $905 \leq T$	1.01	1.415	...	839	905	14
AZ91B	Mg-9Al-0.6Zn-0.2Mn	$C_p = 0.251 + 1.354 \times 10^{-3}T$ $C_p = 1.43$	$742 \leq T \leq 869$ $869 \leq T$	0.98	1.428	...	742	869	14
K1A	Mg-0.7Zr	$C_p = 0.873 + 0.463 \times 10^{-3}T$ $C_p = 1.43$	$T \leq 922$ $923 \leq T$	1.005	1.428	...	922	923	14
ZK51A	Mg-4.6Zn-0.7Zr	$C_p = 1.945 - 6.28 \times 10^{-4}T$ $C_p = 0.90 + 0.516 \times 10^{-3}T$	$822 \leq T \leq 914$ $914 \leq T$	1.022	1.371	...	822	914	14
HM11A	Mg-1.2Mn-1.2Th	$C_p = 0.65 + 8.75 \times 10^{-3}T$ $C_p = 1.482$	$903 \leq T \leq 923$ $923 \leq T$	0.946	1.411	...	905	923	14
EZ33	Mg-3Ce-2Zn-0.6Zr	$C_p = 1.21$ $C_p = 1.336$	818 $913 \leq T$	0.98	1.336	343	818	913	16
<b>Nickel alloys</b>									
Single-crystal CMSX-4	Ni-10Co-6.5Cr-6.5Ta-6.4W-3Re-1Ti-0.15Fe-0.04Si-0.006C	$C_p = 0.675$	$1653 \leq T$	0.397	0.636	240	1593	1653	16
Hastelloy C	Ni-16Mo-16Cr	$C_p = 0.281 + 0.283 \times 10^{-3}T$	$T \leq 1534$	0.283	...	...	1534	1578	14
Hastelloy X	Ni-22Cr-18.5Fe-9Mo-1.5Co-0.6W-0.5Si-0.1C	$C_p = 0.4384 + 1 \times 10^{-4}T + 5 \times 10^{-8}T^2$	1073–1533	0.439	0.677	276	1533	1628	16
Inconel 718	Ni-19Cr-16.7Fe-5.2Nb-3.1Mo-1Co-0.9Ti-0.35Mn-0.35Si-0.08C	$C_p = 0.65$	1443	0.435	0.72	210	1533	1609	16
<b>Titanium alloys</b>									
Ti-6Al-4V	Ti-5.5–6.7Al-3.5–4.5V-0.25(O <sub>2</sub> + N <sub>2</sub> )-0.03Fe-0.0125H <sub>2</sub>	$C_p = 0.4115 + 2 \times 10^{-4}T + 5 \times 10^{-10}T^2$ $C_p = 0.83$	1268–1923 $T \geq 1923$	0.546	0.83	286	...	1923	16
<b>Zinc alloys</b>									
Zn-Al	Zn-4.5Al-0.05Mg	$C_p = 0.50$ $C_p = 0.52 - 6 \times 10^{-5}(T - 387 \text{ °C})$	630 Liquid $T \geq 660$	0.41	0.51	114	630	660	16

**Table 5 Thermal expansion of selected pure metals at temperatures close to melting**

Element	Melting point ( $T_m$ ), K	LE%(a), $\Delta L/L_0$	CTE ( $\alpha$ )(b), $10^{-6}/K$	$T$ (c), K
Ag	1233.7	2.11	28.4	1200
Al	933.5	1.764	37.4	900
Au	1336	1.757	22.1	1300
Be	1562	2.315	23.7	1500
Bi	544.6	0.307	12.4	525
Cd	594	1.028	40	590
Ce	1072	0.512	9.4	1000
Cr	2148	2.02	19	1900
Co	1766	1.5	17.7	1200
Cu	1356	2.095	25.8	1300
$\alpha$ -Fe	1185	1.37	16.8	1185
Fe ( $\alpha$ - $\gamma$ )	1185	0.993	23.3	1185
$\gamma$ -Fe	1811	2.077	23.3	1650
Hf	2216	0.712	8.4	1300
La	1195	0.497	11.3	1000
Li	453.5	0.804	56	450
Mg	924	1.886	37.6	900
Mn	1525	6.604	...	1500
Mo	2880	2.15	16.5	2800
Nb	2741	1.788	10.1	2300
Ni	1727	2.06	20.3	1500
Pb	660.6	0.988	36.7	600
Pd	1825	1.302	16.9	1200
Pt	2042	1.837	14.9	1900
Re	3431	1.941	9.8	2800
Rh	2236	1.526	15.4	1600
Sb	904	0.588	11.7	800
Si	1683	...	3.8	...
Sn	505	0.516	27.2	500
Ta	3250	3.126	24.4	3200
$\alpha$ -Ti	1156	0.918	11.8	1156
Ti ( $\alpha$ - $\beta$ )	1156	0.868	11	1156
Ti- $\beta$	1958	1.411	13.5	1600
V	2185	2.16	17.2	2000
W	3650	2.263	11.6	3600
Zn	692	1.291	34	690
Zr	2123	1.139	11.3	1800

(a) LE% = percent of linear expansion. (b) CTE = coefficient of linear expansion. (c)  $T$  = temperature. Source: Ref 6

The rigid sphere model (Ref 81) assumed a structure of the liquid metal where the collision diameter may be estimated by the molar volume ( $V$ ) at the melting temperature. Then, the surface tension can be expressed by:

$$\gamma = (3.6T_m V^{-2/3}) \times 10^{-3} \text{ J/m}^2 \quad (\text{Eq 11})$$

Alternatively, the surface tension has been correlated to the heat vaporization ( $\Delta H_v$ ) caused by the breaking of the interatomic bonds during evaporation in the liquid state (Ref 82). Usually, metals with large atomic volume have low energies of vaporization:

$$\gamma = 1.8 \times 10^{-9} (\Delta H_v / V^{-2/3}) \quad (\text{Eq 12})$$

The surface tension for pure metals as a function of temperature ( $\gamma$  vs  $T$ ) can also be calculated using Eq 13 and Table 7:

$$\gamma f(T) = \gamma_i^0 + c(T - T_m) \quad (\text{Eq 13})$$

where  $\gamma_i^0$  is the surface tension at the melting point, and  $c$  is  $d\gamma/dT$ ,  $T_m$ , and  $T > T_m$ ;  $T$  and  $T_m$  are in degrees Kelvin.

