time and array size on the CM, while the other algorithms are essentially between 2nd and 3rd order.

The optimum virtual processing ratio VP (where VP is defined as the number of virtual processors per physical processor) is in multiples of 4, since the 64-bit floating point chips have a vector length of 4 in the slicewise model. In terms of computing speed, the number of matrix elements should be as closely matched to the available number of processors, or a factor of 4 times the number of available processors, as possible (this assumption neglects communication and overhead costs). For problems where a large number of nodes are needed, it is wise to develop a computational approach which accounts for resource allocation, developing adaptive grid strategies with this in mind.

V. Conclusions

The results presented illustrate the performance possible using matrix-formulated radiative transfer calculations on a parallel computer architecture. These architectures have the potential of changing the nature of radiative transfer calculations which are CPU and memory intensive. Computations involving complex geometries will be more manageable and much quicker. Parallel computing will be especially effective for nonlinear problems, e.g., those which have temperature-dependent properties. These machines also allow for simpler programming, improving software readability, and reducing source code size in comparison to code written for FORTRAN 77 compilers.

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Internal Structure of Shock Waves in Disparate Mass Mixtures

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Introduction

THE direct-simulation Monte Carlo (DSMC) method developed by Bird[1] is an important technique for numerical simulation of rarefied gas flows. In DSMC simulations, a molecular model is required to calculate collisions between molecules, and the most widely used model is the variable hard sphere (VHS) model of Bird.[2] There are several models which can be considered as extensions of the VHS model, such as the generalized hard sphere model,[3] in which both attraction and repulsion forces are incorporated, or the variable soft sphere model,[4] which is compatible with both the diffusion and viscosity coefficients. However, in predicting the behavior of gas mixtures, there is an unfavorable aspect in the models, i.e., all of the collisions between molecules in a mixture are treated to follow only one common type of molecular interaction rather than differentiating depending on the type of interaction. The realistic treatment of molecular interactions can be an important factor in simulating flowfields involving large changes in mole fraction, especially if detailed behavior of individual components in a gas mixture is to be predicted. To overcome this kind of limitation, Erwin[5] extended an intermolecular-potential-based approach to binary mixtures where heteromolecular collision cross sections obtained from the corresponding intermolecular potentials were employed. The application of the method, however, requires a large cross-sectional data table for each class of molecular collision, and is limited to monatomic gas mixtures. The particle simulation method proposed by McDonald[6] can, in principle, employ different molecular interactions for different kinds of molecular collisions. The method, however, has not been applied to gas mixtures with different molecular interactions. Recently, Chung et al.[7] proposed the variable diameter hard sphere (VDHS) model which can be considered

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a simple extension of the VHS model to handle gas mixtures, and allows different molecular interactions for collisions between different species.

In this article, the internal structure of a shock wave in a helium-xenon mixture is investigated using the DSMC method, and is compared with the experimental data of Gmurczyk et al.[8] It is shown that the use of different molecular interactions for collisions between different species in a mixture can have a substantial effect in predicting the shock structure. It is also shown that an irregular behavior is observed not only in the density, which was shown in the experimental results of Gmurczyk et al.,[8] but also in the parallel temperature of the light-gas component.

Variable Diameter Hard Sphere Model

In the VDHS model, the collision cross section between molecules 1 and 2 (σ_{12}) follows the classical hard-sphere scattering law

$$\sigma_{12} = \pi d_{12}^2 \tag{1}$$

where the effective collision diameter (d_{12}) is approximated by the combining rule

$$d_{12} = \tfrac{1}{2}(d_1 + d_2) \tag{2}$$

Here, the effective diameter of each species, d_p ($p = 1, 2$), is defined from the VHS model as follows:

$$d_p = d_{p0}\left[\frac{m_r C_r^2}{2(2-\omega_p)kT_{p0}}\right]^{-\omega_p/2} \tag{3}$$

where the quantity m_r is the reduced mass, k is the Boltzmann constant, C_r is the relative speed between colliding molecules, d_{p0} is the reference value of the effective diameter of species p at the reference temperature T_{p0}, and the VHS exponent of species p,ω_p, is related to the viscosity-temperature exponent of species p, s_p, by $\omega_p = s_p - 0.5$. The VHS exponent is also related to the exponent of the inverse power law molecular force of species p, η_p, by $\omega_p = 2/(\eta_p - 1)$. From Eqs. (1–3), the collision cross section for a collision involving a particle of species 1 and a particle of species 2 can be written as

