CALCULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES OF ARC FURNACE PLASMAS

H. Dinulescu*, E. Pfender** and H. Wilhelmi*
*Institut für Industrieofenbau und Wärmetechnik im Hüttenwesen, RWTH Aachen, Aachen, West Germany. ** Heat Transfer Division, Department of Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota 55455

ABSTRACT

A general computer program has been developed for the computation of thermodynamic and transport properties of thermal plasmas of complex composition (up to 40 species) in a temperature range from 1,000 K to 40,000 K and a pressure range from 0.1 bar to 10 bar. The computational algorithm is based on the solution of the Boltzmann equation by the method of Chapman and Enskog. As an example selected results for an air/iron plasma are shown.

1. INTRODUCTION

High current electric arcs are used in arc furnaces for scrap melting, for metal refining and alloying, for extractive metallurgy, etc. In a typical arc furnace, the arc is operated in an environment of complex composition and little is known about the actual arc behavior because diagnostics has been limited to the measurement of external arc parameters (current, voltage, arc power, pressure, electrode gap). Presently available information is essentially restricted to empirical relations among these parameters.

With the availability of high speed computers, numerical modeling of arcs becomes feasible. This approach, however, faces two severe problems. First of all, modeling requires knowledge of thermodynamic and transport properties of the arc plasma which represents, in general, a multi-component mixture of gases and vapors. Second, modeling is, at this time, restricted to relative simple arc configurations (two-dimensional situations) which probably differ substantially from actual arcs in arc furnaces. Nevertheless, even severely simplified models will be useful for determining those components in the multi-component mixture which make important contributions to the transport coefficients and, therefore, to the arc behavior. It is, for example, well known that even small percentages of metal vapors dominate the electrical conductivity in regimes of relatively low temperatures (seeding of MHD plasmas).

Modeling of a high intensity arc requires the solution of the conservation equations which consist of a set of highly non-linear, coupled differential equations. These equations contain thermodynamic and transport properties (plasma density ρ, specific heat at constant pressure C_p, viscosity μ, thermal conductivity k, electrical conductivity σ_e, thermal diffusion coefficient for the electrons ϕ_e). In general, the plasma properties are functions of the temperature and of the pressure provided that Local Thermodynamic Thermodynamic Equilibrium (LTE) prevails.

Although plasma transport properties can be measured, this approach is rather expensive and, therefore, available experimental data are restricted to a few inert gases and simple gas mixtures [1,7,11]. Fortunately, the kinetic theory of gases provides a sound basis for the computation of plasma properties. Previous investigations have shown that the Chapman-Enskog solution of the Boltzmann equation applies to arc plasmas even above 1 atmosphere. The results of such calculations are available for a few gases and some simple gas mixtures [2-6]. For specific multi-component mixtures one cannot expect to find suitable data in the literature, i.e., computation of these properties becomes part of the modeling effort.

2. THE METHOD OF COMPUTATION

According to the method of Chapman and Enskog the transport properties can be computed for arbitrary compositions starting from known interaction potentials of any two particles in the mixture. The interaction potentials can be determined by different means, such as from particle beam scattering experiments, from diatomic molecule spectra or, from quantum mechanical calculations[8]. The interaction potential can be expressed as a simple function of the intermolecular distance r. A typical example is the Morse potential

$$\phi = \varepsilon\{\exp[-2\ (\tfrac{C}{\sigma})\ (r-r_e)]\ -2\ \exp\ [-\ (\tfrac{C}{\sigma})\ (r-r_e)]\};\ \frac{r_e}{\sigma} = 1 + \frac{\ln 2}{C}$$

where ε, σ and C are parameters specific for a given pair of colliding atoms.

Although the algorithm is rather involved, it can be easily incorporated into a computer program. The transport properties can then be regarded as functions of the interaction potential with the temperature T, the pressure p, and the composition n_j as parameters, e.g.: $\mu=\mu\{\phi(r);\ T,\ p,\ n_j\}$.

An important simplification is obtained by taking advantage of the small electron mass to decouple the electron Boltzmann equation from those of the heavy species [10]. This allows the electron properties to be computed independently from those of the heavy particles, starting from the momentum transfer cross section of the electrons with neutrals. The electron transport properties can then be regarded as functions of the cross section correlation (of the electron speed, (C_e), e.g.: $\sigma_e = \sigma_e\{Q_{en_j};\ T,\ p,\ n_j\}$ where $Q_{en_j}(C_e)$ is the electron-neutral cross section.

Thus, the main input for the transport property calculation consists of the potential function parameters (ε, C, σ) for the heavy particle collisions and the cross sections for electron-neutral collisions.