There are two definitive compendia of surface tension values by Keene: the first for pure metals (Ref 83) and the other for iron and its binary alloys (Ref 84). The review of elements

**Table 6 Density at the melting point, dimensionless values for the parameters  $a$  and  $b$ , viscosity, and activation energy for viscous flow for selected elements**

Element	Melting point, K	Density, g/cm <sup>3</sup>			Viscosity (Ref 13, 78, 79)		
		Measured (Ref 13) at $T_m$	$\rho_L = a - b(T - T_m)$ (Ref 28)		$\eta$ at $T_m$ , mN·s/m <sup>2</sup>	$\eta_0$ , mN·s/m <sup>2</sup>	$E$ , kJ/mol
			$a$	$b \times 10^{-4}$			
Ag	1233.7	9.346	9.329	10.51	3.88	0.4532	22.2
Al	933.5	2.385	2.378	3.111	1.34	0.185	15.4
Au	1336	17.36	17.346	17.020	5.38	1.132	15.9
B	2448	2.08 at 2346 K	...	...	...	...	...
Be	1550	1.690	1.690	1.165	...	...	...
Bi	544	10.068	10.031	12.367	1.85	0.4458	6.45
Cd	593	8.020	7.997	12.205	2.28	0.3001	10.9
Ce	1060	6.685	6.689	2.270	2.88	...	...
Cr	2148	6.28	6.280	7.230	...	...	...
Co	1766	7.760	7.740	9.500	4.49	0.2550	44.4
Cu	1356	8.000	8.033	7.953	4.10	0.3009	30.5
Fe	1811	7.015	7.035	9.26	5.85	0.191	51.5
Hf	2216	11.10	...	...	...	...	...
La	1203	5.955	5.950	2.370	2.45	...	...
Li	453.5	0.525	0.5150	1.201	0.55	0.1456	5.56
Mg	924	1.590	1.589	2.658	1.32	0.0245	30.5
Mn	1525	5.730	5.750	9.300	...	...	...
Mo	2880	9.35	...	...	...	...	...
Nb	2741	7.830	...	...	...	...	...
Ni	1727	7.905	7.890	9.910	4.60	0.1663	50.2
Pb	660.6	10.678	10.587	12.220	2.61	0.4636	8.61
Pd	1825	10.490	18.909	28.826	...	...	...
Pt	2042	19.00	18.909	28.826	...	...	...
Re	3431	18.80	...	...	...	...	...
Sb	904	6.483	6.077	6.486	1.48	0.0812	22
Si	1683	2.524	2.524	3.487	0.94	...	...
Sn	505	7.000	6.973	7.125	2.00	0.5382	5.44
Ta	3250	15.00	...	...	...	...	...
Ti	1958	4.110	4.140	2.260	5.20	...	...
V	2185	5.700	5.36	3.20	...	...	...
W	3650	17.60	...	...	...	...	...
Zn	692	6.575	6.552	9.502	3.85	0.4131	12.7
Zr	2123	5.800	...	...	8.0	...	...

Source: Ref 129

has recently been updated (Ref 85). Variations on reported surface tension of pure elements and alloys are expected because of the experimental techniques and the strong effect of surface-active impurities such as soluble oxygen, sulfur, and tellurium in liquid metals on their surface tension. Therefore, the levels of impurities in solution should be carefully controlled and taken into account in the determination and assessment of the surface tension of metallic alloys. It should be noted that in practice it is difficult to control soluble oxygen levels.

Marangoni flows are those driven by surface tension gradients. In general, surface tension depends on both the temperature and chemical composition at the interface; consequently, Marangoni flows may be generated by gradients in either temperature or chemical concentration at an interface. Because the temperature coefficient for surface tension,  $d\gamma/dT$ , can change sign from a negative to positive as the impurity concentration increases, the direction of flow in shallow pools of liquid (Marangoni flow) with uneven temperature distributions can be reversed with different materials with different surface-active element concentrations. These effects are established to have implications in melt processes such as the weld quality and flow during melt refining. Fifty ppm of either oxygen or sulfur cause a decrease of 25% in  $\gamma$  and a change from negative ( $d\gamma/dT$ ) to positive

( $d\gamma/dT$ ), which will reverse the direction of any Marangoni convection.

Brooks and Quedest (Ref 86) have recently reviewed both the surface tension ( $\gamma$ ) and  $d\gamma/dT$  for a variety of ferritic and austenitic steels as a function of sulfur content. In general, ( $\gamma$ ) decreases with increasing sulfur levels, and  $d\gamma/dT$  increases from negative to positive with increasing sulfur levels. For detailed compositions of the steels, the reader is referred to Ref 86.

Thermodynamic models to calculate the surface tensions of liquid alloys have been developed (Ref 46, 87–90). These models were based on earlier work on surface tension prediction of binary (Ref 89) and ternary (Ref 90) solutions and on the Buttler equation (Ref 91). In order to calculate the surface tension of a liquid metal using the Buttler equation, the surface tensions and surface areas of the pure constituent elements and the excess Gibbs energy of the liquid metal must be known. The excess Gibbs energy is the same as that used for calculating the phase diagram and thermodynamic properties. In this thermodynamic approach, the description of the alloy system must be established before any property of the multi-component alloy can be calculated. Model parameters for several alloy systems have been determined (Ref 92–103). Table 8 shows the surface tension values for some alloys of industrial interest (Ref 16).

**Table 7 Surface tension for pure liquid metals**

Element	$\gamma_i^0$ at $T_m$ , mN/m	$-d\gamma/dT$ , mN/m · K
Ag	903	0.16
Al	914	0.35
Au	1140	0.52
B	1070	...
Be	1390	0.29
Bi	378	0.07
Cd	570	0.26
Ce	740	0.33
Cr	1700	0.32
Co	1873	0.49
Cu	1285	0.13
Fe	1872	0.49
Hf	1630	0.21
La	720	0.32
Li	395	0.15
Mg	559	0.35
Mn	1090	0.2
Mo	2250	0.30
Nb	1900	0.24
Ni	1778	0.38
Pb	468	0.13
Pd	1500	0.22
Pt	1800	0.17
Re	2700	0.34
Sb	367	0.05
Si	865	0.13
Sn	544	0.07
Ta	2150	0.25
Ti	1650	0.26
V	1950	0.31
W	2500	0.29
Zn	782	0.17
Zr	1480	0.20

Source: Ref 13

**Table 8 Surface tension for some industrial alloys**

Material(a)	Surface tension(b), mN/m	Temperature, K
Cu-Al (Al-bronze)	1240	1350
	1215	1473
Single-crystal	1850	1653
CMSX-4	1850	1873
Hastelloy X	1880	1628
	1865	1773
Inconel 718	1882	1609
	1866	1773
Zn-Al	830	660
	807	773

(a) Chemistries given in Table 4. (b) Values depend on oxygen and sulfur contents. Source: Ref 16

