Kinetic Effects in Spherical Expanding Flows of Binary-Gas Mixtures

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Abstract. Diffusion effects in the spherical expanding flows of argon-helium mixtures have been studied using the direct simulation Monte Carlo technique at the Knudsen numbers from 0.0015 to 0.03 and various pressure ratios. The similarity analysis was used to analyze the flow structure. Kinetic effects influence the shock-wave thickness, parallel and transverse species' temperatures, diffusive velocities, the effectiveness of species separation, and ambient gas penetration. A comparison of the DSMC and Navier-Stokes solutions indicates areas of the continuum-concept applicability for studying diffusive effects in low-density flows.

INTRODUCTION

Diffusive processes have a significant effect on the structure of a low-density gas mixture flow in underexpanded free jets [1-3].The expansion of a binary gas mixture from a spherical source of radius r_* into a flooded space was studied by Skovorodko and Chekmarev [4], Gusev and Riabov [5], and Riabov [6] in terms of numerical and asymptotic solutions of the Navier-Stokes equations. The results could be effectively used for simulating hypersonic vehicle flights in atmospheres of planets [6], as well as for the separation of gas species and isotopes [7,8]. The phenomenon of background gas penetration into underexpanded free jets was described by Brook *et al* [3], Skovorodko and Chekmarev [4], and Gusev and Riabov [5]. The systematic analysis of the diffusive processes in expanding flows based on the direct simulation Monte Carlo (DSMC) technique has not been provided yet. Also the problem of applicability of the Navier-Stokes equations to describe these processes is not solved.

In the present study, diffusion effects in the spherical expanding flows of argon-helium mixtures have been studied using the DSMC technique [9,10] at the Knudsen numbers from 0.0015 to 0.03 and pressure ratios from 100 to 10,000. The similarity analysis [11,12] and analytical asymptotic techniques [5,6] were used to study the flow structure.

DSMC METHOD

The DSMC method [9] and one-dimensional code [9] have been used in this study of spherical low-density binary gas-mixture flows. Molecular collisions in the argon-helium mixture are modeled using the variable hard sphere (VHS) molecular model [9]. The inner boundary conditions have matched the transonic continuum solution at $r/r_* = 1.05$.

Code validation was established [10] by comparing numerical results with experimental data [6]. The mesh size and the number of molecules per cell were varied until independence of the flow profiles from these parameters was achieved for each case. The total number of non-uniform cells is 10,000, the molecules are originally distributed evenly, and a total number of 109,720 molecules corresponds to an average 11 molecules per cell. The error was pronounced when this number falls below five per cell in the most critical flow regions (near the source and shock wave). The cell geometry has been chosen to minimize the changes in the macroscopic properties (pressure and density) across the individual cell [9]. In all cases the usual criterion [9] for the time step Δt_m has been realized, $1\times10^{-10} \le \Delta t_m \le 1\times10^{-8}$ s. Under these conditions, gas-dynamic parameters have become insensitive to the time step. The ratio of the mean separation between collision partners to the local mean free path and the ratio of the time step to the local mean collision time have been well under unity over the flowfield.

CP663, *Rarefied Gas Dynamics: 23rd International Symposium,* edited by A. D. Ketsdever and E. P. Muntz
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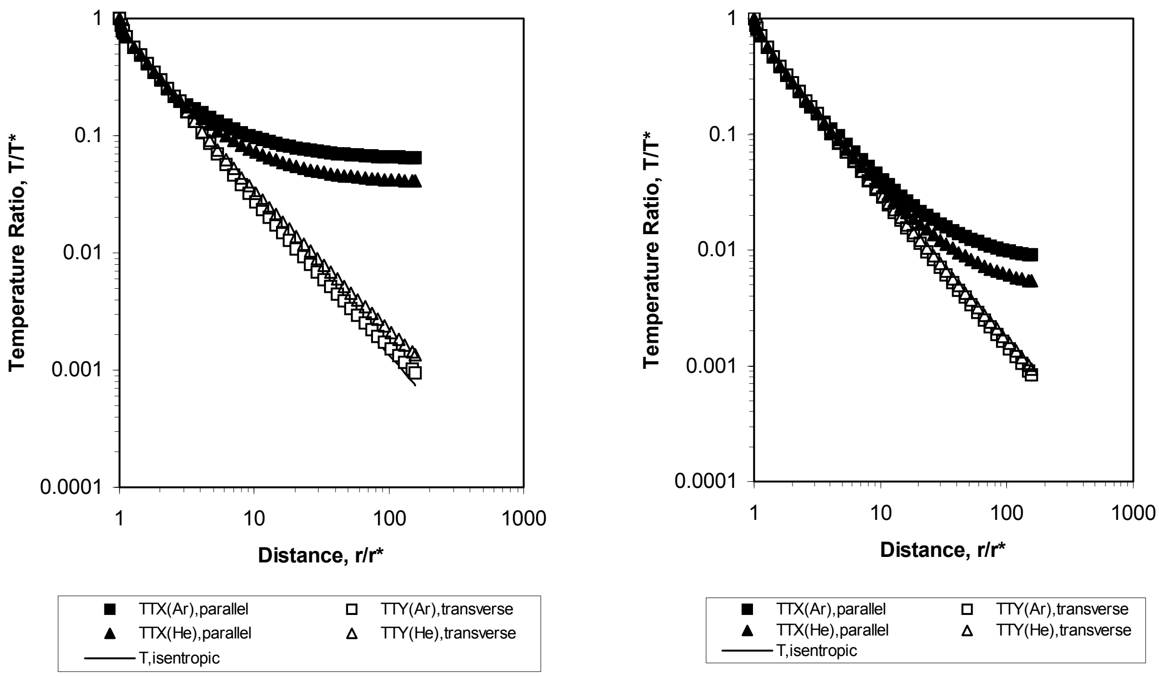
EXPANSION OF A GAS MIXTURE INTO A VACUUM