$$\sigma_{12} = \left[\sum_{i=1}^{2}\sum_{j=1}^{2} A_i A_j C_r^{-(\delta_i+\delta_j)}\right] C_r^{-2\bar{\omega}} \tag{4}$$

where

$$\bar{\omega} = \tfrac{1}{2}(\omega_1 + \omega_2)$$

$$\delta_p = \omega_p - \bar{\omega}$$

$$A_p = \frac{\sqrt{\pi}}{2} d_{p0}\left[\frac{m_r}{2(2-\omega_p)kT_{p0}}\right]^{-\omega_p/2}$$

$$(p = 1, 2)$$

It can be readily seen that Eq. (4) is identical to the VHS model if a common VHS exponent is used, i.e., $\omega_1 = \omega_2 = \bar{\omega}$. Details of the VDHS model including the expressions for internal energy exchange and chemical reactions can be found in Ref. 7.

Results

To compare various methods, the helium-xenon shock wave, for which experimental data is available, is considered. Details of the DSMC simulation can be found in Ref. 10. The results from various methods with the experimental density profile data of Gmurczyk et al.[8] are compared in Fig. 1. The disparate mass mixture is composed of 3% xenon and 97% helium by mole fraction, and the preshock Mach number (M_s) is 3.89. The length coordinate x is normalized by the upstream mean free path L. The VHS exponents of He and Xe are chosen to be 0.173 and 0.292, respectively. The reference diameters of He and Xe are chosen to be 2.278 and 5.181 $\times$ 10^{-10} m, respectively, at a reference temperature of 300 K. The parameters are obtained by the method of Bird[2] from viscosity data over a temperature range of 250–1500 K, which is close to the experimental temperature range implied in the paper of Gmurczyk et al.[8] A common VHS exponent for the results of the VHS model, which is represented by the dot-dashed lines, is 0.177, which is a molar-averaged value; and that for another VHS model case, which is represented by dotted lines, is 0.233, which is a mass averaged value. The results of Piatkowski[9] were obtained from the numerical solution of the Boltzmann equation with the Bhatnagar-Gross-Krook (BGK) model by the moment method using the generalized Mott-Smith assumptions. It can be seen that the VDHS and VHS models give better results than those of Piatkowski[9] in predicting the separation of the species within the shock wave. The results from the VHS models show that the VHS exponent has a substantial effect on the details of the shock profile. The results obtained by using a molar-averaged VHS exponent poorly predict the xenon shock thickness and the species separation within the shock, while they show a better agreement with the helium shock thickness. This is as expected, since the molar-averaged VHS exponent, 0.177, is very close to that of helium which behaves closer to a hard-sphere gas. The use of the mass-averaged VHS exponent improves the results in the xenon shock thickness and the species separation. The helium shock thickness, however, becomes worse. It can be seen that the VDHS model correctly predicts both the individual shock thicknesses and the species separation. Although it is very weak, the results from the VDHS model show the concavity in the helium profile preceded by the first sharp inflection, which cannot be seen in the other results. The numerical results do not predict the overshoot of the helium density profile in the tail part of the shock wave.

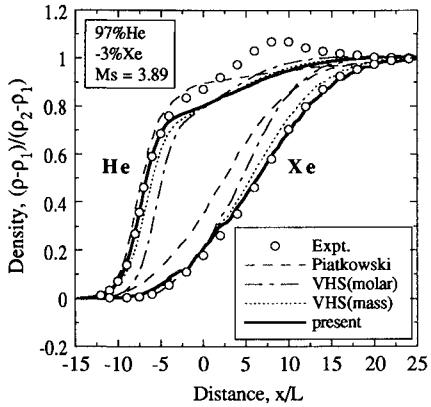

Fig. 1 Density profiles in a shock wave of 97% He, 3% Xe mixture.