The transport property computation requires, in addition, knowledge of the plasma composition at each temperature and pressure, e.g.: $k = k\ (p,T,n_j)$. With the assumption of LTE, the local composition, n_j, can be computed with the system of Saha equations. For this, the partition functions of the various species present must be computed, which proceeds from the knowledge of the energy levels and their statistical weights. Once the partition functions have been determined, the thermodynamic properties (C_p,h,u,ρ) can be also computed. Thus, the main input for the thermodynamic properties consists of the energy levels and statistical weights of the atoms and molecules constituting the mixture. One of the difficulties with gas mixtures is the required knowledge of cross section data for all relevant processes. Since the number of components is large, the required cross sections are, in general, very numerous. It was found in the course of the present investigation that this last difficulty can be overcome easier in a plasma (high temperature, ionized species) than in a low temperature mixture of similar complexity, for the follwoing reasons. First, due to the small electron mass, the electron can be treated independently of the other species by considering only interaction of the electrons with the heavy particles, but not those of the heavy particles among themselves. Second, it can be shown that in the arc range of temperatures the inelastic collisions can be ignored without appreciable loss of accuracy. Third, polar molecules play a minor role in plasmas since the temperature is high enough so that molecules are dissociated and are present only as minority species. An erroneous assumption concerning the cross sections of polar molecules will thus reflect in a negligible error for the complete mixture. Fourth, although the number of components is large in a plasma, the required cross section information is much smaller than for a low temperature mixture of similar complexity because most of the species are ionized and the collision cross section of ions is given by the known Coulomb interaction. Fifth, the number of plasma components which enter the kinetic theory formulas is less than it may appear, because at any given temperature many of the species present are in minority and can be ignored without important loss of accuracy; e.g., at low temperature most ions are in minority while at high temperature the molecules and the neutral atoms can be ignored.

Thus, the main problem in building a general program rests with the availability and gathering of a reasonable amount of cross section data for elastic collision of the various species. Although comprehensive collections of such data do not exist in the literature, a large amount of information is scattered in a variety of publications. Information on atom-atom and atom-ion collisions is provided by molecular spectroscopy.

3. RESULTS

A suitable computer program has been developed in the course of the present investigation. The program has been tested on simple gases (Ar, N_2) and the results were found to agree resonably well with published data. The program is applicable to mixtures with a large number of components. With the cross section data already collected and stored, the program can be applied to some typical arc furnace mixtures. At the present time the program expansion is being continued by collection and storage of additional cross section data. Figures 1, 2, 3 and 4 present the results of calculations for a mixture of air and iron which may be encountered in the atmosphere of an arc scrap melter. The pressure is 1 atmosphere. The various collision cross sections required have been obtained from ref. 9 and 12.

The iron vapor, which originates from arc attachment spots and from the melt, is seen to have a marked effect on the electrical conductivity at temperatures below 12,000 K. This is due to the ionization of iron atoms which provide a large number of electrons starting at a temperature of about 3,000 K. Above 12,000 K the ionization of Fe-atoms is almost complete and they make no noticeable contribution to the electrical conductivity of the base gas.

The influence of iron seeding on the thermal conductivity consists essentially in reducing the peak at around 15,000 K. This is due to a decrease of the reaction component of the thermal conductivity since part of the reacting particles (dissociating N and O atoms) are replaced with non-reacting iron ions and associated electrons.

The viscosity is little affected by iron seeding since the viscosity is essentially a heavy particle property and the Fe-ions have the same collision cross section as the N and O ions being different from these only by their mass.

Finally, the specific heat is increased by the presence of iron seeding at around 4,000 K due to the additional energy absorption by ionizing iron atoms.

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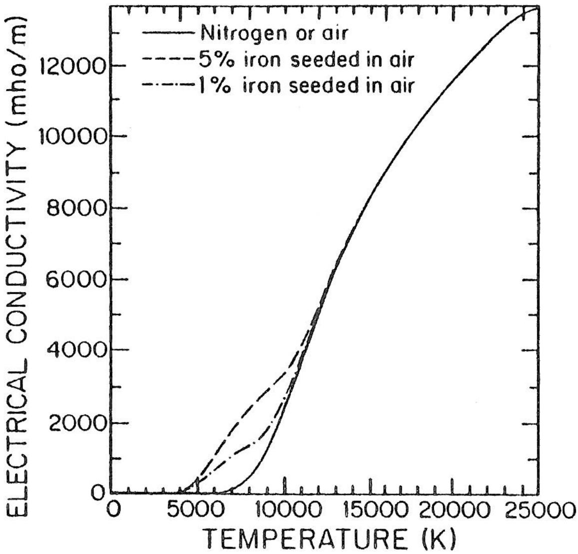

Fig. 1 Electrical conductivity of nitrogen or air and iron seeded air (p = 1 bar).