## Viscosity

The viscosity is the resistance of the fluid to flow when subjected to an external shear force. The shear stress ( $\tau$ ), or the force per unit area, causing a relative motion of two adjacent layers in a liquid is proportional to the velocity gradient ( $du/dy$ ), which is normal to the direction of the applied force ( $\tau = -\eta du/dy$ ), where the proportionality factor,  $\eta$ , is termed the viscosity. This concept is known as Newton's law of viscosity. Most liquid metals are believed to follow a Newtonian behavior. The unit of viscosity is called Poise (P) ( $1P = 1 \text{ dyne} \cdot \text{s}/\text{cm}^2 = 1 \text{ g}/\text{cm} \cdot \text{s} = 1 \text{ mPa} \cdot \text{s}$ ). The parameter ( $\eta/\rho$ ) is referred to as kinematic viscosity and has units ( $\text{m}^2/\text{s}$ ), which

are identical to the units for diffusion coefficients and thermal diffusivity.

Several methods exist to measure the viscosity of liquid metals (Ref 67, 104, 105). However, accurate and suitable methods to measure the viscosity of liquid metals and their alloys are restricted due to the relatively low viscosity, high liquidus temperatures, and chemical reactivity of melts.

The reciprocal of the viscosity is known as the fluidity. The kinematic viscosity is the ratio of the viscosity to density ( $\nu = \eta/\rho$ ). This is an important parameter in fluid mechanics. The kinematic viscosity represents the transverse diffusion of momentum down a velocity gradient that is necessary to describe mold filling in a casting process.

The Arrhenius equation is the most common form of representing the temperature dependence (Ref 104) of viscosity:

$$\eta = A \exp(E_v/RT) \quad (\text{Eq 14})$$

where  $E_v$  is the activation energy for viscous flow, and  $R$  is the ideal gas constant ( $8.3144 \text{ J/K}$ ).

Andrade (Ref 106) derived a semiempirical relation to determine the viscosity of elemental liquid metals at their melting temperatures. Andrade's relationship is based on the quasicrystalline theory that assumes that the atoms in the liquid at the melting point are vibrating in random directions and periods, just as in the solid state.

Modification to Andrade's equation, based on the characteristics of atomic vibration frequency at the melting point, gives (Ref 104):

$$\eta_m = 1.7 \times 10^{-7} \rho^{2/3} T_m^{1/2} M^{-1/6} \text{ (Pa} \cdot \text{s)} \quad (\text{Eq 15})$$

where  $\rho$  is the density,  $M$  is the atomic mass, and  $T_m$  is the melting point in degrees Kelvin.

The temperature dependence of the viscosity for most pure liquid metals can be expressed by:

$$\eta = \eta_0 \exp(2.65T^{1.27}/RT) \text{ (mPa} \cdot \text{s)} \quad (\text{Eq 16})$$

At  $T = T_m$  and  $\eta = \eta_m$ , then the value for  $\eta_0$  is determined as follows:

$$\eta_0 = \eta_m / [\exp(2.65T_m^{1.27}/RT_m)] \quad (\text{Eq 17})$$

With the exception of silicon, manganese, chromium, hafnium, palladium, and vanadium, these equations allow a reasonable prediction of the viscosity as a function of temperature for most pure liquid metals. Further modifications of Andrade's equation have been developed in an attempt to estimate more accurately the viscosity of liquid metals (Ref 107–111).

An empirical relationship between viscosity and surface tension for pure liquid metals has been developed (Ref 111):

$$\eta_m = 2.81 \times 10^{-4} [(M\gamma_m)^{1/2}/V^{1/3}] \quad (\text{Eq 18})$$

where  $M$  is the atomic mass,  $V$  is the atomic volume, and  $\gamma_m$  is the surface tension at the melting point.

Table 6 shows the viscosity of liquid metals at their melting temperature and their activation energy for viscous flow (Ref 78, 79), and Table 9 shows the viscosities of some metals and some alloys of commercial interest (Ref 16).

## Electrical and Thermal Conductivity

Thermal and electrical conductivities are intrinsic properties of materials, and they reflect the relative ease or difficulty of energy transfer through the material. Metals are well known for their high electrical conductivity, which arises from the easy migration of electrons through the crystal lattice. The conductivity on melting for most metals decreases markedly due to the exceptional disorder of the liquid state. Generally, the electrical resistivity of some liquid metals just above their melting points is approximately 1.5 to 2.3 greater than that of the solids just below their melting temperature (Ref 33). Examples of exceptions are iron, cobalt, and nickel.

Mott (Ref 112) derived an empirical equation to estimate the ratio of liquid/solid electrical conductivity ( $\sigma_{e,l}/\sigma_{e,s}$ ) at the melting point of the pure metal. The Mott equation is expressed as follows:

$$\ln(\sigma_{\text{sol}}/\sigma_{\text{liq}}) = C(\Delta H_m/T_m) = C(\Delta S_m) \quad (\text{Eq 19})$$

where  $\Delta H_m$  is the enthalpy of fusion in KJ/mol,  $T_m$  is the melting temperature in degrees Kelvin,  $\Delta S_m$  is the entropy of fusion, and  $C$  is a constant. With the exception of a few metals (e.g., antimony, bismuth, gallium, mercury, and tin), the simple relationship proposed by Mott is in good agreement with experimental measurements.

Reviews of the electrical and thermal conductivity theories can be found in the literature (Ref 113–119). Of particular interest to high-temperature technology, such as casting processes, is the theoretical relation between the thermal ( $k$ ) and electrical ( $\sigma$ ) conductivities known as the Wiedman-Franz law (WFL) and the constant of proportionality known as the Lorentz number,  $L$  (Ref 120). The WFL relationship (Eq 20) appears to hold reasonably well for pure metals around the melting point, but large departures can occur at lower temperatures in the solid:

$$L = (k/\sigma T) = 2.445 \times 10^{-8} \text{ W} \cdot \Omega/\text{K}^2 \quad (\text{Eq 20})$$

Convective flow that usually occurs in the liquid should not have any effect on the electrical conductivity. Therefore, it should be possible to estimate the thermal conductivity of liquid alloys from the electrical conductivity values. The electrical conductivity for molten binary alloy has been estimated using Eq 21 (Ref 33):

$$\sigma_{T1} = \sigma_1 x_1 + \sigma_2 x_2 + \sigma_3 x_3 + \dots \quad (\text{Eq 21})$$

A negative departure of less than 10% from linearity has been observed for most alloys. Similarly, the temperature dependence of the

Table 9 Density, thermal conductivity, surface tension, and viscosity for some commercial alloys

