The Pennsylvania State University
The Graduate School
Department of Aerospace Engineering

MODELING AND SIMULATION OF RADIATION FROM
HYPERSONIC FLOWS WITH MONTE CARLO METHODS

A Dissertation in
Aerospace Engineering

by

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Abstract

During extreme-Mach number reentry into Earth’s atmosphere, spacecraft experience hypersonic non-equilibrium flow conditions that dissociate molecules and ionize atoms. Such situations occur behind a shock wave leading to high temperatures, which have an adverse effect on the thermal protection system and radar communications. Since the electronic energy levels of gaseous species are strongly excited for high Mach number conditions, the radiative contribution to the total heat load can be significant. In addition, radiative heat source within the shock layer may affect the internal energy distribution of dissociated and weakly ionized gas species and the number density of ablative species released from the surface of vehicles. Due to the radiation total heat load to the heat shield surface of the vehicle may be altered beyond mission tolerances. Therefore, in the design process of spacecrafts the effect of radiation must be considered and radiation analyses coupled with flow solvers have to be implemented to improve the reliability during the vehicle design stage.

To perform the first stage for radiation analyses coupled with gas-dynamics, efficient databasing schemes for emission and absorption coefficients were developed to model radiation from hypersonic, non-equilibrium flows. For bound-bound transitions, spectral information including the line-center wavelength and assembled parameters for efficient calculations of emission and absorption coefficients are stored for typical air plasma species. Since the flow is non-equilibrium, a rate equation approach including both collisional and radiatively induced transitions was used to calculate the electronic
state populations, assuming quasi-steady-state (QSS). The Voigt line shape function was assumed for modeling the line broadening effect. The accuracy and efficiency of the databasing scheme was examined by comparing results of the databasing scheme with those of NEQAIR for the Stardust flowfield. An accuracy of approximately 1% was achieved with an efficiency about three times faster than the NEQAIR code.

To perform accurate and efficient analyses of chemically reacting flowfield-radiation interactions, the direct simulation Monte Carlo (DSMC) and the photon Monte Carlo (PMC) radiative transport methods are used to simulate flowfield-radiation coupling from transitional to peak heating freestream conditions. The non-catalytic and fully catalytic surface conditions were modeled and good agreement of the stagnation-point convective heating between DSMC and continuum fluid dynamics (CFD) calculation under the assumption of fully catalytic surface was achieved. Stagnation-point radiative heating, however, was found to be very different. To simulate three-dimensional radiative transport, the finite-volume based PMC (FV-PMC) method was employed. DSMC-FV-PMC simulations with the goal of understanding the effect of radiation on the flow structure for different degrees of hypersonic non-equilibrium are presented. It is found that except for the highest altitudes, the coupling of radiation influences the flowfield, leading to a decrease in both heavy particle translational and internal temperatures and a decrease in the convective heat flux to the vehicle body. The DSMC-FV-PMC coupled simulations are compared with the previous coupled simulations and correlations obtained using continuum flow modeling and one-dimensional radiative transport.

The modeling of radiative transport is further complicated by radiative transitions occurring during the excitation process of the same radiating gas species. This
interaction affects the distribution of electronic state populations and, in turn, the radiative transport. The radiative transition rate in the excitation/de-excitation processes and the radiative transport equation (RTE) must be coupled simultaneously to account for non-local effects. The QSS model is presented to predict the electronic state populations of radiating gas species taking into account non-local radiation. The definition of the escape factor which is dependent on the incoming radiative intensity from overall all directions is presented. The effect of the escape factor on the distribution of electronic state populations of the atomic N and O radiating species is examined in a highly non-equilibrium flow condition using DSMC and PMC methods and the corresponding change of the radiative heat flux due to the non-local radiation is also investigated.
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Nomenclature

$A$ Einstein coefficient for spontaneous emission, s$^{-1}$,

or a chemical species symbol

$A(i, j)$ Einstein coefficient for spontaneous emission from state $i$ to state $j$, s$^{-1}$

$A(c, i)$ Einstein coefficient for spontaneous emission from continuum state to state $i$, cm$^3$s$^{-1}$

$A(i, c)$ Einstein coefficient for photoionization from state $i$ to continuum state, s$^{-1}$

$a_0$ Bohr radius, 5.29167 × 10$^{-9}$ cm

$B$ Einstein coefficient for stimulated emission and absorption, (cm$^3$-µm)/(J-s),

or a chemical species symbol

$BP$ breakdown parameter

$BV_U$ rotational constant, cm$^{-1}$

$b$ exponent, dimensionless

$b_{hw}$ line half width, Å

$c$ speed of light, 2.9979 × 10$^{10}$ cm s$^{-1}$

$\tilde{C}$, $\tilde{D}$ vector assembled by excitation rate coefficients of atom

