Postprint of Research on Computational Method Library for Thermal Radiation Transport in Reentry Vehicle Flow Fields

Authors: Wang Jingying, Hao Jia’ ao, Du Guangsheng, Chunshou Li

Date: 2017-11-07T00:00:00+00:00

Abstract

Based on comparative analyses of one-dimensional radiative equilibrium and temperature discontinuity case results from several thermal radiation transport solution methods, a thermal radiation transport solution method library is proposed, constructed from the discrete ordinates method, P1 approximation, and optically thick limit approximation. This method library can be effectively coupled with the governing equations for thermochemical nonequilibrium flow fields of reentry vehicles for simulation. Using this method library, a spherical nose case at an altitude of 60 km and Mach number 35 was simulated. The calculations indicate that thermal radiation exerts a significant ‘cooling’ effect on high-temperature flow fields; radiative heat transfer is comparable in magnitude to convective heat transfer, and the radiative heat flux calculated using non-coupled flow-field radiative heating exceeds the coupled calculation value by 27%. Numerical simulation studies under such flight conditions should account for thermal radiation coupling effects.

Full Text

Thermal Radiation Solving Method Library for Reentry Vehicle Flowfield Simulation

WANG Jing-Ying[1], HAO Jia-Ao[2], DU Guang-Sheng[1], LEE Chun-Hian[2]
[1] School of Energy and Power Engineering, Shandong University, Jinan 250100, China
[2] School of Aeronautic Science and Engineering, Beihang University, Beijing 100191, China

Abstract

Based on comparisons of the results of one-dimensional radiation equilibrium and temperature discontinuity model cases, a thermal radiation solving method library consisting of the discrete ordinates method, P1 approximation, and the optically limiting approximation is proposed. The library can achieve effective coupled simulation with equations describing the thermo-chemical nonequilibrium flow over reentry vehicles. In the 60 km altitude and Mach number 35 sphere model case, it is found that thermal radiation can 'cool' the high temperature shock layer remarkably. It is also demonstrated that the radiative heating is comparable to the convective heating, and the radiative heating of the simulation uncoupled with radiation overestimates the coupled value by 27%, which illustrates that coupling effects of radiation should be considered in corresponding research.

Key words: radiation; hypersonic; aerothermodynamics; reentry

Reentry vehicles are the core component of deep space exploration missions such as manned lunar missions. When returning to Earth' s atmosphere at extremely high speeds (approximately 10 km/s), the surrounding high-temperature shock layer flowfield (reaching 10^4 K) subjects the vehicle to severe aerothermal heating, posing a grave threat to vehicle safety and potentially causing mission failure [1]. Therefore, accurately predicting the aerothermal environment of reentry vehicles to provide a basis for thermal protection design has become a critical technical challenge for corresponding deep space exploration missions.

The high-temperature atmospheric flowfield characteristics of high-speed reentry vehicles are extremely complex, with thermochemical nonequilibrium processes such as molecular vibrational energy excitation and multi-component chemical reactions strongly coupled with thermal radiation. For aerothermal heating prediction under these conditions, thermal radiation coupling effects must be considered in addition to conduction and convection. Candler and Park [2] employed a one-dimensional tangent slab formula to solve radiative transfer coupled with thermochemical nonequilibrium flowfield calculations, reporting that for the AFE model at an altitude of 78 km and velocity of 9 km/s, the stagnation point radiative heat transfer was approximately 6\$×10^{4}\$ W/m^2. Feldick [3] combined one-dimensional tangent slab approximation, Monte Carlo simulation, and a P1-Monte Carlo hybrid method with the DPLR (Data Parallel Line Relaxation) program to conduct nonequilibrium flowfield coupled radiation simulations for the MPCV (Multi-Purpose Crew Vehicle) return capsule, finding that the tangent slab approximation overestimated radiative heat flux by 30% compared to Monte Carlo simulation. Gao Tiesuo et al. [4] obtained radiative heat flux by integrating the emission coefficient along spatial paths under the optically thin limit assumption, while the high-temperature flowfield was obtained by solving chemically nonequilibrium N-S equations, concluding that in severe reentry heating regions, radiative heat flux from the return capsule contributed up to 30% of the total heat flux.

Monte Carlo simulation results can be considered accurate solutions for radiative transfer when the sample size is sufficiently large [6]; therefore, the results from tangent slab approximation and Monte Carlo simulation serve as benchmarks for our one-dimensional case studies. The optically thin approximation generally requires characteristic optical thickness τL 1, while the optically thick approximation requires τL 1. Detailed principles and expressions for each method can be found in references [6] and [7]. All methods were implemented through self-programmed FORTRAN calculations.