Material(a)	Density, g/cm <sup>3</sup> T in K	Thermal conductivity(b), W/m · K (temp. range in K)	Estimated viscosity(c), mPa · s	
<b>Aluminum alloys</b>				
<b>Aluminum alloys</b>	<b>273 K</b>			
A319	2.75	$\rho_s = 2.753 - 22.3 \times 10^{-2} (T - 298)$ $\rho_l = 2.492 - 27.0 \times 10^{-2} (T - 894)$ $k_s = 76.64 + 0.2633T - 2 \times 10^{-4}T^2$ $k_l = 70$ $k_i = 71$	(T: 298–773) (T: 894) (T: 1073)	1.3 at 894 K 1.1 at 1073 K
LM25 (A356)(d)	2.68	$\rho_s = 2.68 - 21.2 \times 10^{-2} (T - 298)$ $\rho_l = 2.401 - 26.4 \times 10^{-2} (T - 887)$ $k_s = 149.7 + 0.0809T - 1 \times 10^{-4}T^2$ $k_l = 65.8$ $k_i = 70$	(T: 298–840) (T: 887) (T: 1073)	1.38 at 887 K 1.1 at 1073 K
2003(e)	...	...	...	...
3004	2.72	$\rho_s = 2.72 - 23.4 \times 10^{-2} (T - 298)$ $\rho_l = 2.4 - 27.0 \times 10^{-2} (T - 929)$ $k_s = 124.7 + 0.56T + 1 \times 10^{-5}T^2$ $k_l = 61$	(T: 298–890) (T: $\geq 929$ )	1.15 at 929 K 1.05 at 973 K
2024-T4	2.785	$\rho_s = 2.785 - 21.3 \times 10^{-2} (T - 298)$ $\rho_l = 2.50 - 28.0 \times 10^{-2} (T - 905)$ $k_s = 188$ $k_l = 85.5$	(T: 473–573) (T: 811–905)	1.30 at 905 K 1.1 at 1073 K
6061-T6	2.705	$\rho_s = 2.705 - 20.1 \times 10^{-2} (T - 298)$ $\rho_l = 2.415 - 28.0 \times 10^{-2} (T - 915)$ $k_s = 7.62 + 0.995T - 17 \times 10^{-4}T^2 + 1 \times 10^{-6}T^3$ $k_l = 66.5$ $k_i = 90$	(T: 298–773) (T: 873) (T: 915)	1.15 at 915 K 1.0 at 1073 K
7075-T6	2.805	$\rho_s = 2.805 - 22.4 \times 10^{-2} (T - 273)$ $\rho_l = 2.50 - 28.0 \times 10^{-2} (T - 901)$ $k_s = 196$ $k_l = 193$ $k_i = 85$	(T: 673–773) (T: 805) (T: 901)	1.3 at 901 K 1.1 at 1073 K
<b>Copper alloys</b>				
Cu-Al (Al-bronze)	7.262	$\rho_s = 7.262 - 48.6 \times 10^{-2} (T - 298)$ $\rho_l = 6.425 - 65.0 \times 10^{-2} (T - 1350)$ $k_s = 7.925 + 0.1375T - 6 \times 10^{-5}T^2$ $k_l = 42$ $k_i = 27$	(T: 373–773) (T: 1313) (T: 1373)	6.3 at 1350 K 5.2 at 1473 K
Brass(e)	...	...	...	...
70Cu-30Zn	...	$k_s = 140.62 + 112.14 \times 10^{-4}T$ $k_{s/l} = 2430.3 - 191.61 \times 10^{-2}T$ $k_l = 45.43 + 26 \times 10^{-3}T$	(T: 460–1188) (T: 1188–1228) (T: $\geq 1228$ )	...
Brass(e)	...	...	...	...
60Cu-40Zn	...	$k_s = 182.95 + 366.1 \times 10^{-4}T$ $k_{s/l} = 16479.5 - 13.93 T$ $k_l = 39.724 + 26 \times 10^{-3}T$	(T: 620–1173) (T: 1173–1178) (T: $\geq 1178$ )	...
Copper-nickel(e)	...	...	...	...
70Cu-30Ni-Fe-Mn	...	$k_s = 16.041 + 438.9 \times 10^{-4}T$ $k_{s/l} = 796.018 - 502.63 \times 10^{-3}T$ $k_l = -3.8 + 26 \times 10^{-3}T$	(T: $\leq 1443$ ) (T: 1443–1513) (T: $\geq 1513$ )	...
<b>Iron and steel alloys</b>				
Steel AISI 1008(e)	7.86	$\rho_l = 7.0$ at 1823 K $k_s = 13.58 + 11.3 \times 10^{-3}T$ $k_l = 280.72 - 14.0 \times 10^{-3}T$ $k_i = 14.53 + 105.0 \times 10^{-4}T$	(T: 1122–1768) (T: $\geq 1768$ ) (T: 1073–1693)	...
1% Cr steel(e)	...	...	...	...
Fe-0.3C-0.69Mn-0.2Si-1.1Cr-0.7Ni	...	$k_{s/l} = 91.74 - 351.0 \times 10^{-4}T$ $k_l = 7.85 + 116.8 \times 10^{-4}T$	(T: 1693–1793) (T: $\geq 1793$ )	...
304 stainless steel	8.02	$\rho_s = 8.02 - 50.1 \times 10^{-2} (T - 298)$ $\rho_l = 6.90 - 80.0 \times 10^{-2} (T - T_m)$ $k_s = 10.33 + 15.4 \times 10^{-3}T - 7.0 \times 10^{-7}T^2$ $k_{s/l} = 355.93 - 196.8 \times 10^{-3}T$ $k_l = 6.6 + 12.14 \times 10^{-3}T$	(T: 298–1633) (T: 1644–1672) (T: $\geq 1793$ )	8.0 at 1727 K
316 stainless steel	7.95	$\rho_s = 7.95 - 50.1 \times 10^{-2} (T - 298)$ $\rho_l = 6.881 - 77.0 \times 10^{-2} (T - T_m)$ $k_s = 6.31 + 27.2 \times 10^{-3}T - 7.0 \times 10^{-6}T^2$ $k_{s/l} = 355.93 - 196.8 \times 10^{-3}T$ $k_l = 6.6 + 12.14 \times 10^{-4}T$	(T: 298–1573) (T: 1644–1672) (T: $\geq 1672$ )	8.0 at 1723 K
420 stainless steel(e)	7.7	$\rho_l = 7.0$ at 1823 K $k_s = 20 + 61.5 \times 10^{-4}T$ $k_{s/l} = 133.4 - 594.9 \times 10^{-4}T$ $k_l = 6.5 + 116.8 \times 10^{-4}T$	(T: $\leq 1727$ ) (T: 1727–1783) (T: $\geq 1783$ )	...
Ductile iron	7.3	$\rho_s = 7.06$ at 1373 K $\rho_l = 6.62$ at 1451 K $\rho_i = 6.586$ at 1573 C $k_s = 31$ $k_l = 28$ $k_i = 29$	(T: 1373) (T: 1451) (T: 1673)	14.0 at 1451 K 11.5 at 1573 K 9.0 at 1673 K
Gray cast iron	7.2	$\rho_s = 6.992$ at 1273 K $\rho_l = 6.964$ at 1353 K $\rho_i = 7.495 - 77.0 \times 10^{-2}T$ $k_s = 29$ $k_l = 26$ $k_i = 28$	(T: 1353) (T: 1463) (T: 1673)	14.3 at 1463 K 14.0 at 1473 K 10.5 at 1573 K
<b>Magnesium alloys</b>				
AZ31B(e)	...	...	...	...
AZ91B(e)	...	$k_s = 67.12 + 655.7 \times 10^{-4}T$ $k_{s/l} = 830.9 - 844.8 \times 10^{-3}T$ $k_l = 3.05 + 70.0 \times 10^{-3}T$	(T: 499–839) (T: 839–905) (T: $\geq 905$ )	...
KIA(e)	...	...	...	...
ZK51A(e)	...	$k_s = 18.27 + 112.11 \times 10^{-3}T$ $k_{s/l} = 372 - 364.6 \times 10^{-3}T$ $k_l = -5.63 + 7.0 \times 10^{-2}T$	(T: $\leq 742$ ) (T: 742–869) (T: $\geq 869$ )	...
HM11A(e)	...	...	...	...
EZ33	1.8	$\rho_s = 1.8 - 14.3 \times 10^{-2} (T - 298)$ $\rho_l = 1.663 - 27.0 \times 10^{-2} (T - 913)$ $k_s = 127.16 + 142.9 \times 10^{-4}T$ $k_l = 11.66 + 7.0 \times 10^{-2}T$ $k_i = 71.96 + 154.35 \times 10^{-3}T - 93.8 \times 10^{-6}T^2$ $k_{s/l} = 688 - 672.2 \times 10^{-3}T$ $k_l = 9.62 + 70.0 \times 10^{-3}T$ $k_i = 73.35 + 133.43 \times 10^{-3}T - 73.9 \times 10^{-6}T^2$ $k_{s/l} = 2887 - 305.0 \times 10^{-2}T$ $k_l = 8.0 + 70.0 \times 10^{-3}T$	(T: 520–922) (T: $\geq 923$ ) (T: $\leq 822$ ) (T: 822–914) (T: $\geq 914$ ) (T: $\leq 903$ ) (T: 903–923) (T: $\geq 923$ )	1.5 at 913 K 1.4 at 973 K
<b>Nickel alloys</b>				
Single crystal	8.7	$\rho_s = 8.7 - 45.8 \times 10^{-2} (T - 298)$ $\rho_l = 7.754 - 90.0 \times 10^{-2} (T - 1653)$ $k_s = 27.2$ $k_l = 25.6$	(T: 1573)(f) (T: 1653–1673)	6.7 at 1653 K 5.3 at 1773 K

