Numerical Simulations of Gas Cloud Expansion in Rarefied Environment

Virendra K. Dogra
The Johns Hopkins University Applied Physics Laboratory
Laurel, Maryland 20723, USA

Dean C. Wadsworth
ERC, Inc.,
Edwards AFB, California 93524, USA

Abstract. Time accurate numerical simulations of a high temperature source cloud of gas expanding into an ambient atmosphere are performed using a multiple temperature gas model and the direct simulation Monte Carlo (DSMC) method. The multi-temperature approach uses continuum conservation equations derived from the Boltzmann equation via first-order Chapman-Enskog expansion and zero-order non-isotropic velocity distribution function. These equations are solved numerically using a kinetic flux splitting method for inviscid fluxes and a central difference scheme for the viscous fluxes in a time accurate manner. The DSMC technique is a well-established particle approach for rarefied flows. The source and ambient densities and temperatures are varied to establish the range of applicability and relative accuracy of the two methods. For most of the source and the ambient parameter considered, the two methods give similar predictions of the basic flowfield evolution, and of the degree of translational non-equilibrium that arises.

INTRODUCTION

The expansion of a highly energetic gas cloud into a rarefied environment is a phenomenon that arises in many practical problems, including supernova explosions, high altitude rocket plumes, and active space experiments where interaction of the artificial plasma and neutral gas cloud with the ambient atmosphere is studied. During the rapid expansion of the gas cloud, the spherical gas front or contact surface propagates outward through the ambient atmosphere, while a rarefaction wave propagates inward into the source cloud. Recent time-accurate continuum simulations[1] of a high-temperature metallic gas cloud at high altitude with radiation transport show the flow field generally includes continuum, transitional, and rarefied regions depending on the absolute and relative densities and thermal energies of the source cloud and ambient atmosphere. Thus it seems that particle simulation methods such as the direct simulation Monte Carlo (DSMC) method[2] would be more suitable for simulating these flows. However, the unsteady nature of these flows makes the particle approach a formidable computational task. Other features that add further complexity to the particle treatment are the presence of very dense gas in the source region and the potential for phase change as well as coupled radiative transport. Moreover, the dilute gas assumptions made in these particle simulation methods make them unsuitable for dense regions of the cloud. This suggests that at present a continuum method, which to some extent accounts for the non-equilibrium nature of the flow, may provide efficient and accurate simulations of the gas cloud expansion.

The purpose of this study is to improve the fundamental understanding of the initial evolution of the gas cloud expansion, including the formation of the shock wave in the ambient atmosphere and

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
JUN 2004		**-**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Numerical Simulations of Gas Cloud Expansion into a Rarified Environment	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) **Virendra Dogra; Dean Wadsworth**	5d. PROJECT NUMBER **2308**
	5e. TASK NUMBER **M19B**
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Air Force Research Laboratory (AFMC),ERC,10 E. Saturn Blvd.,Edwards AFB,CA,93524-7680**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

Time accurate numerical simulations of a high temperature source cloud of gas expanding into an ambient atmosphere are performed using a multiple temperature gas model and the direct simulation Monte Carlo (DSMC) method. The multi-temperature approach uses continuum conservation equations derived from the Boltzmann equation via first-order Chapman-Enskog expansion and zero-order non-isotropic velocity distribution function. These equations are solved numerically using a kinetic flux splitting method for inviscid fluxes and a central difference scheme for the viscous fluxes in a time accurate manner. The DSMC technique is a well-established particle approach for rarefied flows. The source and ambient densities and temperatures are varied to establish the range of applicability and relative accuracy of the two methods. For most of the source and the ambient parameter considered, the two methods give similar predictions of the basic flowfield evolution, and of the degree of translational non-equilibrium that arises.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
unclassified	**unclassified**	**unclassified**		**6**	

the degree of translational non-equilibrium that arises. Time accurate numerical simulations of a rapidly expanding high temperature gas cloud are performed using both a multi-temperature gas dynamics model[3-4] and the DSMC method[2]. The influence of the source radius and source and ambient density are evaluated. Comparison of results for the two methods establishes the range of applicability and the relative accuracy of each.