[Figure 1: see original paper] Sketch of one-dimensional radiative transfer model

1. One-Dimensional Radiative Transfer Model

A unified one-dimensional model case was adopted for comparative analysis of existing radiative transfer solving methods. The geometric description follows reference [5] and is illustrated in Figure 1: the space between two infinite, isotropic, diffuse parallel walls is filled with participating gray medium, with thermodynamic and radiative properties independent of temperature. The distance between parallel walls is L, with normal coordinate y and optical thickness coordinate $\tau =$ y, where is the medium' s radiative absorption coefficient. Wall 1 and Wall 2 have temperatures Tw1 and Tw2, and emissivities 1 and 2, respectively. The radiation intensity I makes angle γ with the y-axis and azimuthal angle ϕ. This model possesses one-dimensional axisymmetric properties. For convenience, uniform spatial discretization is employed with total discrete points N+1, physical interval Δy = L/N, and optical thickness interval $\Delta\tau = \tau$L/N.

2. Comparative Analysis of Methods Using One-Dimensional Model Cases

Multiple commonly used radiative transfer solving methods were selected for comparative analysis using one-dimensional model cases. The methods examined include: Tangent Slab Approximation (TSA), Monte Carlo Method (MC), Discrete Ordinates Method (DOM), P1 Approximation (P1), and two optically limiting approximation methods: Optically Thin Approximation (THIN) and Optically Thick Approximation (THICK). The tangent slab approximation is essentially a one-dimensional integral analytical solution of the radiative transfer equation. For the configuration shown in Figure 1, the tangent slab approximation yields radiative heat flux:

$$q_r = 2\pi \int_0^\infty \int_0^1 I(\tau, \mu)\mu \, d\mu \, d\nu$$

where T represents temperature, and E$_2$ and E$_3$ are second- and third-order exponential integral functions [6].

2.1 Radiative Equilibrium Assuming radiative equilibrium of the medium between the two walls in Figure 1, the spatial gradient of radiative heat flux qr is zero, i.e., dqr/dy = 0 W/m^3. Wall temperatures are set as Tw1 = 1000 K and Tw2 = 700 K, with emissivities 1 = 2 = 1.0. Cases with absorption coefficients = 0.7, 1.5, and 3.0 m^{-1} are calculated, with L = 1.0 m. The nondimensional radiative heat flux is defined as:

$$\Psi = \frac{q_r}{\sigma(T_{w1}^4 - T_{w2}^4)}$$

To determine the discrete point number N, grid independence calculations were performed for the benchmark tangent slab approximation, with results shown in Figure 2 [Figure 2: see original paper]. The figure demonstrates that when the number of discrete grid points N > 30, the radiative heat flux values from the tangent slab approximation become essentially stable, and the nondimensional temperature distribution data no longer changes with grid refinement. Therefore, all N values in our one-dimensional cases exceed 30 to ensure calculation accuracy of the tangent slab approximation method. For the radiative equilibrium case in this section, N = 50 is adopted.

Currently, domestic and international research mostly employs a single existing radiative transfer solving method directly coupled with flowfield numerical schemes. However, the high-precision methods' characterization of thermal radiation in infinite-dimensional spectral and propagation directions undoubtedly brings enormous computational and storage requirements to coupled simulations, while simplified radiation models suffer from insufficient prediction accuracy. Consequently, a single radiative transfer solving method cannot meet the current demand for efficient simulation of reentry vehicle aerothermal environments. Based on analysis of one-dimensional radiative transfer model cases and full consideration of flowfield optical thickness characteristics and numerical scheme features under reentry flight conditions, this paper constructs a radiative transfer solving method library suitable for coupled simulation with reentry vehicle thermochemical nonequilibrium flowfield equations, and successfully implements flowfield-radiation coupled simulation for a sphere case under Ma = 35 reentry flight conditions using this method library.