$\tilde{C}_m$, $\tilde{D}_m$ vector assembled by excitation and dissociation rate coefficients of molecule

$D$ a photon traveling distance, cm

$d$ parameter in the Voigt width, dimensionless (See Eq. (4.4))

$d_{ff}$ correction factor for free-free radiation, dimensionless

$D_w$ Doppler line half width, cm

$e$ electron charge, 4.8030 × 10$^{-10}$ statcoul
$E$ radiative energy, W

$E_{abs}$ radiative energy absorbed by cell, W

$E_{bundle}$ radiative energy carried by photon bundle, W

$E_{emis}$ total emission energy, $W/cm^3$

$E_i$ electronic term energy for atomic level $i$, $cm^{-1}$

$E_k$ kinetic energy of free electron, $cm^{-1}$

$E_{trans}$ transmitted radiative energy, W

$E_\infty$ ionization energy of an atom, $cm^{-1}$

$\Delta E$ net kinetic energy of a free electron, $cm^{-1}$

$F$ rotational term energy for a molecule, $cm^{-1}$

$F_i$ assembled collisional and radiative coefficient of electronic state $i$, dimensionless

$G$ vibrational term energy for a molecule, $cm^{-1}$

$G_i$ assembled collisional and radiative coefficient of electronic state $i$, dimensionless

$G_\lambda$ incoming radiative intensity integrated over all directions, $W/cm^2-\mu m$

$GF$ Gaunt factor for bound-free radiation, dimensionless

$g$ degeneracy, dimensionless

$H$ data points of electron number density and electron temperature

$\Delta H$ data point interval

$h$ Planck’s constant, $6.6262 \times 10^{-34} Js$

$I_H$ ionization potential of atomic hydrogen, $109.679 cm^{-1}$

$I_\lambda$ radiative intensity, $W/cm^2-\mu m-sr$

$J$ rotational quantum number, dimensionless
$j$ data point index  

$K_n$ Knudsen number, dimensionless  

$K^{e\,(i,j)}$ excitation rate coefficient of collisional transition from state $i$ to state $j$ by electron impact, cm$^3$s$^{-1}$  

$K(i,c)$ excitation rate coefficient of collisional transition from state $i$ to continuum state, cm$^3$s$^{-1}$  

$K(c,i)$ recombination rate coefficient of collisional transition from continuum state to state $i$, cm$^6$s$^{-1}$  

$K_{Wi}$ heavy particle induced recombination rate coefficient, cm$^3$s$^{-1}$  

$K^{e\,ci}$ electron induced recombination rate coefficient, cm$^3$s$^{-1}$  

$K_{W(i,j)}$ heavy particle induced molecular excitation rate coefficient from state $i$ to state $j$, cm$^3$s$^{-1}$  

$k_B$ Boltzmann’s constant, $1.3806 \times 10^{-23}$ JK$^{-1}$  

$k,k_1,k_2$ line-center index, dimensionless  

$L$ nose radius of the Stardust blunt body, m  

$l$ number of electronic states for bound-free transition,  

$l_{1,2}$ ratio between face endpoints, m  

$l_m$ number of electronic state energy levels for diatomic QSS, dimensionless  

$Ma$ Mach number, dimensionless  

$M$ matrix assembled excitation rate coefficients of atom, or a chemical species symbol  

$M_m$ matrix assembled excitation and dissociation rate coefficients of molecule
m  mass, kg
max  maximum value of vibrational or rotational line, dimensionless
N  number density, cm$^{-3}$
$N_i$  number density of electronic state $i$, m$^{-3}$
$N_{\text{rays per cell}}$  number of rays emitted from one cell
$N_{\text{total rays}}$  initial total number of rays
$n$  principal quantum number, dimensionless
$n_a$  atom number density, m$^{-3}$
n_e  electron number density, m$^{-3}$
n_+  ion number density, m$^{-3}$
P  number of data points
Q  partition function, dimensionless
$Q_{\text{emis}}$  total integrated emission coefficient, W/cm$^3$-sr
$Q_{\text{emis},k}$  accumulated atomic emission lines from $i = 1$ to $k$, W/cm$^3$-sr
$Q_{\text{emis},\lambda}$  partially integrated emission coefficient, W/cm$^3$-sr
$q_{V_UV_L}$  Franck Condon factor, dimensionless
$q_c$  convective heat flux, W/m$^2$
$q_R$  radiative heat flux, W/m$^2$
R  transition moment, statcoul-cm
$R$  random number, dimensionless
$R_c$  radius of curvature, m
Re  electronic transition moment for a vibrational band ($V_U$, $V_L$)
normalized by $ea_0$, dimensionless