COMPUTATIONAL APPROACHES

Conservation equations of the multi-temperature gas dynamic model in spherical symmetric coordinates (Ref.1) are solved numerically in a time accurate manner. The inviscid part of the flux is calculated at each cell interface using a kinetic flux splitting method.[1] A local ellipsoidal distribution function of the form

$$f_0 = f_{0r}\, f_{0p}\, f_{0t}$$

where

$$f_{0r} = \frac{1}{\sqrt{2p\,RT_r}} \exp\langle -\frac{1}{2RT_r} c_r'^{\,2} \rangle,$$

$$f_{0p} = \frac{1}{\sqrt{2p\,RT_p}} \exp\langle -\frac{1}{2RT_p} c_p'^{\,2} \rangle,$$

$$f_{0t} = \frac{1}{\sqrt{2p\,RT_t}} \exp\langle -\frac{1}{2RT_t} c_t'^{\,2} \rangle,$$

is then defined for each cell and used to formulate analytical expressions for the inviscid fluxes in the radial (r) and perpendicular (p) directions. The c'_r, c'_p, and c'_t are the components of the random molecular velocity in the above expressions. As with other flux-splitting techniques, this inviscid flux is formally first-order accurate in space. The second-order accuracy in space is achieved by using a MUSCL variable-extrapolation scheme[5] in conjunction with a minmod slope limiter to ensure monotonicity. The viscous fluxes are calculated with a second-order accurate central difference scheme. Fourth-order accuracy in time is obtained using a Runge-Kutta time integration method[6]. The time step chosen is the minimum of a Courant-based time step and a step based on the magnitude of energy exchange between the radial and perpendicular directions.

The DSMC calculations are performed using a wholly conventional one-dimensional method well described in reference 2. Some features of the current implementation are given in, e.g., reference 7. Profiles of macroscopic properties at a given time are generated as instantaneous snapshots of sampled molecular quantities.

RESULTS AND DISCUSSION

The source cloud is assumed to be spherical with uniform initial density and temperature. The source is pure argon with an assumed Maxwellian (inverse fourth power law) inter-atomic potential ($T_{ref} = 273\,K$ *and* $m_{ref} = 2.517 x 10^{-5}\ kg/ms$). Two values of source gas density r_s at a temperature of T_s

= 3000 K are considered in the present calculations. The outer boundary condition is assumed to be the standard atmosphere at the given altitude (70 or 85 km). To focus on cloud expansion and not on molecular diffusion and other multi-species issues, the ambient atmosphere is simulated as pure argon at the ambient atmospheric density and temperature.

In the multi-temperature continuum calculations the initial spherical source volume and flow domain are divided into uniformly distributed spherical cells of constant width 0.0002m. One cell is added to the outer boundary after each time step, allowing the grid to grow in time as the gas cloud expands. This procedure reduces the computational task during early phases of the solution because computation may need very large number of cells at later times.

The DSMC calculations use a uniform radial grid with cell dimension comparable to the initial source mean free path. Collision sub cells were utilized to further improve the spatial fidelity. Maxwell molecule collision interaction was approximated using the Maxwell limit of the VHS model. Sensitivity studies (not shown) confirm the results to be grid and timestep independent. Since spatial weight factors are not used, initial molecular population of a cell is controlled only by the local gas number density and the cell volume. Control of statistical noise present in the sampled snapshots is possible in this case only by recourse to large numbers of simulated molecules. The typical simulation required 40 million molecules, 1000 cells, 10 subcells per cell, and 2500 timesteps.