2.2 Temperature Discontinuity Mimicking the high-temperature shock layer flowfield of reentry vehicles, a temperature discontinuity case is designed: the medium temperature between the two walls is divided into two uniform layers with piecewise positioning. Near Wall 1 at position y/L = 0.3 is the high-temperature layer with temperature equal to wall temperature Tw1 = 10000 K; near Wall 2 is the low-temperature layer with temperature equal to wall temperature Tw2 = 300 K. Cases with absorption coefficients = 0.01, 0.1, 1.0, and 5.0 m^{-1} are calculated, with L = 1.0 m and N = 1000. The nondimensional radiation energy source term is defined as:

$$\Phi = \frac{\nabla \cdot q_r}{\kappa \sigma T_{w1}^4}$$

The nondimensional radiation energy source term values calculated by each method are shown in Figure 4 [Figure 4: see original paper]. Under all optical thickness conditions, the discrete ordinates method results are highly consistent with the benchmark tangent slab approximation, while the P1 approximation shows slight deviation. At small optical thickness τL = 0.01, the optically thin approximation yields results similar to the tangent slab approximation, but gradually loses validity as τL increases. The optically thick approximation radiation energy source term values remain zero at all times.

The nondimensional radiative heat flux results for each method are presented in Table 1 , where the error is the relative error calculated based on tangent slab approximation heat flux values as the benchmark. The table shows that the tangent slab approximation and Monte Carlo simulation differ minimally, the discrete ordinates method predicts radiative heat flux with high accuracy, while P1 approximation has errors within 5%. However, both optically limiting approximation methods have large heat flux value errors.

Figure 3 [Figure 3: see original paper] shows the temperature distribution results for each method in the radiative equilibrium case. The temperature values from the discrete ordinates method (DOM) are almost identical to the benchmark methods of tangent slab approximation (TSA) and Monte Carlo simulation (MC), and the P1 approximation (P1) calculations are also close to the benchmark solutions. The optically thin approximation (THIN) yields fixed temperature values, while the optically thick approximation (THICK) shows large differences from tangent slab approximation data, though its prediction accuracy gradually improves as the total optical thickness value τL increases.

3. Characteristics of Different Radiative Transfer Solving Methods

The tangent slab approximation solution is exact but can only integrate along one-dimensional paths, making it unreasonable for high-dimensional calculations with difficult-to-define accuracy. Monte Carlo simulation can be considered an exact solution with sufficient sample size but brings corresponding computational cost issues. The discrete ordinates method shows high consistency with benchmark methods (tangent slab approximation and Monte Carlo simulation) in one-dimensional solutions. It is a direct discretization method based on the complete radiative transfer equation and is easily extensible to high dimensions. The P1 approximation solves a simplified radiative transfer equation with moderate accuracy. Optically thin and thick approximations are only reasonable under extremely small (generally τL < 0.01) or extremely large optical thickness conditions.

Regarding computational resource consumption, the tangent slab approximation performs numerical integration along one-dimensional paths, requiring modest storage but demanding upstream-downstream point-by-point integration at each grid point, completing N^2 algebraic operations per calculation (where N is the number of discrete grid points), making the computational cost considerable. Monte Carlo simulation requires tracking the history of each energy bundle' s absorption and emission, with enormous energy bundle sample sizes often consuming large storage resources and computational effort. The discrete ordinates method requires storing radiative intensities in each angular direction and solving M algebraic equations (where M is the number of discrete angular directions) at each grid point, occupying certain storage and computational costs. The P1 approximation only solves a second-order differential equation for incident radiation, with modest storage and computational requirements. Optically limiting approximations explicitly calculate radiation quantities directly from the temperature field, with very low solution cost.

Table 4 lists the CPU time consumed by each method in solving the radiative equilibrium case in Section 2, where the Monte Carlo simulation required an energy bundle sample size of [MATH_{{{sample}}_{{size}}}]. As can be seen from Table 4, the actual computational time consumed by each method is consistent with the qualitative analysis in Table 3 . The tangent slab approximation and Monte Carlo simulation consume substantial computational time, while the discrete ordinates method and P1 approximation offer higher computational efficiency, and the optically limiting methods consume almost no time.

Except for the tangent slab approximation, which is difficult to extend to high dimensions, the remaining methods are easily extensible to high-dimensional cases. Meanwhile, the tangent slab approximation encounters cross-region integration issues during parallel solution processes, requiring large amounts of data transfer between parallel regions. The discrete ordinates method and P1 approximation both transfer radiation-related quantities at adjacent region interfaces. The optically limiting approximation only needs to transfer temperature values at adjacent region interfaces.