$r$ radial component of photon travel distance in a cell, m

$r_c$ internuclear distance, unit of length, not explicitly evaluated

$S$ distance from stagnation point, m

$S_{J_UJ_L}$ rotational line strength factor, dimensionless

$S_c$ source function, W/cm²-μm-sr

$S_d$ distance from emission point to cell face intersection point, m

$s_x, s_y, s_z$ unit directional cosines in a Cartesian coordinate system

$T_{trn}$ translational temperature, K

$T_{rot}$ rotational temperature, K

$T_{vib}$ vibrational temperature, K

$T_e$ electron temperature, K

$T_{eU}$ upper state electronic energy of the term symbol for molecular radiation, cm⁻¹

$T_{eL}$ lower state electronic energy of the term symbol for molecular radiation, cm⁻¹

$t$ time, s

$V$ vibrational quantum number, dimensionless

$V_{cell}$ cell volume, m³

$V_\infty$ freestream velocity, m/s

$w_l$ Lorentzian width, Å

$w_g$ Gaussian width, Å

$w_s$ Stark width, Å

$w_{s,0}$ reference Stark width, Å
$w_v$  
Voigt width, Å

$X$  
horizontal coordinate of DSMC computational domain for the Stardust geometry, m

$x_i, y_i, z_i$  
intersection points of a photon bundle with a cell face, m

$x_e, y_e$  
emission locations, m

$x_1, x_2$  
coordinates of cell boundary along X-axis, m

$X_{i,\text{data}}$  
emission or absorption coefficients from the database

at the $i$-th wavelength data point

$X_{i,\text{NEQ}}$  
emission or absorption coefficients from NEQAIR

at the $i$-th wavelength data point

$Y$  
vertical coordinate of DSMC computational domain for the Stardust geometry, m

$y_1, y_2$  
coordinates of cell boundary along Y-axis, m

$\alpha$  
optical length, dimensionless

$\varepsilon_i$  
emission coefficient of a bound-bound transition

at the line-center wavelength, W/cm$^3$-sr

$\varepsilon_{\lambda}$  
emission coefficient, W/cm$^3$-µm-sr

$\varepsilon_{\lambda}^c$  
assembled parameter for emission coefficient, W/sr

$\theta$  
polar angle, radian

$\kappa_{\lambda}$  
absorption coefficient, cm$^{-1}$

$\kappa_{\lambda}^c$  
assembled parameter for absorption coefficient, cm$^3$

$\lambda$  
wavelength, Å

$\lambda_1$  
wavelength where line broadening starts, Å

$\lambda_2$  
wavelength where line broadening ends, Å
\[ \lambda_{k_1} \] wavelength at line-center index \( k_1, \text{Å} \)

\[ \lambda_{k_2} \] wavelength at line-center index \( k_2, \text{Å} \)

\[ \nu \] frequency, s\(^{-1}\)

\[ \tilde{\nu} \] transition energy of emitted photon, cm\(^{-1}\)

\[ \Omega \] solid angle, sr

\[ \Delta \lambda \] distance from line center, Å

\[ \tilde{\nu} \] wavenumber, cm\(^{-1}\)

\[ \rho \] mass density, kg/m\(^3\)

\[ \rho_i \] ratio of non-equilibrium to equilibrium population of electronic state \( i \), dimensionless

\[ \rho_{ij} \] escape factor of transition from state \( i \) to state \( j \), dimensionless

\[ \rho_{\infty} \] freestream mass density, kg/m\(^3\)

\[ g \] collision rate

\[ \sigma \] standard deviation

\[ \sigma_{\lambda H} \] ionization cross-section of hydrogen atom, cm\(^2\)

\[ \sigma_{\lambda}^{bf} \] bound-free absorption cross-section, cm\(^2\)

\[ \sigma_{H}^{ff} \] hydrogenic free-free cross-section, cm\(^5\)

\[ \tau_{\lambda} \] optical thickness, dimensionless

\[ \phi_{\lambda} \] line broadening function, \( \mu \text{m}^{-1} \)

\[ \chi \] ratio of summation of non-equilibrium electronic state populations to that of equilibrium state, dimensionless

\[ \Psi \] vibrational wave function, units of length\(^{-1/2}\), not explicitly evaluated
\( \varphi \) \quad \text{cell face intersection angle, radian}