The DSMC results of the gas-mixture expansion ($f_{Ar,*} = 0.5$) from a spherical source into a vacuum are shown in Fig. 1 for two values of the Knudsen number, $Kn_* = 0.015$ (Reynolds number $Re_* = 124$) and 0.0015 ($Re_* = 1240$). The major effect of freezing the parallel temperature can be observed. The freezing comes first for heavier molecules of argon at smaller values of the Knudsen number. Cercignani [13] discussed the latter feature in detail. The parallel temperature for both species follows the temperature in the isentropic expansion [5,6]. The concentration of species remains about the constant, $f_{Ar} = 0.5$, along the streamlines.



a) $\boldsymbol{Kn_* = 0.015}$ **b)** $\boldsymbol{Kn_* = 0.0015}$

FIGURE 1. Parallel and Transverse Temperature Distributions in the Spherical Expansion of Ar-He Mixture into Vacuum.

EXPANSION OF A GAS MIXTURE INTO A FLOODED SPACE

The flow pattern is different in the case of gas-mixture expansion into a flooded space [5,6]. The distributions of argon concentration, pressure, stream and diffusion velocities, overall, species, parallel and transverse temperatures are shown in Figs. 2-7 at $Kn_* = 0.015$ and various pressure ratios $p_{0*}/p_a = 10^2$, 10^3, and 10^4 (filled squares, circles, and triangles, respectively). The results for $Kn_* = 0.0015$ and $p_{0*}/p_a = 10^4$ are also shown for comparison purposes.

It was found that the spherical flow could be separated by the coordinate[5,11] $r_+ \approx r_*(p_{0*}/p_\infty)^{1/2}$, at which the stream parameters are extreme, into two regions with significantly different properties. In the first "internal" region at $r < r_+$ the flow is supersonic (this region was studied in Refs. 5,10). The supersonic parameters depend on two similarity factors of Knudsen numbers Kn_* and Kn_+, based on the critical radius of a spherical source r_* and a coordinate [5,11] r_+. In the second "external" region at $r > r_+$, there is a transition of supersonic flow into subsonic stream at the infinity (see Figs. 2-7). The Knudsen number Kn_∞ based on the length scale parameter at infinity $l = (Qa_\infty/4\pi\gamma p_\infty)^{1/2}$ is the major similarity parameter in the second region. Another important similarity factor $K_2 = Re_*(p_\infty/p_{0*})^{1/2} \approx Re_{\infty l}$ can be used to study the flow structure in this region [5,12]. Correlations between Kn_*, Kn_∞, and Kn_+, are given in Ref. 10. For $K_2 = 12.4$ ($Kn_\infty = 0.17$), the concentration of argon changes insignificantly in the supersonic region. Because of the large gradients of the flow parameters in the shock wave front, the considerable increase in the velocity of the light helium component in this region is realized. Accumulation of the light component occurs in the leading front of the spherical shock wave, just as in the normal shock-wave case considered by Bird [9]. The enrichment of the mixture with the light component begins with the increasing of the pressure. It indicates that baro-diffusion effect dominates in this part of the shock wave. The DSMC data correlates well with the solutions of the Navier-Stokes equations [5] (see Fig. 2).