Figures 1-4 show the evolution of the density, temperature, and velocity profiles for a source cloud expanding into a 70 km altitude ambient. The initial source density and radius for this case are r_s = 0.005 kg/m^3 and r_s =0.1 m, corresponding to a source Knudsen number of $Kn_s \sim 5.6\text{x}10^{-4}$. The source to ambient density ratio is approximately 60. The initial source energy is 19.6 J with energy-density of $4.68\text{x}10^3$ J/m^3. These figures show that a well-defined shock wave propagates outward in the ambient atmosphere. The shock is followed by a contact surface, which separates the expanding gas from the ambient environment. A strong rarefaction wave travels behind the contact surface towards the center of the source. The final time shown (t=$1\text{x}10^{-4}$ s) corresponds to approximately one acoustic time (based on the initial source radius and speed of sound).

Translational non-equilibrium arises in the shock wave as the gas cloud expands (Fig. 3). The ratio of the radial temperature to the parallel temperature (T_r/T_s) as a function of normalized gas cloud radius is shown in Fig. 3 for three different times. The maximum value of this ratio is more than two which occurs in the shock wave region (Fig. 3). This suggests that the shock wave region is in a highly non-equilibrium thermal state. The majority of the expanding gas cloud remains in translational equilibrium, due to the relatively high source density. A slight overshoot is observed in the radial temperature just behind the shock wave (Fig. 2), but no overshoot is present in the perpendicular temperature (not shown).

The radial velocity increases linearly with radius through the cloud for most of the flow field (Fig. 4). Also, the radial velocity gradient decreases with time as the gas cloud expands into the ambient atmosphere.

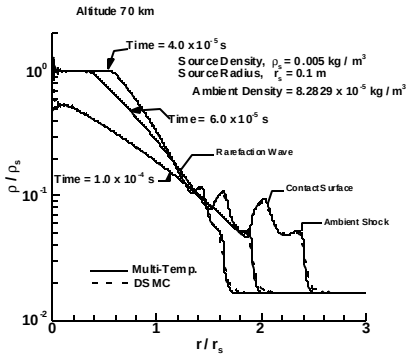


Fig. 1 Density Profiles

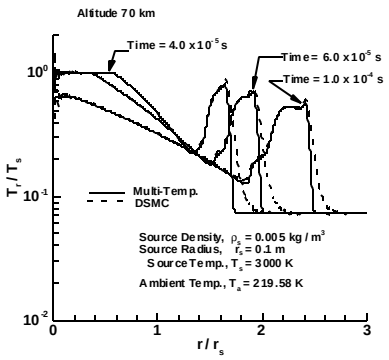
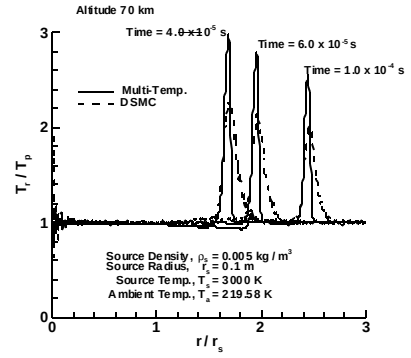


Fig. 2 Radial Temperature Profiles



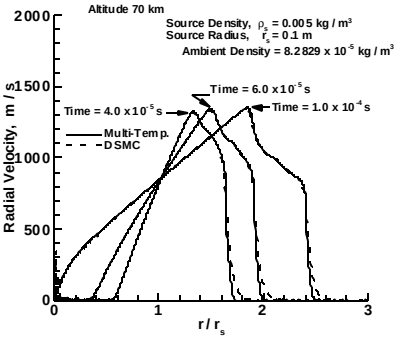


Fig. 3 Parallel Temperature Profiles

Fig. 4 Radial Velocity Profiles

DSMC calculations predict a slightly thicker shock than predicted by the multi-temperature continuum model (Figs. 1-4). The DSMC results are expected to be more accurate than the continuum method in the highly non-equilibrium leading edge of the shock. Also, the difference in shock wave thickness is slightly more pronounced in the temperature profiles because temperature is calculated based on higher moments of the distribution function. The DSMC results show relatively large scatter near the origin due to the small cell volumes present, but this does not obscure interpretation of the remainder of the flowfield. The overall qualitative and quantitative comparison of the flow field predictions by the two methods is very good for this case.

