Table 1: Properties of some gases

Gas	Molar mass in g/mol	Thermal conductivity in W/m/K
H2	2.016	0.1805
O2	32.00	0.0263
N2	28.02	0.0258
CO2	44.01	0.0166
CH4	16.04	0.0341
Ar	39.95	0.0177
He	4.0026	0.1513

1 Thermal Conductivity of Mixtures

The determination of the thermal conductivity of gas mixtures is a central aspect of modeling transport phenomena, particularly in high-temperature and high-pressure processes. Among the most established approaches is the empirical equation introduced by Wassiljewa, which was subsequently refined by Mason and Saxena to improve its applicability to multicomponent systems. This model offers a reliable means of estimating the thermal conductivity of gas mixtures based on the properties of the pure components and their molar interactions.

The thermal conductivity of a gas mixture, denoted by λ_{mix}, can expressed as shown in equation 1.

$$\lambda_{extmix} = \sum_{i=1}^{n} \frac{x_i \lambda_i}{\sum_{j=1}^{n} x_j \Phi_{ij}} \tag{1}$$

In this equation, x_i represents the molar fraction of component i within the mixture, while λ_i denotes the thermal conductivity of the pure substance i. The denominator contains the interaction parameter Φ_{ij}, which describes the influence of component j on the transport properties of component i.

The interaction parameter Φ_{ij} is given by the relation shown in equation 2.

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j}\right)^{-1/2} \left[1 + \left(\frac{\lambda_i}{\lambda_j}\right)^{1/2} \left(\frac{M_j}{M_i}\right)^{1/4}\right]^2 \tag{2}$$

Here, M_i and M_j are the molar masses of the components i and j, respectively. Molar masses and thermal conductivity of the pure substances are listed in table 1. The structure of this expression illustrates the nonlinear dependence of the interaction term on both the molar mass ratio and the square root of the conductivity ratio of the involved species.

This formulation acknowledges that the transport properties of a gas mixture are not a simple linear combination of the individual conductivities. Rather, they are governed by intermolecular interactions, which affect the energy exchange and diffusion behavior of each component. These interactions are particularly significant at elevated pressures or in cases where the gas components exhibit widely differing molecular masses or transport properties.

The equation proposed by Wassiljewa and refined by Mason and Saxena assumes that binary interactions dominate the behavior of the mixture, while higher-order (three-body or more) interactions are neglected. It also presumes that the gases approximate ideal

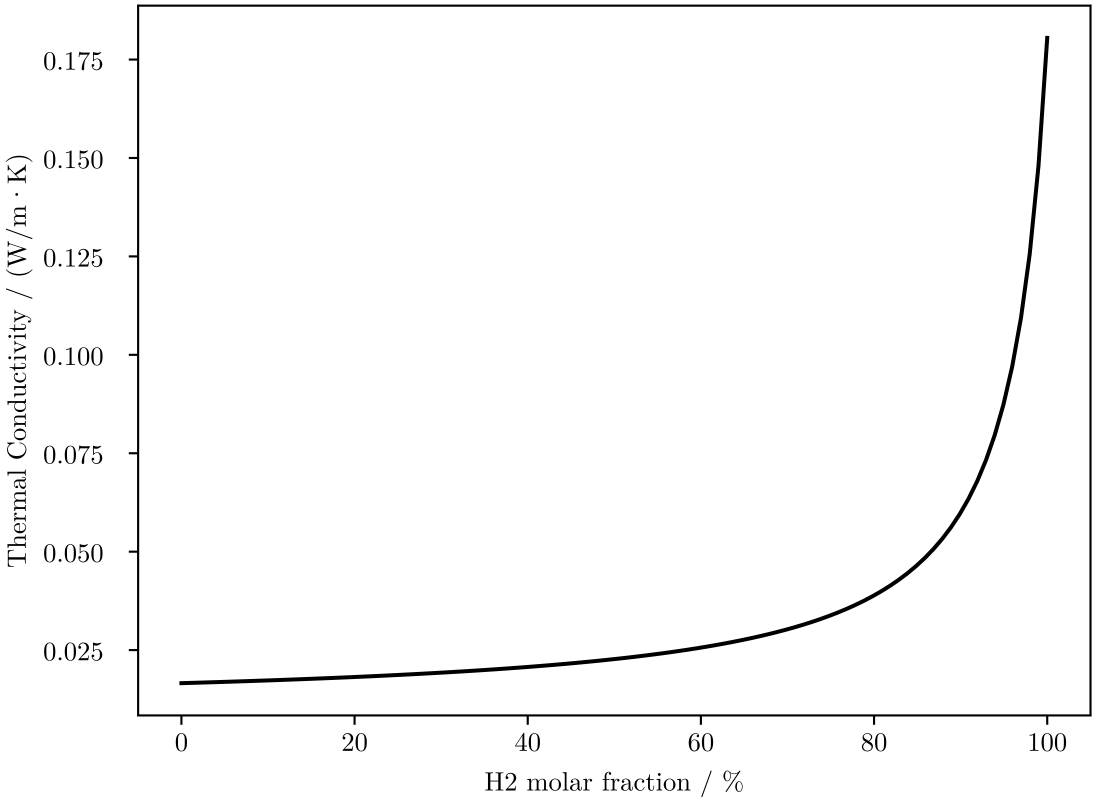

Figure 1: Thermal Conductivity of H2/CO2 mixtures

behavior, although in practical applications, moderate deviations from ideality are tolerated without significant loss of accuracy. In figure 1 the resulting thermal conductivity of an H2/CO2-mixture is shown.

In engineering practice, the accurate determination of λ_{mix} is essential for the prediction of heat transfer in systems such as membrane modules, chemical reactors, and combustion chambers. In the context of membrane-based gas separation, for instance, the thermal conductivity of the gas mixture influences the local temperature distribution, which in turn affects both the permeation behavior and the structural stability of the membrane.

It is important to note that the calculated mixture conductivity reflects only the gas phase behavior. In porous systems such as carbon membranes, additional effects must be considered. These include the solid-phase thermal conduction through the membrane matrix, radiative transport in pore channels at high temperatures, and transport in the Knudsen regime for narrow pores. To account for these complexities, models based on effective medium theory, such as those of Maxwell-Eucken or Bruggeman, are frequently employed. These models combine the conductivities of individual phases (gas and solid) with geometrical factors that reflect the morphology of the porous structure.

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