Arc Electrique et Procédés Plasmas Thermiques

Calculation of combined diffusion coefficients for Ar-Cu, Ar-He and Ar-Fe mixtures

Abstract : This work is devoted to the diffusion in argon-copper, argon-helium and argon-iron thermal plasma mixtures, at atmospheric pressure. The diffusion is studied through combined diffusion coefficients that we have calculated according to the Murphy's concept. The collision integrals and parameters used to obtain these coefficients are presented and the combined diffusion coefficients due to gradients of densities and gradients of electric fields are plotted for several mixtures, temperatures between 300K and 30000K, and the atmospheric pressure.

Diffusion phenomena in thermal plasma

The role of diffusion is to restore the medium homogeneity by diffusion flows generated by the ***gradients*** of concentration, temperature, pressure and eventually the gradients of external forces. The flow of particles is defined at first approximation by the ***Fick law*** applied to species i :

$$\vec{\Gamma}_i = n_i \vec{\upsilon}_i = -D_i \vec{\nabla} n_i$$

Where D_i is the diffusion coefficient. In the case of a mixture with several species, this flow of particles is definitely more complex. ***Murphy [1]*** has shown that the mass flow of a particle i inside a plasma containing ν chemical species can be written as :

$$J_i = n_i m_i \overline{V_i} = \frac{n^2 m_i}{\rho} \sum_{j=1}^{\nu} m_j D_{ij} d_j - D_i^T \nabla \ln T$$

Where d_j is a term containing the gradients of pressure, and gradients of forces which are often weak in comparison to the gradients of densities.

$$d_j = \nabla x_j + \left(x_j - \frac{\rho_j}{\rho}\right) \nabla \ln P - \frac{\rho_j}{P\rho}\left(\frac{\rho}{m_j} F_j - \sum_{l=1}^{\nu} n_l F_l\right)$$

[1] A.B. Murphy, Phys. Rev E, **55**, 7433 (1997)

The combined diffusion coefficients

Murphy [2] has developed an interesting concept which consists in combining diffusion flows and separating all the species in two **gas A** (with p species) **and B** (with q species).

Advantages : independent of the number of chemical species, depends only on the elementary constituents present in the plasma, only one coefficient to treat the diffusion.

Drawbacks : only binary mixtures, homo-nuclear and non-reactive gases supposed to be established in LTE.

Combined diffusion coefficients $\overline{D_{AB}^x}$ (due to the gradients of densities) and $\overline{D_{AB}^E}$ (due to the gradients of electric field) can be written as:

$$\overline{D_{AB}^x} = \frac{1}{m_B} \sum_{i=2}^{p} s_i \sum_{j=1}^{q} m_j D_{ij}^a \frac{\partial x_j}{\partial x_B}$$

$$\overline{D_{AB}^E} = -\frac{e}{k_B T} \cdot \frac{1}{m_B} \sum_{i=1}^{p} s_i \sum_{j=1}^{q} m_j x_j Z_j D_{ij}$$

Two expressions checking the following relations :

$$\overline{D_{AB}^x} = \overline{D_{BA}^x} \quad \text{and} \quad \overline{D_{AB}^E} = -\overline{D_{BA}^E}$$

[2] A.B. Murphy, Phys. Rev. E, **48**, 3594, (1993)

The collision Integrals

The combined diffusion coefficients are strongly influenced by the species and their collisions. These numerous collisions are treated through functions called ***collision integrals*** $\Omega_{ij}^{(\ell,s)}$. The method used to calculate these functions are given by Hirschfelder [3]:

$$\Omega_{ij}^{(\ell,s)} = \left(\frac{k_b T}{2\pi\mu_{ij}}\right)^{1/2} \int_0^{\infty} \exp\left(-\gamma_{ij}^2\right) \cdot \gamma_{ij}^{2s+3} \cdot Q_{ij}^{(\ell)}(\varepsilon_r) \cdot d\gamma_{ij}$$

Where $Q_{ij}^{(\ell)}$ is the total transport cross section, $\gamma_{ij} = (\varepsilon_r / k_b T)^{1/2}$, μ_{ij} the reduced mass, ε_r the kinetic energy $\varepsilon_r = \mu_{ij} g_{ij}^2 / 2$.