\( \psi \) \quad \text{azimuthal angle, radian}

**Subscripts**

\( a \) \quad \text{atom}

\( b \) \quad \text{blackbody}

\( c \) \quad \text{line-center}

\( \text{cell} \) \quad \text{computational cell}

\( \text{cross section} \) \quad \text{cell cross-section}

\( e \) \quad \text{electron}

\( \text{emis} \) \quad \text{emission}

\( \text{end} \) \quad \text{ending data}

\( E \) \quad \text{equilibrium state}

\( H \) \quad \text{hydrogenic}

\( i,j \) \quad \text{index of electronic state, or index of cell}

\( \text{init} \) \quad \text{initial data}

\( k \) \quad \text{kinetic}

\( L \) \quad \text{lower state}

\( LU \) \quad \text{lower to upper state}

\( W \) \quad \text{heavy particle}

\( m \) \quad \text{molecule}

\( \text{max} \) \quad \text{maximum value}

\( \text{min} \) \quad \text{minimum value}
min  cutoff limit
NEQ  NEQAIR
n  principal quantum number
R  rotational state
total  all cells of computational domain
U  upper state
UL  upper to lower state
V  vibrational state
θ  polar angle
λ  wavelength
ψ  azimuthal angle
+  ion
∞  ionization, or freestream

Superscripts
bf  bound-free
c  constant
e  electronic state
ff  free-free
rad  radiative transition
*  normalized quantity
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Chapter 1

Introduction

1.1 Background

For high-speed reentry into Earth’s atmosphere, spacecraft such as Stardust[1, 2, 3, 4, 5, 6], Crew Exploration Vehicle[7], or MUSES-C[8] experience hypersonic non-equilibrium flow conditions where molecules are dissociated and atoms are weakly ionized. These complex phenomena occurring behind the shock wave lead to high temperature flows and ionization that generate a severe heating load on the thermal protection system (TPS) and cause radar communications blackout to the vehicle.[9] Since the internal energy states of atomic species are strongly excited for high Mach number conditions, the radiative contribution to the total heat load becomes significant.[10] In fact, the radiative heating to the stagnation region can readily exceed the convective heating rates at superorbital reentry velocities.[11] In addition, radiative energy within the shock layer may affect the macroscopic flow properties and internal energy distribution of dissociated and weakly ionized air species and ablative products released from the surface of vehicles. Due to the radiation total heat load to the heat shield surface of the vehicle may be altered beyond mission constraints. Therefore, the effect of radiation on the flowfield and TPS must be taken into account and radiation analyses coupled with flow solvers have to be implemented to improve the reliability of the vehicle design stage.
The radiative heat loads resulting from high temperature gases have been an area of significant research over the past fifty years with the goal of developing spacecraft TPS, that can withstand the severe flow conditions such as high temperature and air plasma. The field has progressed by developing accurate numerical and experimental methods for aerodynamics and chemistry modeling to predict chemical reactions in high temperature gas dynamics. Zhigulev et al.[12] carried out a systematic examination of the effect of radiation under a high temperature gas flow past a vehicle body by a theoretical approach. It was verified that radiation contributed to the change of the characteristics of hypersonic flows around the vehicle - especially at the temperature and the species concentration of the radiating gas flow. The influence of radiation to convective heating was studied by Goulard[13] using approximate inviscid flowfields with transparent or gray-gas radiation, estimating that the flowfield temperature decreased and the convective heat transfer was also reduced as a result of radiative cooling effects. Viscous flowfields coupled with equilibrium gas radiation were studied to examine the effect of radiation cooling and contribution of the convective and radiative heating to an ablating body[14]. In that work, only the absorption coefficients of continuum radiation were employed for atomic radiation and the smeared band model was used for evaluating the molecular line absorption coefficients.

In the 1970s, non-gray equilibrium radiation models were adopted to the radiative heating problem for the entry into Earth and other planetary atmospheres. Moss[15] performed radiative viscous shock layer calculations with a coupled ablation injection model in the Earth reentry equilibrium flowfields surrounding axisymmetric blunt bodies. A non-gray radiation model including atomic line and continuum transitions were used in
that work. It was found that an ablation injection rate greater than 0.2 kg/s resulted in only small additional reductions in the surface heating. The investigation of stagnation region radiative heating for Venus entry was carried out using coupled viscous shock layer equations with a non-gray radiation model by Page et al.[16] and Sutton et al.[17]. Sutton applied a coupled inviscid and boundary layer approach with an equilibrium line-by-line radiation model for Venusian entry[18] and outer planet entry[19]. He showed that the radiative heat flux toward the body was attenuated in the boundary layer of the downstream regions of the body as well as at the stagnation point, and the attenuation of radiation by the boundary layer reduced the radiative heating to the body by 10 - 20 % for the Venusian entry conditions.

