ON THE DETERMINATION OF HIGH-PRESSURE MASS DIFFUSION COEFFICIENTS FOR BINARY MIXTURES

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Recent Direct Numerical Simulations of supercritical temporal mixing layers for several binary-species systems have shown that one of the most important characteristics of a three-dimensional supercritical mixing layer is the existence of regions of high density-gradient magnitude (HDGM). At the transitional state, the HDGM regions resemble convoluted threads, such as observed by Chehroudi and Talley (1999). Visualizations of the time sequence leading to transition showed that the HDGM regions form due to two coupled processes: the convolution/distortion of the original density boundary, and the mixing of the species. Independent of the species system, as one probes deeper into the HDGM regions, one finds that the mass fraction of the heavier, lower stream species increases but that even very deep into those regions, the fluid is not the pure heavier species. Traces of the lighter fluid are present, as that species dissolved/diffused into the heavier one. For example, for heptane/nitrogen mixing layers, the HDGM mixture inhomogeneity is attributed to the mixture non-ideality (Harstad and Bellan (2000, 2001), Okong'o and Bellan (2002)) expressed through the mass diffusion factor, which decreases the effective molecular diffusivity and impedes the molecular mixing; this is thus a molecular process combined with a thermodynamic effect. Therefore, this indicates that molecular diffusion, altered by thermodynamic processes, plays an important role in transitional supercritical mixing.

Generic models for calculating high-pressure diffusion coefficients are, however, not available. Therefore, a model for high-pressure binary-diffusion coefficient calculation is then proposed based on considerations originating from re-casting both the low pressure kinetic theory and the Stokes-Einstein infinite dilution expressions into forms consistent with corresponding states theory. These considerations lead to an ansatz that is an expression reflecting departures from the kinetic-theory relationship through a division factor that is a function of the reduced species density and that becomes unity in the limit of low-pressure gases. Available high-pressure data sets extracted from the literature are used to derive correlations for the factor that are eventually categorized according to the species system. The typical uncertainty in these correlations is estimated as 10 to 15 %, with a maximum uncertainty of about 30% for the high-density regime. Further, simulations of heptane drops in nitrogen under zero gravity and at high-pressure conditions are performed to investigate the sensitivity of the drop diameter predictions to this typical range of uncertainty in the prescribed diffusivity. Results show that the RMS deviation variation in the drop diameter value is approximately a factor of four less than the corresponding imposed change in the diffusivity.

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ACKNOWLEDGMENT

This study was conducted at the Jet Propulsion Laboratory, California Institute of Technology, sponsored by the NASA Microgravity Combustion program with Dr. Merill King as contract monitor and Dr. Jackie Sung as technical contact with the National Center for Microgravity Research on Fluids and Combustion.