

Shear viscosity of n -alkanes in the zero density region

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The shear viscosity of n -alkanes in the zero-density limit has been calculated by the classical-trajectory method that has been successfully used to predict the viscosity of real dilute gases [1]. The n -alkane molecules were modelled as rigid linear chains consisting of n_c-1 spherical segments (n_c being the number of carbon atoms) that interact through a combination of site-site Mie $n-6$ potentials ($n=9-14$). The moment of inertia of each n -alkane was used to determine the site-site separation. The work builds on the specific case of the 12-6 (Lennard-Jones, LJ) site-site potential [2], where it was demonstrated [3] that it is not possible to find a unique pair of LJ parameters, ϵ and σ , to reproduce the measured viscosity values of all n -alkanes. However, based on the best fit values of ϵ and σ , for C_3H_8 , $n-C_4H_{10}$, $n-C_6H_{14}$ and $n-C_7H_{16}$, it has been shown that the ratio $\sqrt{\epsilon}/\sigma^2$ is a linear function of n_c . Hence, a model was developed that predicts the viscosity values to within $\pm 5\%$, of experimental ones, for n -alkanes from C_3H_8 to $n-C_9H_{20}$ and within $\pm 5-10\%$ for longer n -alkanes. Here, new results that allow for a greater flexibility in the steepness of the repulsive wall by employing the Mie site-site potential, are presented. Based on the best scaling parameters (n , σ , and ϵ) obtained by fitting to the experimental viscosity of C_3H_8 , $n-C_4H_{10}$, $n-C_6H_{14}$ and $n-C_7H_{16}$, a new model was developed that predicts shear viscosities of long n -alkanes to within $\pm 5\%$. The limiting case of the site-site potential, namely the representation by an effective spherical LJ 12-6 potential, is also discussed [4]. This correlative approach, which makes use of a semi-empirical relationship for the LJ parameter σ , yields viscosities to within $\pm 2-3\%$ of experimental ones.

References

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