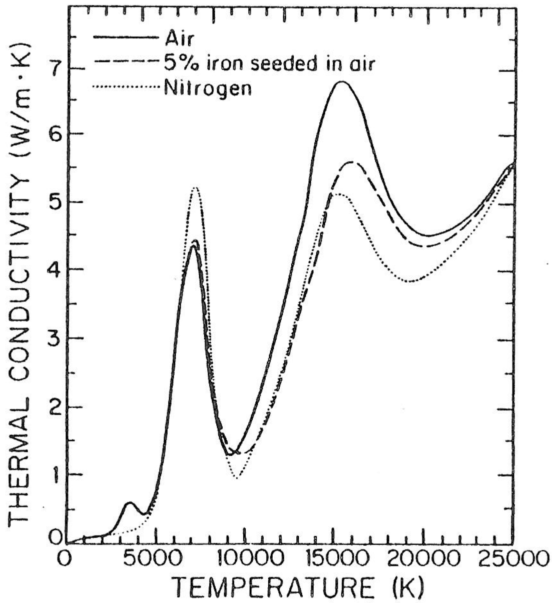

Fig. 2 Total thermal conductivity of nitrogen, air and iron seeded air (p = 1 bar).

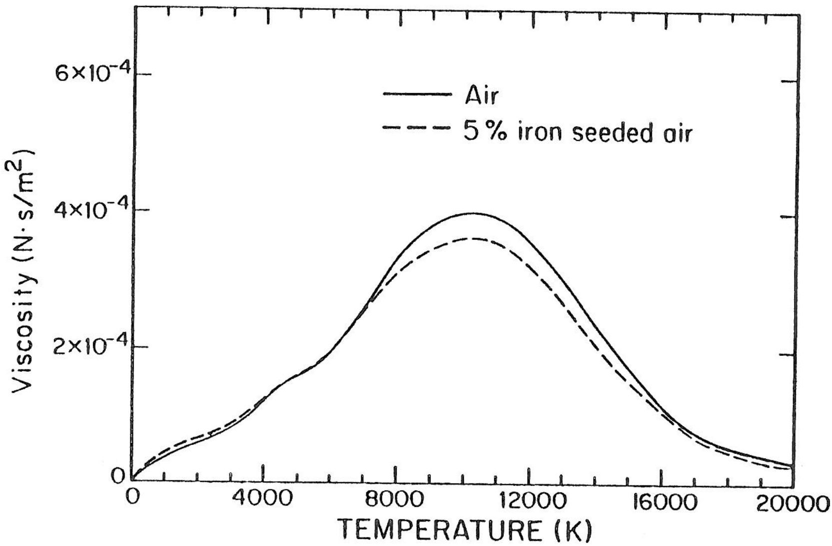

Fig. 3 Dynamic viscosity of air and iron seeded air (p = 1 bar).

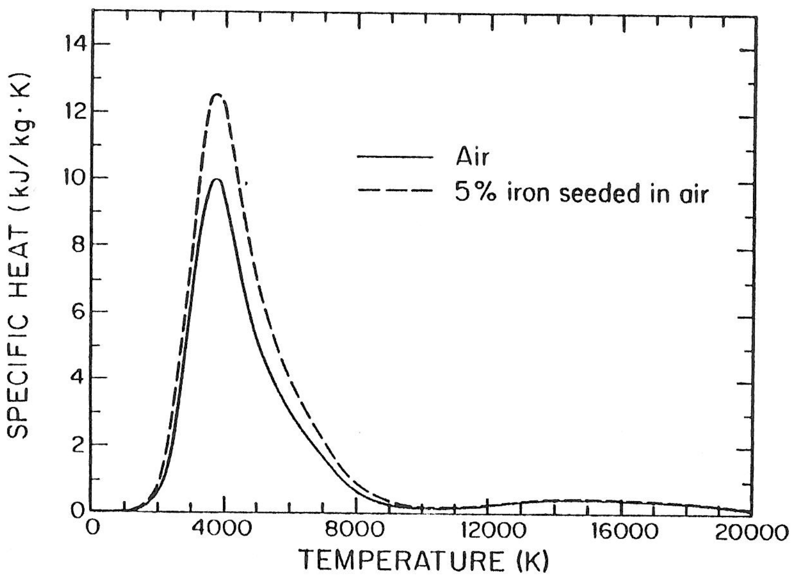

Fig. 4 Specific heat of air and iron seeded air (p = 1 bar).