A second set of calculations (Figs. 5-8) is also performed at 70 km altitude for expansion of a gas cloud with five times smaller source density and half the radius of the previous case. For this case, r_s = 0.05 m and r_s = 0.001 kg/m^3, resulting in $Kn_s \sim 5.6\text{x}10^{-3}$ and $r_s / r_a \sim 12$. The source energy is 0.489 J, and the energy density is 934 J/m^3. These calculations illustrate the effect of initial source energy on the gas cloud expansion for given ambient conditions. Figures 5-8 show the same general features of the gas cloud expansion as are observed in the first set of calculations (Fig. 1-4) except that a shock wave does not form in the ambient because there is not enough source energy to raise the expansion front velocity to high supersonic value (Fig. 8). Comparison of Fig. 6 and Fig. 7 of the temperature profiles shows considerable thermodynamic non-equilibrium in the expansion front region.

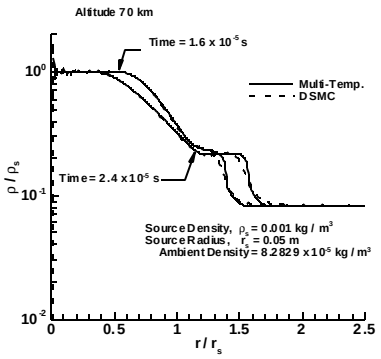


Fig. 5 Density Profiles

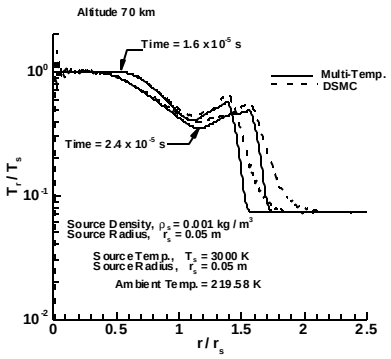
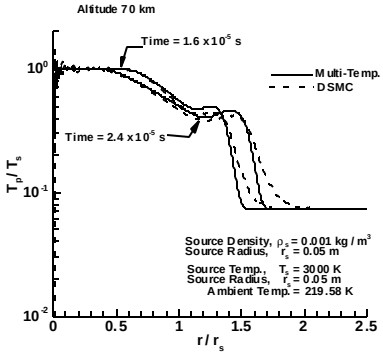


Fig. 6 Radial Temperature Profiles



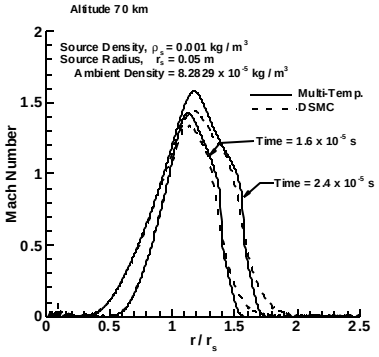


Fig. 7 Parallel Temperature Profiles Fig.8 Radial Velocity Profiles

In order to see the effect of ambient rarefaction on the gas cloud expansion, a third set of calculations is performed for the source conditions used in the first set (Fig. 1-4), but with an ambient corresponding to an altitude of approximately 85 km. The ambient values of density and temperature are r_a = 8.2196 x 10^{-6} kg/m^3 and T_a =188.893 K, giving a density ratio $r_s / r_a \sim 600$. Figures 9 and 10 show normalized plots of density and radial temperature as a function of normalized radial distance. Fig. 9 shows that the multi-temperature model predicts a well-defined thin shock in the ambient, whereas the DSMC calculations predict a thick and diffused shock wvae. The multi-temperature model cannot resolve the large non-equilibrium effects present in the leading edge of the disturbance, and for this reason the radial temperature in the shock region predicted by the multi-temp model is lower than predicted by the DSMC method (Fig.10). The difference in parallel temperatures in the shock wave region (not shown) is much smaller than for radial temperatures. Also, the difference in radial velocity predicted by the two methods in the shock wave region (not shown) is small. The overall comparison of flow field predictions by two methods is reasonably good.