(continued)

(a) Chemistry of the alloys is given in Table 4. (b) The polynomial equations that represent the thermal conductivity for most of the alloy systems shown in this table are estimated from the data recommended in Ref 16. Other data indicated as (e) have been obtained from Ref 14. For further analysis of the data it is recommended to consult the original source cited in the given literature. (c) Estimated values of viscosity may vary from  $\pm 10$  to  $\pm 30\%$  (Ref 16). (d) Aluminum alloy with the British designation LM25 is equivalent to the Aluminum Association designation of A356. (e) Data from Ref 14. (f) Based on estimated  $C_p$  value from  $\lambda_s = \text{ap}C_p$  (Ref 16)



Table 9 (continued)

Material(a)	Density, g/cm <sup>3</sup> T in K	Thermal conductivity(b), W/m · K (temp. range in K)	Estimated viscosity(c), mPa · s
Hastelloy X	8.24 $\rho_s = 8.24 - 38.1 \times 10^{-2}(T - 298)$ $\rho_l = 7.42 - 83.0 \times 10^{-2}(T - 1628)$	$k_s = 3.36 + 17.3 \times 10^{-3}T + 2.0 \times 10^{-6}T^2$ (T: 1073–1533) $k_l = 29.0$ (T: 1428–1773)	7.5 at 1628 K 5.5 at 1773 K
Inconel 718	8.19 $\rho_s = 8.19 - 39.2 \times 10^{-2}(T - 298)$ $\rho_l = 7.40 - 88.0 \times 10^{-2}(T - 1609)$	$k_s = 39.73 + 32.4 \times 10^{-3}T + 2.0 \times 10^{-5}T^2$ (T: 1173–1443) $k_l = 29.6$ (T: 1609–1873)	7.2 at 1609 K 5.31 at 1773 K
<b>Titanium alloys</b>			
Ti-6Al-4V	4.42 $\rho_s = 4.42 - 15.4 \times 10^{-2}(T - 298)$ $\rho_l = 3.92 - 68.0 \times 10^{-2}(T - 1923)$	$k_s = -0.797 + 18.2 \times 10^{-3}T - 2.0 \times 10^{-6}T^2$ (T: 1268–1923) $k_l = 33.4$ (T: 1923) $k_l = 34.6$ (T: 1973)	3.25 at 1923 K 2.66 at 2073 K
<b>Zinc alloys</b>			
Zn-Al	6.7 $\rho_s = 6.7 - 60.3 \times 10^{-2}(T - 298)$ $\rho_l = 6.142 - 97.7 \times 10^{-2}(T - 660)$	$k_s = 98.0$ (T: 630) $k_l = 40.0$ (T: 660)	3.5 at 673 K 2.6 at 773 K

(a) Chemistry of the alloys is given in Table 4. (b) The polynomial equations that represent the thermal conductivity for most of the alloy systems shown in this table are estimated from the data recommended in Ref 16. Other data indicated as (e) have been obtained from Ref 14. For further analysis of the data, it is recommended to consult the original source cited in the given literature. (c) Estimated values of viscosity may vary from +10 to -30% (Ref 16). (d) Aluminum alloy with the British designation LM25 is equivalent to the Aluminum Association designation of A356. (e) Data from Ref 14. (f) Based on estimated  $C_p$  value from  $\lambda_s = \alpha C_p$  (Ref 16)