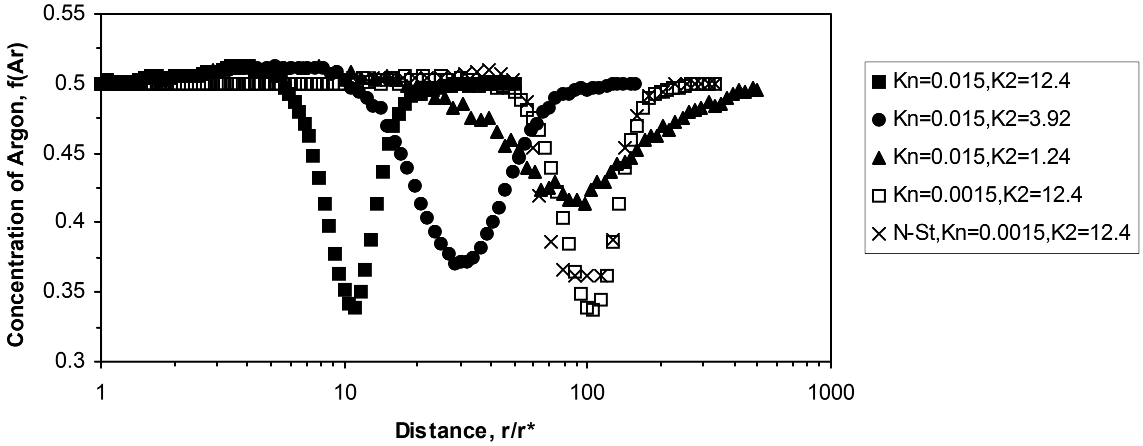


FIGURE 2. Argon Concentration in Spherical Expanding Flow at Different Rarefaction Parameters K_* and Kn_2.

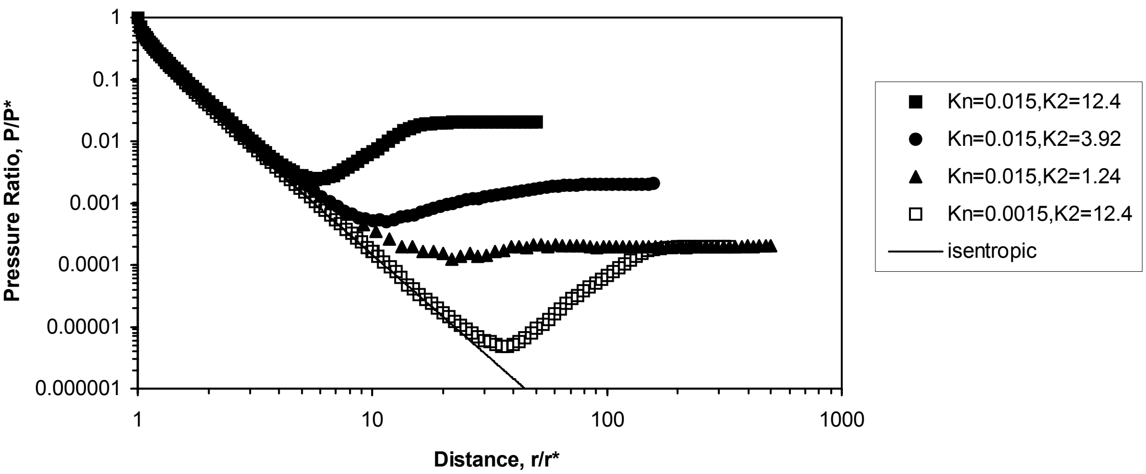


FIGURE 3. Pressure in a Spherical Expanding Flow of Ar-He Mixture at Different Rarefaction Parameters K_* and Kn_2.

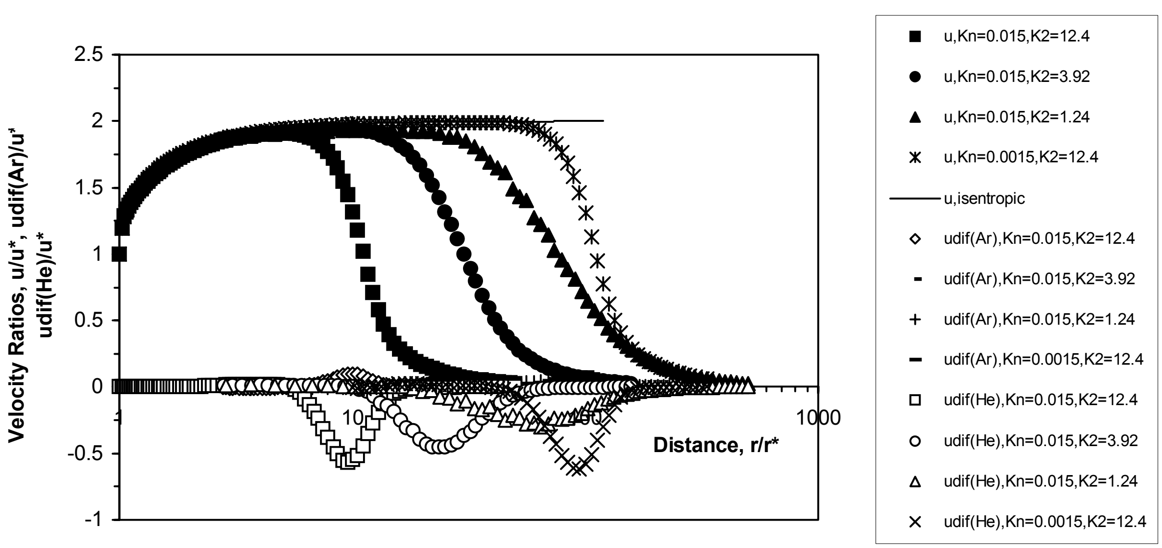


FIGURE 4. Stream and Diffusion Velocities of Argon and Helium in Expanding Flows at Different Parameters K_* and Kn_2.