In summary, this paper abandons the tangent slab approximation (unfavorable for high-dimensional solution and parallel processing) and Monte Carlo simulation (high computational cost). The final radiative transfer solving method library consists of three methods at different levels: the discrete ordinates method, P1 approximation, and optically limiting approximation (including optically thin and thick approximations). The general execution principle of this method library for radiative transfer solving is: for non-coupled precise solution with the flowfield, directly select the discrete ordinates method; for coupled solution with the flowfield, if the flowfield' s optical thickness satisfies limiting conditions, first use the optically limiting approximation for coupled simulation, then switch to the discrete ordinates method after convergence to save computational cost; if limiting conditions are not satisfied, first use the P1 approximation for coupled solution, then switch to the discrete ordinates method after convergence. These usage principles are illustrated in Figure 5 [Figure 5: see original paper].

[Figure 5: see original paper] Operation procedures of the thermal radiation solving method library

4. Demonstration of Coupled Simulation for Reentry Flight Case

A sphere model with R = 1.0 m at Ma = 35 is selected for coupled simulation of high-temperature flowfield and thermal radiation under reentry flight conditions, demonstrating the effectiveness of the constructed radiative transfer solving method library coupled with flowfield numerical schemes. The free-stream density is ∞ = 3.1$\times10^{-4}$ kg/m^3, temperature T∞ = 247 K, with atmospheric mass fraction composition YN$_2$ = 0.77, YO$_2$ = 0.23, corresponding to Earth atmospheric parameters at 60 km altitude. The high-temperature flowfield solution employs the numerical scheme from references [8-10], using Park' s two-temperature thermodynamic nonequilibrium model [11] and Gupta' s 11-species 20-reaction chemical kinetics model [12]. Thermal radiation properties are calculated using Anderson' s two-step model [7]. Wall temperature is Tw = 1000 K, wall emissivity = 1.0, with fully catalytic wall conditions. The flowfield-radiation coupling algorithm is described in reference [8]. Both flowfield solving and radiation method library are implemented through self-programmed FORTRAN. The computational grid is 60$\times70, withthefirstgridspacingnormaltothewallat1.0\times10^{-6}$ m [13] as required for aerothermal heating prediction. The computational cost for this sphere model is relatively small, so the high-precision discrete ordinates method in the solving method library can be directly used for flowfield-radiation coupled solution.

Figure 6 [Figure 6: see original paper] presents the pressure and temperature distributions from coupled flowfield-radiation calculations, showing a very thin shock layer with shock standoff distance less than 1/15 of the sphere radius. The post-shock stagnation region translational-rotational temperature and vibrational-electronic temperature both exceed 10000 K. Figure 7 [Figure 7: see original paper] shows the thermal radiation quantity distributions within the flowfield, where the radiation energy source term and total absorption coefficient distributions completely correspond to the flowfield temperature distribution. Although the maximum incident radiation is distributed within the shock layer, high incident radiation values also extend to the upstream flow ahead of the shock, demonstrating greater diffusivity.

Under Ma = 35 flight conditions, the radiation energy source term has reached considerable magnitude (approximately 10^8 W/m^3), and thermal radiation effects on the flowfield are significant. However, the shock layer optical thickness remains very small, less than 0.005. Therefore, this paper also employs the optically thin approximation from the solving method library for coupled calculation with the flowfield. Figure 8 [Figure 8: see original paper] compares stagnation line temperature results for flowfield calculations without radiation coupling (uncoupled), coupled with optically thin approximation (coupled_{thin}), and coupled with discrete ordinates method (coupled_{dom}). Compared to the uncoupled case, coupled calculations show lower shock layer temperatures and thinner shock layers, highlighting the radiation cooling effect [7]. The optically thin approximation shows more pronounced radiation cooling than the discrete ordinates method because it neglects radiation absorption and only considers radiation emission, resulting in larger radiation energy source term values and more significant flowfield effects.

Figure 9 [Figure 9: see original paper] presents the stagnation line mass fraction distributions of N^+ and e^- for uncoupled and coupled radiation calculations. The coupled calculations show significantly lower N^+ and e^- mass fractions than uncoupled values, likely because radiation cooling effects inhibit ionization reactions. Therefore, significant coupling effects exist between high-temperature atmospheric chemical reactions and thermal radiation under high-speed reentry flight conditions. Additionally, the optically thin approximation coupled calculation shows more significant radiation cooling effects, with N^+ and e^- mass fractions lower than those from discrete ordinates method coupled calculations.