Table 10 Electrical resistivity ( $\rho_e$ ) and thermal conductivity of solid and liquid metals

Element	$T_m, K$	Electrical resistivity (Ref 13, 33)					$T$ range $T_m$ to $T, K$	Thermal conductivity (Ref 122)			
		$\rho_{e,s}, \mu\Omega \cdot cm$	$\rho_{e,l}, \mu\Omega \cdot cm$	$\rho_{e,l}/\rho_{e,s}$	$\rho_{e,l} = \alpha T + \beta$			$k_{sm}$	$k_{lm}$	$\Delta S_m, J/mol \cdot K$	$K$
					$\alpha, \mu\Omega \cdot cm/K$	$\beta, \mu\Omega \cdot cm$					
Ag	1233.7	8.2	17.2	2.09	0.0090	6.2	1473	362	175	9.15	0.0794
Al	931	10.9	24.2	2.20	0.0145	10.7	1473	211	91	10.71	0.0785
Au	1336	13.68	31.2	2.28	0.0140	12.5	1473	247	105	9.39	0.0911
B	2448	...	210.0	...	...	...	...	...	...	...	...
Be	1550	...	45.0	...	...	...	...	...	...	...	...
Bi	544	...	129.0	...	...	...	...	7.6	12	20.75	0.022
Cd	593	17.1	33.7	1.97	Not linear	...	...	$37 \pm 3$	90	10.42	...
Ce	1060	...	126.8	...	...	...	...	21	22	2.99	...
Cr	2148	...	31.6	...	...	...	...	45	35	9.63	0.0261
Co	1766	97	102	1.05	0.0612	-6.0	1973	45	36	9.16	0.0243
Cu	1356	9.4	20.0	2.1	0.0102	6.2	1873	330	163	9.77	0.0722
Fe	1809	122	110	0.9	0.033	50	1973	34	33	7.62	0.0039
Hf	2216	...	218.0	...	...	...	...	39	...	10.9	...
La	1203	...	138	...	...	...	...	...	17	5.19	...
Li	453.5	...	240.0	...	...	...	...	71	43	6.6	0.076
Mg	924	15.4	27.4	1.78	0.005	22.9	1173	145	79	9.18	0.066
Mn	1525	66	40	0.61	No data	...	...	24	22	8.3	0.0102
Mo	2880	...	60.5	...	...	...	...	87	72	12.95	...
Nb	2741	...	105.0	...	...	...	...	78	66	10.90	...
Ni	1727	65.4	85.0	1.3	0.0127	63	1973	70	60	10.11	0.0152
Pb	660.6	49.0	95.0	1.94	0.0479	66.6	1273	30	15	7.95	0.0872
Pd	1825	...	...	...	...	...	...	99	87	9.15	...
Pt	2042	...	73.0	...	...	...	...	80	53	10.86	0.0392
Re	3431	...	145	...	...	...	...	$65 \pm 5$	55	17.5	...
Sb	904	183	113.5	0.61	0.270	87.9	1273	17	25	22	...
Si	1683	...	75	...	...	...	...	25	56	29.8	...
Sn	505	22.8	48.0	2.10	0.0249	35.4	1473	59.5	27	13.9	0.0567
Ta	3250	...	118.0	...	...	...	...	70	58	11.1	0.0169
Ti	1958	...	172	...	...	...	...	31	31	7.28	0.0
V	2185	...	71.0	...	...	...	...	51	43.5	9.85	0.0161
W	3650	...	127	...	...	...	...	95	63	14.2	0.029
Zn	692	16.7	37.4	2.24	Not linear	...	...	90	50	10.6	0.055
Zr	2123	...	153	...	...	...	...	38	36.5	9.87	0.0041

electrical conductivity can be estimated using Eq 22:

$$\sigma_T = \sigma_{T1} \{1 + (d\sigma/dT)_{alloy}\} \quad \text{(Eq 22)}$$

where:

$$d\sigma/dT = x_1(d\sigma_1/dT) + x_2(d\sigma_2/dT) + x_3(d\sigma_3/dT) + \dots \quad \text{(Eq 23)}$$

Once  $\sigma_T$  is calculated at a given  $T$ , then the thermal conductivity is calculated using the WLF equation (Eq 20).

Excellent compilations of conductivity properties of pure elements can be found in the literature (Ref 13, 121, 122). Table 10 shows the

electrical resistivity for some solid and liquid metals at the melting point. The resistivity data for the liquid,  $\rho_{e,l}$ , from the melting point to a given temperature in Table 9 can be calculated by the expression:

$$\rho_{e,l} = \alpha T + \beta \quad \text{(Eq 24)}$$

The values for constants  $\alpha$  and  $\beta$  for the various metals are given in Table 10. Note also that the electrical resistivity data given in Table 10 are for bulk metals and may not be applicable to thin films.

Mills and co-workers (Ref 122) combined Mott (Eq 19) and WLF (Eq 20) to establish a relationship between the thermal conductivity

of the solid,  $k_{sm}$ , and liquid,  $k_{lm}$ , at the melting point:

$$\ln\left(\frac{k_{sm}}{k_{lm}}\right) = K\Delta S_m \quad \text{(Eq 25)}$$

where  $K$  is a constant. This equation would be useful to estimate the thermal conductivity of a liquid alloy by determining the thermal conductivity (or electrical conductivity) at the melting point. The only limitation is the constant  $K$ , which would not have a uniform value for all metals and alloys (Ref 122).

Table 10 shows the thermal conductivity for pure metals in the solid and liquid state at the melting point as well as the estimation of the