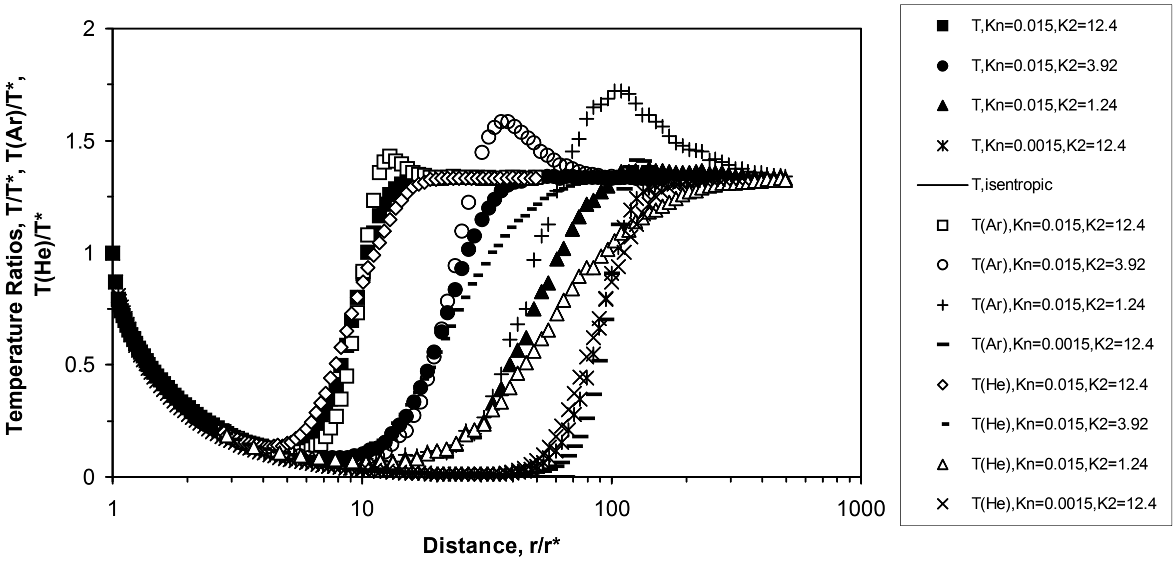


FIGURE 5. Overall and Species Temperatures in Spherical Expanding Flows at Different Parameters K_* and Kn_2.

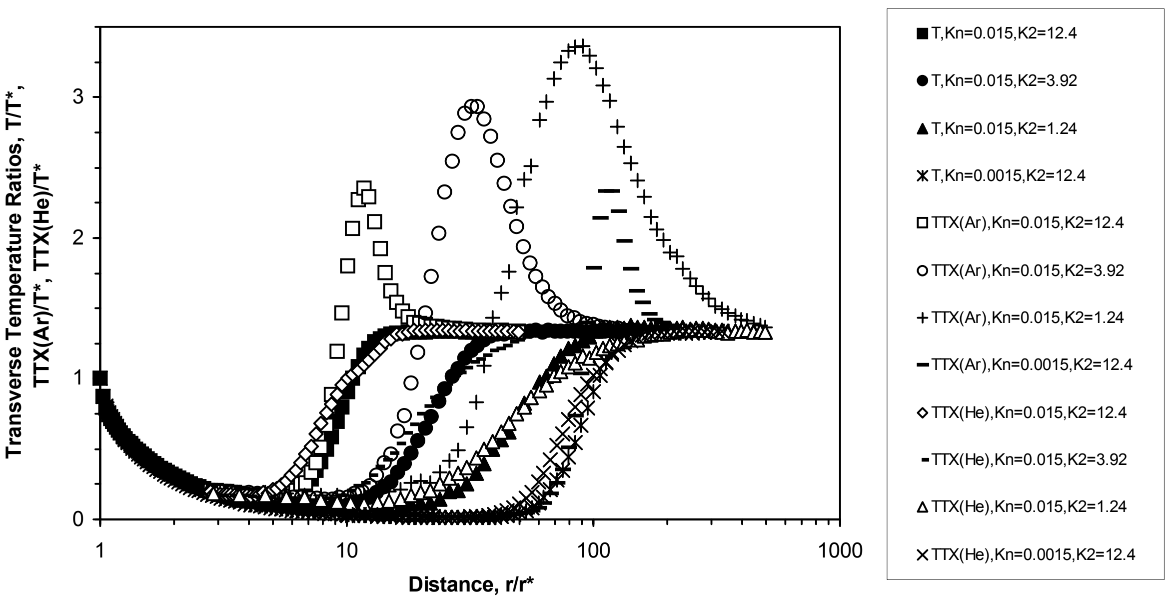


FIGURE 6. Parallel Temperature in Spherical Expanding Flows of Ar-He Mixture at Different Parameters K_* and Kn_2.

In all cases, the hypersonic stream velocity is slightly different from the speed of the isentropic flow (see Fig. 4) and correlates well with the velocity predicted by the Navier-Stokes (continuum) approach.

The pressure ratio significantly influences the thickness of the spherical shock wave, which can be measured differently by using the distributions of the species concentration, pressure, diffusive velocities, or heavy-component parallel temperature (see Figs. 2-6).