Figure 10 [Figure 10: see original paper] shows the stagnation line thermal radiation results for uncoupled and coupled calculations. The absolute values of thermal radiation quantities from coupled calculations are all smaller than uncoupled values, with the optically thin approximation coupled calculation showing more pronounced reduction in absolute thermal radiation values.

Table 5 lists the stagnation point heat flux values for uncoupled and coupled radiation calculations at $\mathrm{Ma} = 35$ (unit: $\mathrm{MW/m^2}$). The convective heat transfer is similar between uncoupled and coupled radiation calculations, but the radiative heat flux from uncoupled calculation is much larger than the coupled value. Meanwhile, coupled simulation predicts that radiative heating is comparable to convective heating.

Conclusion

This paper designed two one-dimensional radiative transfer model cases (radiative equilibrium and temperature discontinuity) to comparatively analyze the performance of various radiative transfer solving methods. The storage, computational cost, and parallelization characteristics of each method in practical solution processes were examined. Abandoning the one-dimensionally exact tangent slab approximation and computationally expensive Monte Carlo simulation, a radiative transfer solving method library was proposed, constructed from three methods at different levels: the discrete ordinates method, P1 approximation, and optically limiting approximation. The usage principles for this method library were also provided. This solving method library can accurately solve radiative transfer, efficiently couple with flowfield numerical schemes, and is suitable for large-scale parallel computing.

Using the constructed radiative transfer solving method library coupled with reentry vehicle high-temperature thermochemical nonequilibrium flowfield numerical solving schemes, a demonstration simulation was successfully implemented for a sphere case at $\mathrm{Ma} = 35$. Under corresponding reentry flight conditions, flowfield-radiation coupling effects are significant, with thermal radiation having a "cooling" effect on the flowfield. Convective heat transfer is similar between uncoupled and coupled radiation calculations, but uncoupled radiative heat flux is much larger than the coupled value. Meanwhile, coupled simulation predicts radiative heating comparable to convective heating. Flowfield-radiation coupling effects should be considered in relevant simulation studies.

References

[1] BIAN Yingui, XU Ligong. Aerothermodynamics[M]. Hefei: University of Science and Technology of China Press, 2011: 1-2

[2] Candler G, Park C. The Computation of Radiation from Nonequilibrium Hypersonic Flows[C]// Thermophysics, Plasmadynamics and Lasers Conference. San Antonio: AIAA, 1988: 1-12

[3] Feldick A. Coupled Nonequilibrium Flow, Energy and Radiation Transport for Hypersonic Planetary Entry[D]. Park: The Pennsylvania State University, 2013

[4] GAO Tiesuo, JIANG Tao, DING Mingsong, et al. Numerical Study of Radiative Heating Influence on Aerothermal Environment over a Reentry Capsule[J]. Acta Aerodynamic Sinica, 2015, 33(1): 36-41

[5] Wang J Y, Gao Z X, Lee C H. An Iterative Technique for Coupled Conduction-Radiation Heat Transfer in Semitransparent Media[J]. Numerical Heat Transfer, Part A: Applications, 2015, 67(11): 1208-1231

[6] Modest M F. Radiative Heat Transfer[M]. San Diego: Academic Press, 2003: 423-432

[7] Anderson J D. Hypersonic and High-Temperature Gas Dynamics[M]. New York: McGraw-Hill Book Company, 1989: 653-674

[8] WANG Jingying. Numerical Study on Coupled Chemical Nonequilibrium and Thermal Radiation Effects in High Speed and High Temperature Flows[D]. Beijing: Beihang University, 2015

[9] Wang J Y, Gao Z X, Lee C H, et al. A Decoupled Procedure for Convection-Radiation Simulation in Scramjets[J]. Science China: Technological Science, 2014, 57(12): 2551-2566

[10] Hao J A, Wang J Y, Lee C H. Numerical Study of Hypersonic Flows over Reentry Configurations with Different Chemical Nonequilibrium Models[J]. Acta Astronautica, 2016, 126: 1-10

[11] Park C. Nonequilibrium Hypersonic Aerothermodynamics[M]. New York: Wiley, 1990

[12] Gupta R N, Yos J M, Thompson R A, et al. A Review of Reaction Rates and Thermodynamic and Transport Properties for an 11-Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30000 K[C]// Technical Report. Washington: NASA, 1990: 1-73

[13] Bertin J J, Cummings R M. Critical Hypersonic Aerothermodynamic Phenomena[J]. Annual Review of Fluid Mechanics, 2006, 38: 129-157

Note: Figure translations are in progress. See original paper for figures.