**Table 11 Heat capacity and thermal conductivity of some mold materials**

Mold material	Dry density, g/cm <sup>3</sup>	Specific heat capacity, kJ/Kg · K	Thermal conductivity, W/m <sup>-1</sup> · K
Silica molding sands			
20–30 mesh	1.730	$C_p = 0.5472 - 1.147 \times 10^{-3}T - 5.401 \times 10^{-7}T$ ( $T < 1033$ )	$k = 0.604 - 0.767 \times 10^{-3}T + 0.795 \times 10^{-6}T^2$ ( $T < 1033$ )
50–70 mesh	1.634	$C_p = 1.066 + 8.676 \times 10^{-5}T$ ( $T > 1033$ )	$k = 0.676 - 0.793 \times 10^{-3}T + 0.556 \times 10^{-6}T^2$ ( $T > 1033$ )
80–120 mesh	1.458		
Silica sand (–22 mesh)			
+ 7% bentonite	1.520	$C_p = 0.4071(T - 273)^{0.154}$ ( $T \leq 1600$ )	$k = 0.946 - 0.903 \times 10^{-3}T + 0.564 \times 10^{-6}T^2$ ( $T < 1500$ )
+ 4% bentonite	1.60		$k = 1.26 - 0.169 \times 10^{-2}T + 0.105 \times 10^{-5}T^2$ ( $T < 1500$ )
Olivine sand	1.83	$C_p = 0.3891(T - 273)^{0.162}$ ( $T \leq 1300$ )	$k = 0.713 + 0.349 \times 10^{-4}T$ ( $T < 1300$ )
+ 4% bentonite	2.125		$k = 1.82 - 1.88 \times 10^{-2}T + 0.10 \times 10^{-5}T^2$ ( $T < 1300$ )
Zircon sand	2.780		$k = 1.19 - 0.948 \times 10^{-3}T + 0.608 \times 10^{-6}T^2$ ( $T < 1500$ )
+ 4% bentonite	2.96	$C_p = 0.2519(T - 273)^{0.170}$ ( $T \leq 1300$ )	$k = 1.82 - 0.176 \times 10^{-2}T + 0.984 \times 10^{-6}T^2$ ( $T < 1500$ )
Chromite sand			
3.9% bentonite	2.75	$C_p = 0.318(T - 273)^{0.158}$ ( $T \leq 1300$ )	$k = 941 - 0.753 \times 10^{-3}T + 0.561 \times 10^{-6}T^2$ ( $T < 873$ )
Graphite (chill foundry grade)	1.922	$C_p = -0.11511 + 2.8168 \times 10^{-3}T$ (505–811)	$k = 135.99 - 8.378 \times 10^{-2}T$ ( $T > 873$ )
		$C_p = 0.6484 + 1.305 \times 10^{-3}T$ ( $T > 811$ )	$k = 103.415 - 4.647 \times 10^{-2}T$ ( $T > 873$ )
		$C_p = 1.3596 + 4.2797 \times 10^{-4}T$ ( $T > 811$ )	
Investment casting			
Zircon-30% alumina-20% silica	2.48–2.54	...	$k = 3.03 - 3.98 \times 10^{-4}T + 508 T^{-1}$ ( $T: 375\text{--}1825$ )

Source: Ref 14

constant  $K$  based on the WFL (Ref 122). The experimental errors in the measurement of the thermal conductivity of the liquid can be larger than 5% for the thermal conductivity and  $\pm 3\%$  for electrical conductivity (Ref 122). Calculating thermal conductivity from measured thermal diffusivity values may reduce some of the experimental errors.

Thermal diffusivity is the ability of a material to self-diffuse thermal energy. This is determined by combining the material ability to conduct heat and its specific heat capacity. The density is involved due to the given specific heat capacity in units of heat per unit mass, while conductivity relates to the volume of material. Thus, the thermal conductivity ( $k$ ) and thermal diffusivity ( $\alpha$ ) that measure the heat flow within materials are related by their specific heat capacity ( $C_p$ ) and density ( $\rho$ ) by the relationship:

$$k = \alpha C_p \rho \quad (\text{Eq 26})$$

Table 9 shows some of the data available in the literature for ferrous and nonferrous alloys (Ref 14).

In casting processes, the need for thermal conductivity data for mold materials becomes more crucial. Mold materials are usually bulk, porous, complex sand-polymer mixtures and ceramic materials, and their thermal conductivity is certainly different from the intrinsic thermal conductivity of the base material. Methods to estimate the thermal conductivity of these materials can be found in the literature (Ref 123). Table 11 shows the thermal conductivity for some mold materials (Ref 14).

## Emissivity

Thermal radiation is an important heat-transfer phenomenon in casting processes, since heat losses during pouring of the molten metal and heat radiation from the mold contribute to the overall heat balance during solidification of the cast product. The thermal radiation

is defined by Plank's law. The integrated form of Plank's equation gives the total emissive power of a body ( $e$ ). This is known as the Stefan-Boltzmann equation and is represented by:

$$e = \varepsilon \sigma T^4 \quad (\text{Eq 27})$$

where  $\varepsilon$  is the emissivity, and  $\sigma$  is the Stefan-Boltzmann constant. The Stefan-Boltzmann constant is given by:

$$\sigma = \frac{2\pi^5 \kappa^4}{15c^2 h} = 5.67 \times 10^{-8} \text{ J/m}^2 \cdot \text{s} \cdot \text{K}^4 \quad (\text{Eq 28})$$

where  $\kappa$  and  $h$  are the Boltzmann's and Plank's constants, respectively, and  $c$  is the speed of light.

Because emissivity data throughout the wavelength spectrum are not available for most metallic materials, the following empirical equation has been employed to represent the total emissivity as a function of temperature (Ref 124):

$$\varepsilon_t = K_1 \sqrt{(\rho T)} - K_2 \rho T \quad (\text{Eq 29})$$

where  $K_1$  and  $K_2$  are constants,  $K_1 = 5.736$ ,  $K_2 = 1.769$ , and  $\rho$  is the electrical resistivity in  $\Omega \cdot \text{m}$ .

Equation 29 is in reasonable agreement with experimental data, and it shows an increase of  $\varepsilon_t$  with  $T$ . However, deviations for some materials at high temperatures can be expected because of the spectral emissivity that changes with the wavelength and direction of emission. Nevertheless, in most practical situations, including in casting processes, an average emissivity for all directions and wavelengths is used. The emissivity values of metals or other nonmetallic materials depend on the nature of the surfaces, such as the degree of oxidation, surface finish, and the grain size. Table 12 gives some total normal emissivity for some pristine and oxidized metals, while Table 13 gives the total emissivity for some alloys and refractory materials (Ref 125).

Additional emissivity data for various materials have been compiled and can be found in the literature (Ref 5, 124, 126–128).

The data quoted in Tables 12 and 13 provide a guideline and must be used with discretion since, in practical applications, the values of emissivity may change considerably with oxidation and roughening of the surfaces. Therefore, it is important that the total emissivity should be determined for the actual surface conditions of the materials in question.

## Typical Thermophysical Properties Ranges of Some Cast Alloys

Tables 14 to 17 show the typical range of thermophysical properties for aluminum, magnesium, cast iron, and nickel alloys. Unfortunately, numerical values of those thermophysical properties in the mushy zone or even in the liquid state are not available. However, one could infer the expected trends as noted in the tables.