At decreasing the similarity rarefaction parameter K_2, the flow pattern is changed dramatically in the shock wave and behind it. For K_2 = 1.24 (Kn_∞ =1.7), the diffusion zone is wider than in the latter case. In the region behind the shock wave, multi-temperature regime of the flow is identified. At the same time, the significant enrichment of the mixture with the heavy component inside the wave front, described by Gusev and Riabov [5] by means of the continuum concept, has not been found.

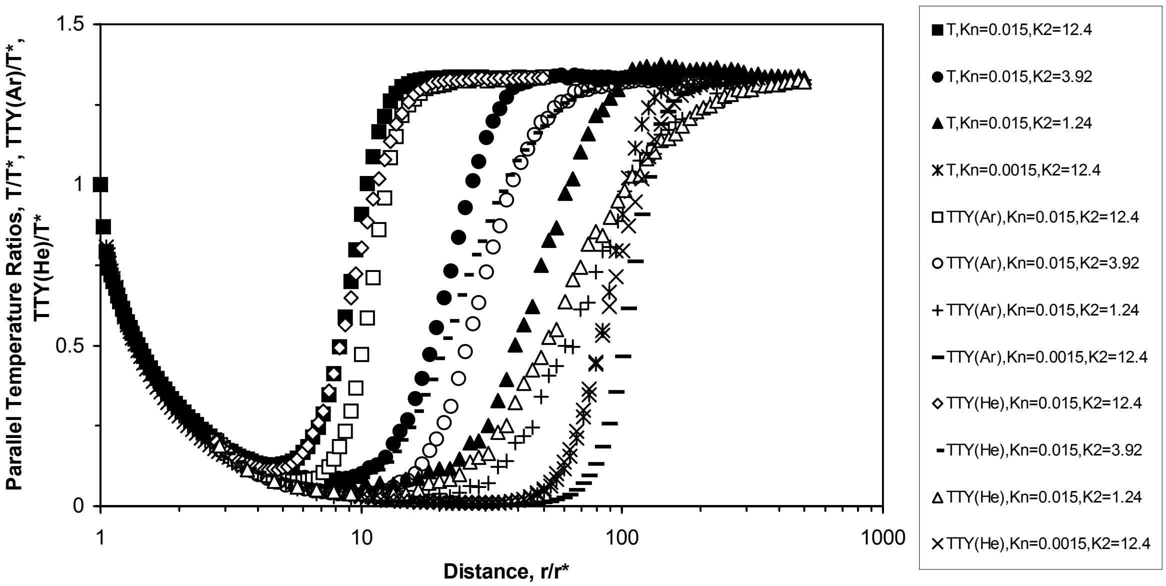


FIGURE 7. Transverse Temperature in Spherical Expanding Flows of Ar-He Mixture at Different Parameters K_* and Kn_2.

Similarity Of Flows Behind The Spherical Shock Wave

The similarity analysis [12] has been used to analyze the flow structure in the "external" region at $r > r_+$. The following dimensional parameters are used for normalization purposes: $R_a = r_*(p_{0*}/p_\infty)^{1/2}$, ρ_∞, $U_a = a_\infty$, $p_a = p_\infty$, and $T_a = T_0$. In this case, index "*a*" refers to the *ambient* medium conditions at the infinity. The renormalized characteristics of the spherical expending flow in the "external" region are shown in Figs. 8-13. All considered flow characteristics (species concentration, pressure, stream and diffusion velocities, overall, species, parallel and transverse temperatures) correlate well in the region ($r \geq R_a$) at the same rarefaction parameters ($K_2 = 12.4$) and various "internal" parameters of the Knudsen number Kn_*.

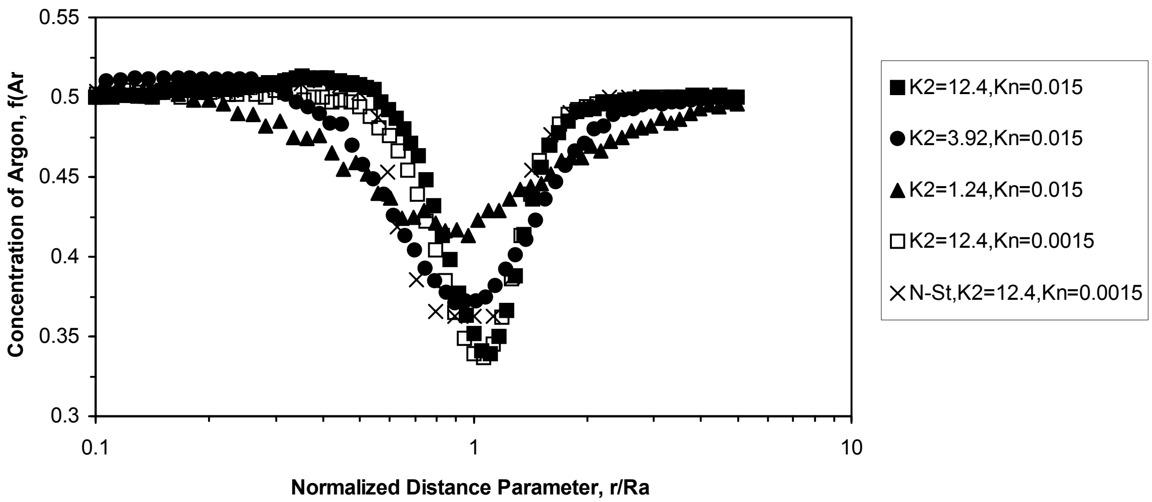


FIGURE 8. Argon Concentration in a Spherical Shock Wave at Different Rarefaction Parameters K_2 and Kn_*.