The data necessary to estimate them are given by the literature. When the collision integrals are not available, the last have been calculated according to empirical formulas given by ***Hirschfelder [3].*** The latter are defined for several potentials as the Lennard-Jones, the polarisability or the rigid spheres potentials. They can not be calculated without the knowledge of these parameters :

Species	ε/k (K)	σ (Å)	ξ (A^{-3})	r_m (A)
Ar	93.3	3.542	1.6411	1.56
He	10.8	2.576	0.2049	1.40
Fe	3000.0	4.300	8.4000	1.93
Cu	2983.0	5.058	7.3100	1.56

[3] J.O. Hirschfelder, C.F. Curtis and R. Byron Bird, Molecular Theory of Gases and Liquids, John Wiley and Sons, NY, (1964)

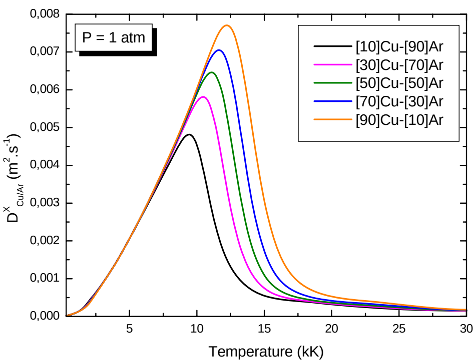

Figure 1: D^x Combined diffusion coefficients for Ar-Cu mixtures

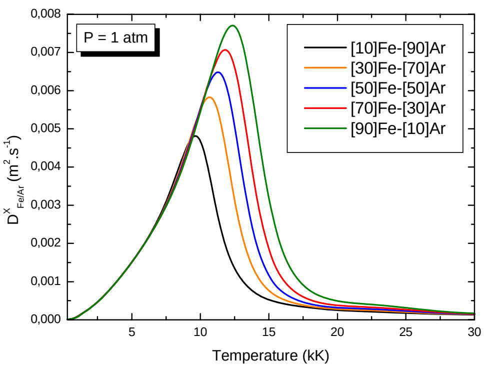

Figure 2: D^x Combined diffusion coefficients for Ar-Fe mixtures

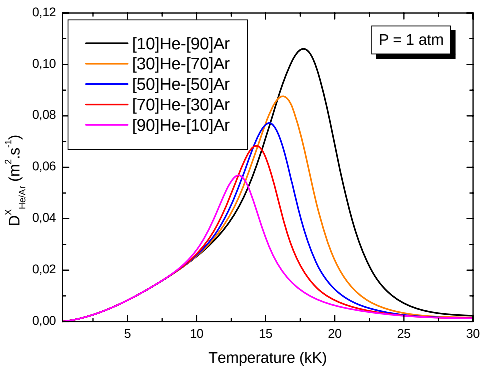

Figure 3: D^x Combined diffusion coefficients for Ar-He mixtures

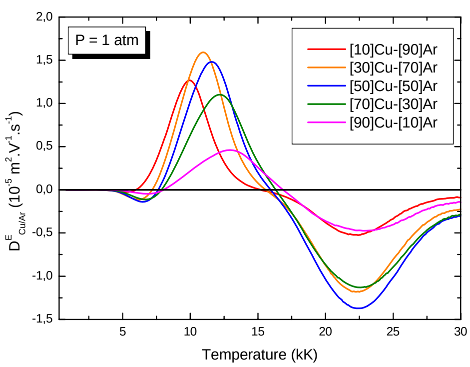

Figure 4: D^E Combined diffusion coefficients for Ar-Cu mixtures

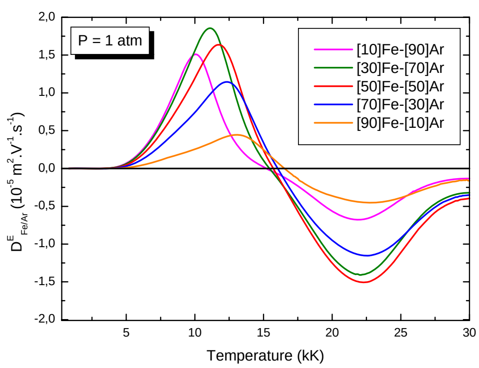

Figure 5: D^E Combined diffusion coefficients for Ar-Fe mixtures

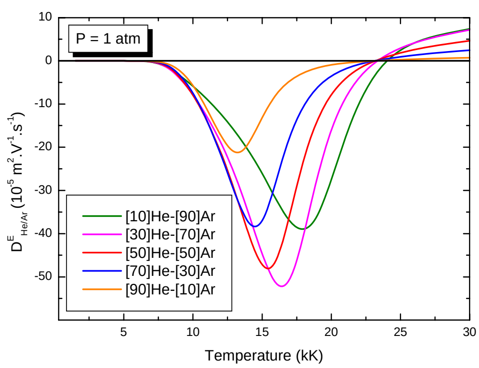

Figure 6: D^E Combined diffusion coefficients for Ar-He mixtures