Figure 2 shows the density profiles in a shock wave of a disparate mass mixture composed of 1.5% xenon and 98.5% helium by mole fraction. The preshock Mach number is 3.61. A mass-averaged VHS exponent of 0.213 is used for the results obtained by the VHS model. The results of Erwin are also shown in the figure. All three methods correctly predict the helium shock thickness. In predicting the separation of the species, the result obtained by the VDHS model shows better agreement with the experimental data than those obtained by the VHS model or the results of Erwin. The xenon shock thickness, however, becomes worse in the results of the VDHS model.

Figure 3 shows the calculated parallel temperature profiles, i.e., the temperature due to the motion of the molecules in the x direction, in a He-Xe shock wave of various xenon mole fractions. In the figure, X_{Xe} and M_s are the mole fraction of

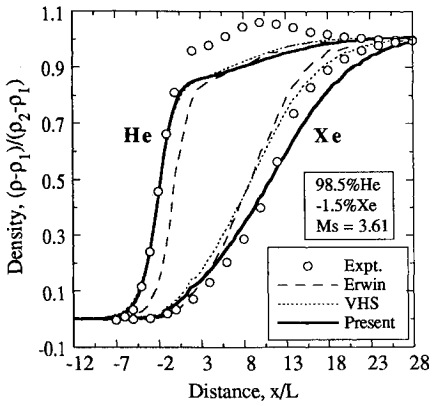

Fig. 2 Density profiles in a shock wave of 98.5% He, 1.5% Xe mixture.

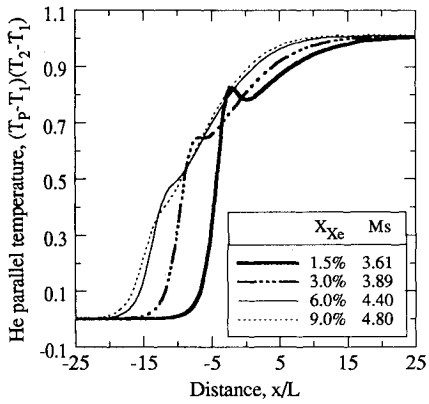

Fig. 3 Parallel temperature of helium in shock waves of He-Xe mixtures.

xenon and the preshock Mach number, respectively. Contrary to common expectations for a shock wave in a single component gas or a mixture composed of gases with a similar mass ratio, shock waves with less xenon mole fraction show a steeper parallel temperature profile in spite of higher preshock Mach numbers. An unusual aspect of the results in Fig. 3 is the hump in the helium parallel temperature profiles resulting from a strong species separation due to pressure diffusion of helium into the front part of the shock, which has never been reported either theoretically or experimentally. It is interesting to see that the location of the concavities preceded by the humps coincides with the location of the sharp inflection point in the density profiles shown in Figs. 1 and 2. The hump fades away when the mole fraction of xenon increases, as can be seen in the parallel temperature profiles for 6 and 9% xenon.

Conclusions

It has been shown that a realistic treatment of the molecular interactions of the colliding molecules can have a substantial effect in predicting the structure of a shock wave in disparate mass mixtures which involve large changes in mole fraction. The VDHS model was shown to offer better agreement with experimental data in predicting the separation of the species within helium-xenon shock waves. It is expected that the use of the VDHS model should offer more accurate results in predicting the separation of species in nonequilibrium flowfields of disparate mass mixtures which involve large changes in mole fraction, such as the flowfield in the plume and backflow regions of nuclear thermal rockets. The highly irregular behavior in the parallel temperature profile of the light species was observed in the DSMC simulation results, and this behavior has never been reported either theoretically or experimentally. This irregular behavior is thought to be physically more plausible than a smooth behavior, and future theoretical and experimental investigations of this phenomenon are recommended.

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Use of Adaptive Finite Elements for Compressible Flow

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Introduction

ADAPTIVE mesh refinement procedures with finite elements have been used for some time in computing compressible high-speed flows. Mesh refinement procedures for triangular finite element meshes were initially detailed by Zienkiewicz et al.[1] Applications of these procedures to compressible flow have been extensively demonstrated by Ramakrishnan et al.[2] Adaptive procedures for finite element meshes with quadrilateral elements are discussed in Oden et al.[3] and Shapiro and Murman.[4]

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