In all considered cases, the stream velocity changes in accordance with the hyperbolic law ($u \sim (r/R_a)^{-2}$) behind the shock wave (see Fig. 10).

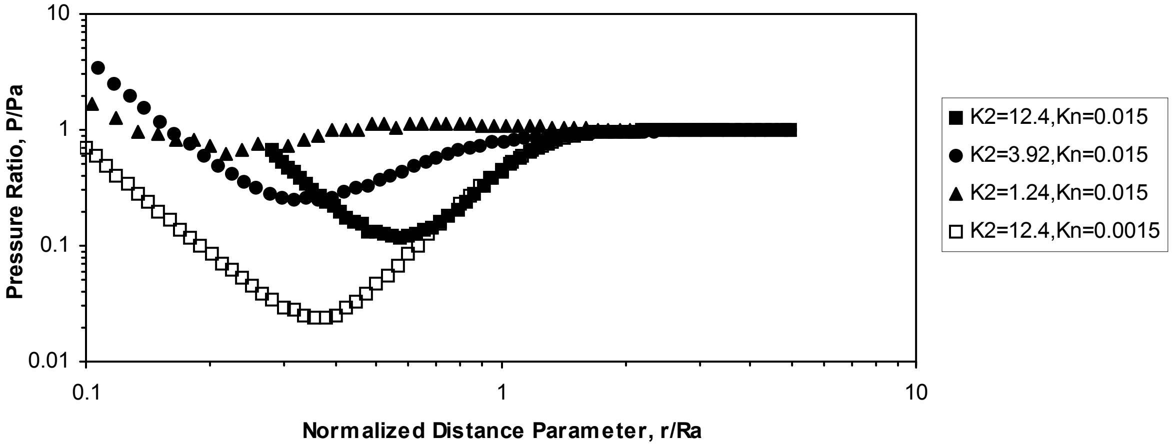


FIGURE 9. Pressure in a Spherical Shock Wave at Different Values of Rarefaction Parameter K_2 and Kn_*.

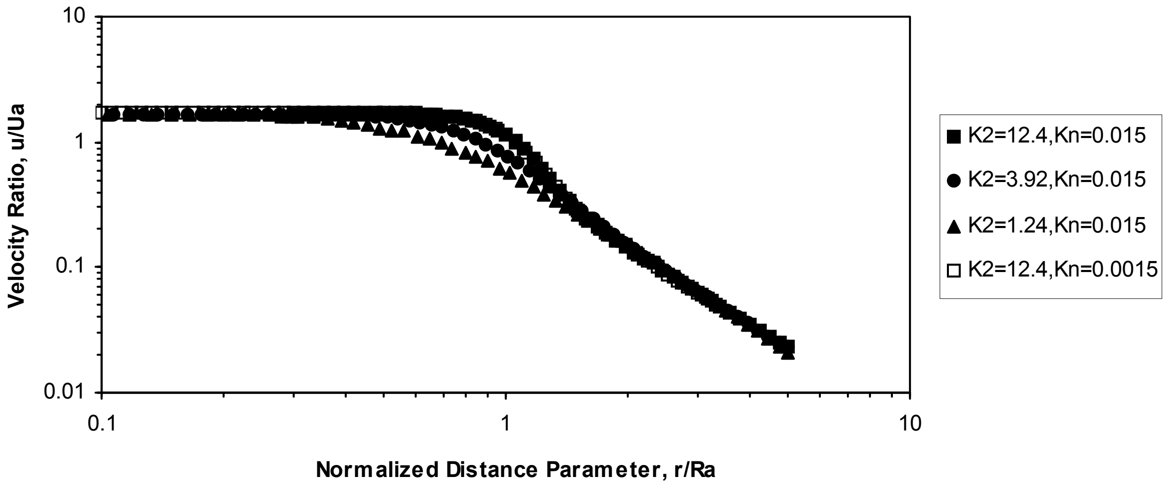


FIGURE 10. Stream Velocity of Ar-He Mixture in a Spherical Shock Wave at Different Parameters K_2 and Kn_*.