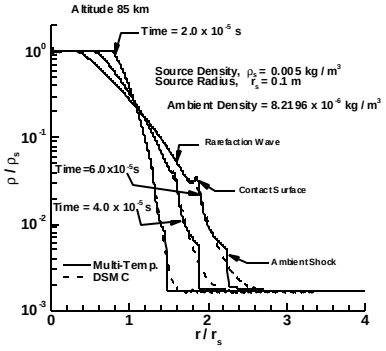


Fig. 9 Density Profiles

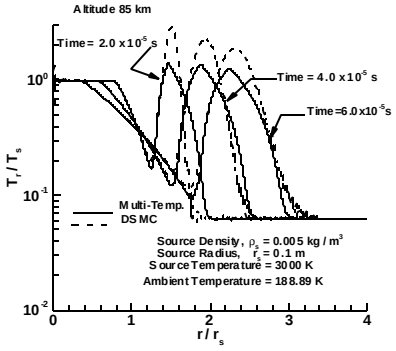


Fig. 10 Radial Temperature Profiles

CONCLUSIONS

Computations carried out for a variety of source and ambient conditions demonstrate the effects of source energy and ambient rarefaction on the evolution of the gas cloud. For the low source energy conditions at 70 km altitude, no shock wave propagates in the ambient because the gas front velocity is barely supersonic. Higher source energy conditions at the same altitude result in a well defined shock wave, with considerable translational non-equilibrium present in the shock wave region. The multi-temperature continuum model and the DSMC method predict a radial temperature overshoot in the gas front region for the dense and high energy source conditions at 70 km altitude. No radial temperature overshoot is predicted for the same source expanding at 85km altitude where ambient

atmosphere is more rarefied by an order of magnitude. The comparison of flow structure of the gas cloud expansion predicted by the multi-temperature model and the DSMC method shows the multi-temperature model is a reasonably good computational tool for low to moderate rarefied and non-equilibrium conditions.

REFERENCES

1. Dogra, V. K., Nance, R. P., Taylor, J. C., Swaminathan, P. K., Erlandson, R. E., and Meng, C.-I., "Modeling of Gas Cloud Expansion at High altitude with Radiation Transport," *Journal of Thermophysics and Heat Transfer*, Vol. 14, No. 3, July-September 2000.
2. Bird, G.A., Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Clarendon Press, Oxford, England, 1994.
3. Candler, G. V., Nijhawan, S., Bose Deepak, and Boyd, I.D., "A Multiple Translational Temperature Gas Dynamics Model," *Physics of Fluids*, Vol. 6, No. 11, 1994.
4. Dogra, V. K., et., al., "Simulations of Gas Cloud Expansion Using a Multi-Temperature Gas Dynamics Model," RGD 22nd International Symposium, AIP conference proceedings, vol. 585, (2000).
5. Van Leer, B., " Towards the Ultimate Conservative Difference Scheme. A Second Order Sequel to Godunov's method," *Journal of Computational Physics*, Vol. 32, 1979, pp. 263-275.
6. Jameson, A., Schmidt, W., and Turkel, E., "Numerical Simulations of the Euler Equations by Finite Volume Methods using Runge-Kutta Time Stepping Schemes," AIAA Paper 81-1259, 1981.
7. Wysong, I. J. and Wadsworth, D. C., "Assessment of direct simulation Monte Carlo phenomenological rotational relaxation models", *Physics of Fluids*, Vol. 10, Number 11, 1998, pp. 2983-2994.