## Summary

This article introduces the methods, concepts, and typical values for the main types of thermophysical data needed for processing modeling of castings. The following conclusions can be drawn:

- Throughout this survey, values have been quoted. These should be used with discretion and taken as representative values for materials and not necessarily values for a particular system.
- The properties considered are specific heat capacity, enthalpy of melting, solidus and liquidus temperatures, coefficient of thermal expansion, density, surface tension, viscosity, electrical and thermal conductivity, and emissivity appropriate to metals, alloys, and molds.
- The measurement of these properties presents the experimentalist with several challenges

**Table 12 Total normal emissivity of pristine and oxidized metals**

Metal	Pristine	Temperature, K	Oxidized	Temperature, K
Ag	0.02–0.03	773	...	...
Al	0.064	773	0.19	873
Be	0.87	1473	...	...
Cr	0.11–0.14	773	0.14–0.34	873
Co	0.34–0.46	773	...	...
Cu: solid	0.02	773	0.24	1073
Cu: liquid	0.12	1473	...	...
Hf	0.32	1873	...	...
Fe	0.24	1273	0.57	873
Mo	0.27	1873	0.84	673
Ni	0.14–0.22	1273	0.49–0.71	1073
Nb	0.18	1873	0.74	1073
Pd	0.15	1473	0.124	1273
Pt	0.16	1473	...	...
Rh	0.09	1673	...	...
Ta	0.18	1873	0.42	873
Ti(a)	0.47	1673	...	...
W	0.17	1673	...	...
	0.18	1873	...	...
	0.23	2273	...	...
Alloys	...	...	...	...
Cast iron	0.29	1873	0.78	873

(a) Spectral normal emissivity at 65  $\mu\text{m}$  wavelength. Source: Ref 124**Table 13 Total normal emissivity of various alloys and refractory materials**

Alloys	$\epsilon$	Temperature, K
Commercial aluminum	0.09	373
Oxidized	0.11–0.19	472–872
Cast iron: Solid	0.60–0.70	1155–1261
Liquid	0.29	1873
Commercial copper: heated at 872 K	0.57	472–872
Liquid	0.16–0.13	1349–1550
Steel: plate rough	0.94–0.97	273–644
Steel liquid	0.42–0.53	1772–1922
<b>Refractory materials</b>		
Alumina: 85–99.5Al <sub>2</sub> O <sub>3</sub> –0–12SiO <sub>2</sub> –0–1Fe <sub>2</sub> O <sub>3</sub>	0.5–0.18	1283–1839
Alumina-silica: 58–80Al <sub>2</sub> O <sub>3</sub> –16–18SiO <sub>2</sub> –0.4Fe <sub>2</sub> O <sub>3</sub>	0.61–0.43	1283–1839
Fireclay brick	0.75	1273
Carbon rough plate	0.77–0.72	373–773
Magnesite brick	0.38	1273
Quartz, fused	0.93	294
Zirconium silicate	0.92–0.80	510–772
	0.80–0.52	772–1105

Note: A linear interpolation of the emissivity values with temperature can be done when the emissivity values are separated by a dash. It should be noted that some materials (such as alumina) are semitransparent, and their measured emissivity depends on the thickness of the sample. Source: Ref 125

**Table 14 Range of thermophysical and mechanical properties of cast aluminum alloys**

Property	At room temperature	At solidus temperature	In the mushy zone	In the liquid range
Thermal conductivity, W/K · m	100–180	150–210	Dropping	60–80
Heat capacity, J/kg · K	880–920	1100–1200	Almost constant	1100–1200
Density, kg/m <sup>3</sup>	2600–2800	2400–2600	Dropping	2200–2400
Viscosity, mm <sup>2</sup> /s			Sharply decreasing	0.4–0.5
Young's modulus, GPa	68–75	40–50		Dropping to zero
Thermal expansion, $\mu\text{m}/\text{m} \cdot ^\circ\text{C}$	20–24		25–30	Sharply increasing
Heat of fusion, kJ/kg			400–500	

Source: Ref 26

associated with high temperatures and the reactivity of the materials with containers and atmospheres.

- The prediction of properties has advanced in recent years, but some care is needed in validating the data.
- Before commissioning expensive work to measure properties, the modeler is advised to check the sensitivity of the

required predictions to changes in the input thermophysical data. This will enable measurement efforts to concentrate on the critical data.

- Among properties not considered are:
  - a. Chemical diffusion coefficients and partition coefficients, which can strongly affect the chemistry at the microstructural scale

- b. Mechanical properties of the metal close to the solidus temperature where it is very weak, with implications to the strength such as susceptibility to hot tearing and cracking
- c. Mechanical properties of molds at appropriate temperatures during casting

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**Table 15 Range of thermophysical and mechanical properties of cast magnesium alloys**

Property	At room temperature	At solidus temperature	In the mushy zone	In the liquid range
Thermal conductivity, W/K · m	50–85	80–120	Dropping	50–70
Heat capacity, J/kg · K	1000–1050	1150–1250	Almost constant	1200–1350
Density, kg/m <sup>3</sup>	1750–1850	1650–1750	Dropping	1550–1650
Viscosity, μm <sup>2</sup> /s			Sharply decreasing	0.6–0.7
Young's modulus, GPa		42–47	30–35	Dropping to zero
Thermal expansion, μm/m · °C		24–26	30–34	Sharply increasing
Heat of fusion, kJ/kg				280–380

Source: Ref 26

**Table 16 Range of thermophysical and mechanical properties of cast iron**

Property	At room temperature	At solidus temperature	In the mushy zone	In the liquid range
Thermal conductivity, W/K · m	30–50	25–30	Almost constant	25–35
Heat capacity, J/kg · K	460–700	850–1050	Dropping	800–950
Density, kg/m <sup>3</sup>	6900–7400	6750–7350	Shrinking/expanding	6700–7300
Viscosity, μm <sup>2</sup> /s		...	Sharply decreasing	0.5–0.8
Young's modulus, GPa	80–160	60–100	Dropping to zero	...
Thermal expansion, μm/m · °C	11–14	17–22	Sharply increasing	...
Heat of fusion, kJ/kg		...	200–250	...

Source: Ref 26

**Table 17 Range of thermophysical and mechanical properties of nickel-base superalloys**

Property	At room temperature	At solidus temperature	In the mushy zone	In the liquid range
Thermal conductivity, W/K · m	8–14	28–32	Slightly dropping	25–35
Heat capacity, J/kg · K	420–470	620–700	Rising	700–800
Density, kg/m <sup>3</sup>	8200–8700	7500–8000	Dropping	7000–7500
Viscosity, μm <sup>2</sup> /s			Sharply decreasing	0.6–1.0
Young's modulus, GPa	180–220	100–120	Dropping to zero	...
Thermal expansion, μm/m · °C	12–13	12–13	20–23 Sharply	...
Heat of fusion, kJ/kg			200–220 increasing	...

Source: Ref 26

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