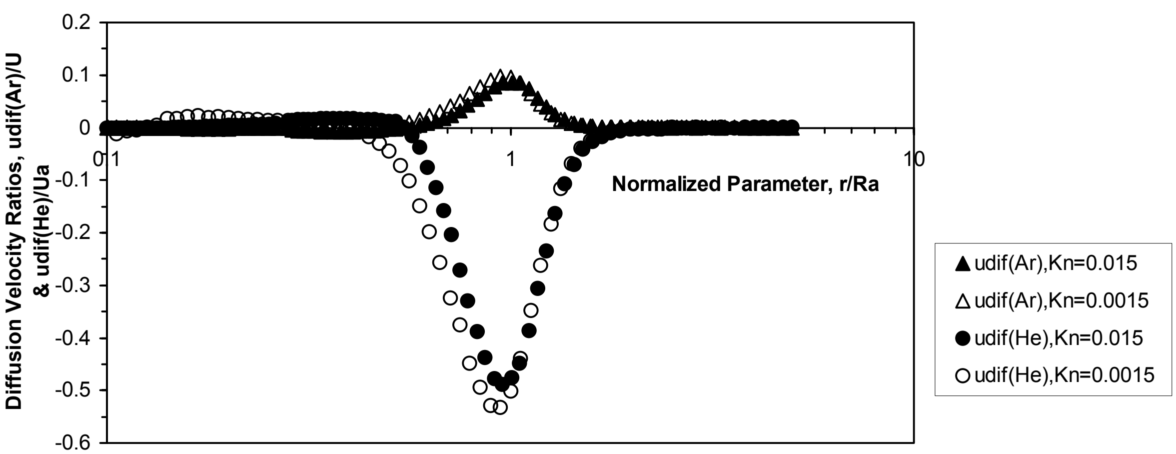


FIGURE 11. Diffusion Velocities of Argon and Helium in a Spherical Shock Wave at K_2 =12.4, Kn_* =0.015 and 0.0015.

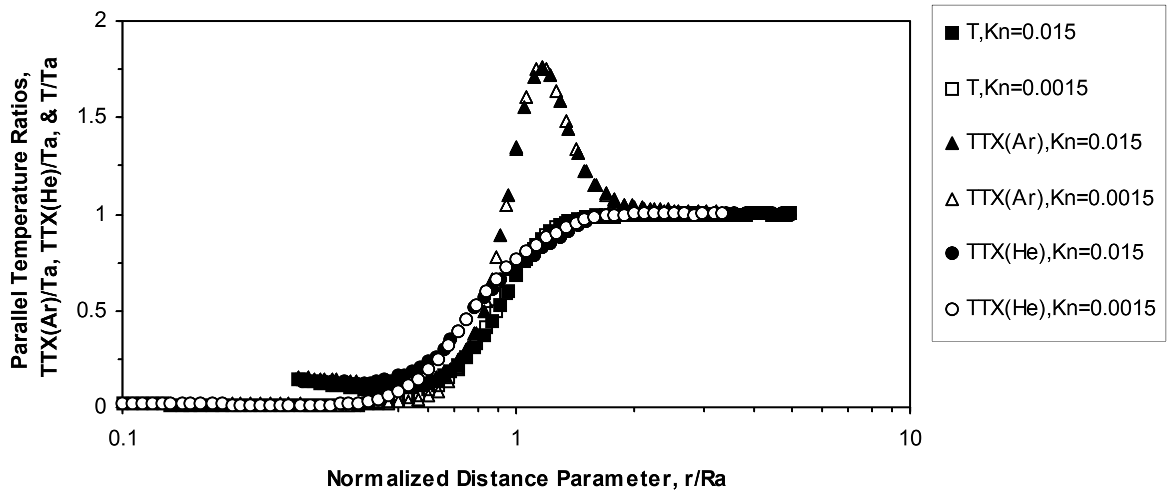


FIGURE 12. Parallel Temperature of Argon and Helium in a Spherical Shock Wave at K_2 =12.4, Kn_* =0.015 and 0.0015.

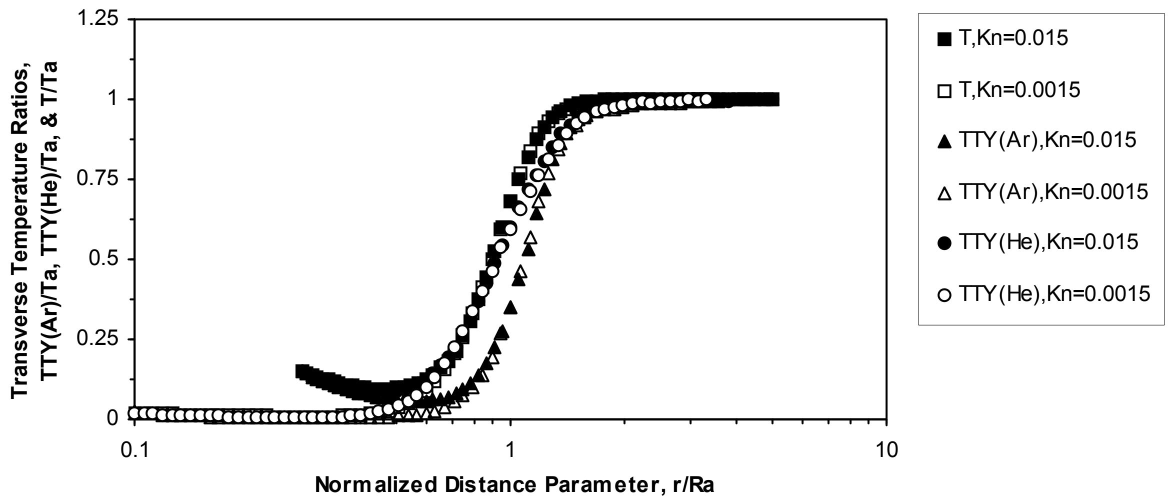


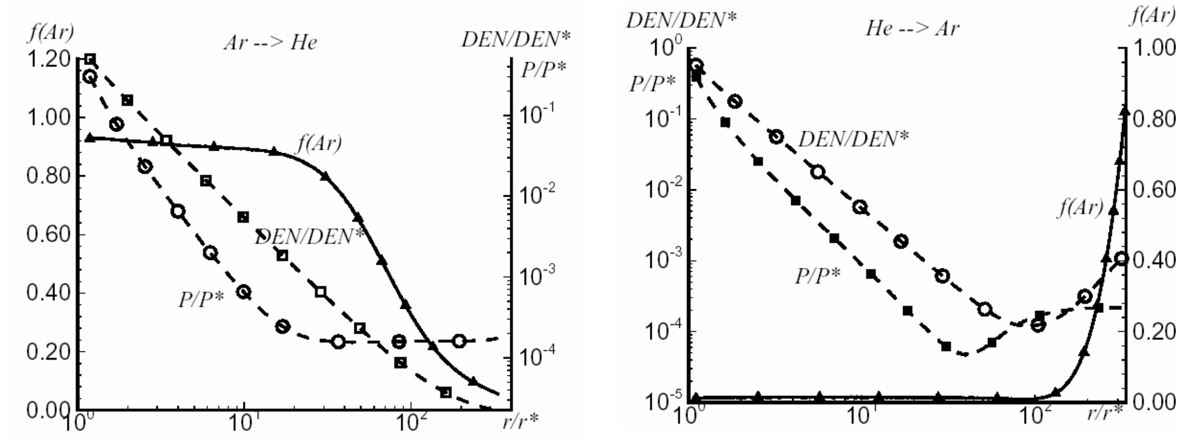
FIGURE 13. Transverse Temperature of Argon and Helium in Spherical Shock Waves at K_2 =12.4, Kn_* =0.015 and 0.0015.

Expansion Of Argon To Helium And Helium To Argon

The spherical expansion of a binary gas mixture into a flooded space has been analyzed in the case of the presence of a diffusive flux at the infinity $r >> r_+$. The numerical results were calculated for the case of the expansion of argon with little helium content ($f_{Ar,*}$ = 0.99) into a space filled by helium with a small admixture of argon ($f_{Ar,\infty}$ = 0.02). The distributions of the argon concentration f_{Ar}, density, and pressure related to this case with Kn_* = 0.014, Re_* = 78.5, and K_2 = 0.785 are presented in Fig. 14a.

The other case of the expansion of helium with a little content of argon ($f_{Ar,*}$ = 0.011) into a space filled by argon with small admixture of helium ($f_{Ar,\infty}$ = 0.9) was also analyzed. The distributions of the argon concentration f_{Ar}, density, and pressure, in flow at Kn_* = 0.03 (Re_* = 453) and K_2 = 4.53 are shown in Fig. 14b.

The results demonstrate that in both cases the gas of the surrounding space does not penetrate through the shock wave into the inner supersonic region of the flow. This property was noted in experiments of Skovorodko and Chekmarev [4]. In the considered cases the continuum approach is not applicable in the flow regions behind the shock waves. The discussed phenomena and the results of previous studies [5,6] were used for estimating the flow parameters and the axisymmetric jet structure in various aerodynamic applications [6].



a) Expansion of Argon into Helium **b) Expansion of Helium into Argon**

FIGURE 14. Argon Concentration, Pressure and Density Ratios in Expansion of Argon into Helium ($Kn_* = 0.014$, $K_2 = 0.785$) and Helium into Argon ($Kn_* = 0.003$, $K_2 = 4.53$).

CONCLUSION

The direct simulation Monte-Carlo and similarity methods have been used in the studies of kinetic and gasdynamic effects in the expanding flows of the argon-helium mixture from a spherical source. The diffusive effects are significant for estimation of the shock-wave width, the effectiveness of species separation, and ambient gas penetration. The group of similarity parameters (Kn_*, Kn_+, Kn , K_2, Re_*, etc.) was found to identify the rarefaction flow regimes, as well as the limits of applicability of the continuum concepts for studying diffusive effects in low-density gas-mixture flows. The kinetic effects play a significant role in "freezing" the parallel temperature of the species in the hypersonic zone; in enriching flow with the light (helium) component in the spherical shock wave, and in abnormally increasing the parallel temperature of the species in the flow behind the shock wave. The rarefaction parameter K_2 is the major criterion for simulating flows in the latter flow area.

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