Perhaps the most of significant development of non-equilibrium radiation in air[20, 21] and thermo-chemical non-equilibrium kinetics models[22, 23, 24, 25] was made by Park in the 1980 and 1990s. Two temperature kinetic model has been widely used to calculate chemical reactions in Navier-Stokes flow solvers[26, 27]. In that model, the rotational temperature of molecules is assumed to be identical to the heavy particle translational temperature and the electron-electronic temperature is identical to the vibrational temperature. The activation temperature for chemical reactions among molecules was defined by a weighted product of the translational and vibrational temperatures. This model, however, cannot explain directly the electron temperature, which was assumed to be identical to the vibrational temperature. Since the electron temperature is an important parameter for both equilibrium and non-equilibrium radiation calculations, its modeling electron is crucial.
More recently, atomic and molecular radiation models have been improved by the development of sophisticated spectroscopic databases and the prediction modeling of excited state population for electronic, rotational and vibrational energy modes. Hypersonic non-equilibrium flowfield and radiation modeling have been performed for the analysis of Stardust and Fire II vehicles, using established radiation models such as the Langley Optimized Radiative Nonequilibrium (LORAN) code and the Nonequilibrium Air Radiation (NEQAIR) code. In addition, coupled flowfield-radiation interactions have been also performed for the Huygens probe for conditions close to peak heating for reentry into Titan atmosphere, Saturn’s largest moon. In that study, the viscous shock layer (VSL) technique for the calculation of the stagnation region of the flow and a modified smeared-rotational band model for the radiation calculation were combined to reduce CPU time rather than solving the full Navier-Stokes equations and a line-by-line radiation model such as LORAN and NEQAIR. The approach provided frequency-integrated heat flux values within 5% of a line-by-line calculation over a range of conditions for Huygens entry.

Recently, closely coupled radiation calculations with advanced hypersonic continuum fluid dynamics (CFD) tools such as DPLR and LAURA and a newly developed efficient line-by-line radiation database based on NEQAIR have been performed for the Stardust and Fire II reentry conditions. A one-dimensional tangent slab (TS) method to solve the radiative transport equation (RTE), using the exact analytical solutions based on exponential integrals was used. The coupled CFD-radiation
studies assumed the governing electronic temperature to be equal to the heavy particle translational temperature (in the case of DPLR) or the vibrational temperature (LAURA).

However, under transitional flow conditions, continuum breakdown occurs.[39] Therefore, kinetic methods, such as direct simulation Monte Carlo (DSMC)[40], are required to simulate high Mach number reentry flowfields. Modeling of chemical reactions including ionization and energy exchange processes was successfully implemented in DSMC for the Stardust blunt body between 68.9 and 100 km altitudes,[41] but radiation coupling was not considered. Since the electronic excited state populations of atoms are produced predominantly due to collisions with electrons, an accurate model of the molecular nitrogen collisions with electrons was included in the DSMC simulations of Ref. [41]. This model is also useful for radiation coupling analyses because the precise modeling of electron temperature is needed to accurately simulate the vacuum-ultraviolet (VUV) shock layer radiation. In other DSMC simulations, Gallis and Harvey[42, 43] modeled non-equilibrium thermal radiation as well as electronic excitation processes to investigate the radiation effect on the flowfield. However, for their method, accurate cross-sections for electronic excitation and absorption coefficients were required and the uncertainty in these cross-sections could not be assessed for all the required species and electronic states. Recently, state-specific electronic state excitations for a few key energy levels of atomic N and O species have been modeled in DSMC, and applied to the stagnation-point radiative heat flux calculation.[44, 45]

In the simulation of coupled hypersonic shock layer radiation, the fidelity of both the gas dynamic approach as well as the RTE must be considered. The statistical
radiative transport using the photon Monte Carlo (PMC) approach has been successfully used to simulate radiation for arbitrarily complex geometries and flow conditions.[46, 47, 48] The approach is basically three-dimensional and is important for modeling radiative transport in optically thick media where the optical thickness gradients may be quite high. The PMC approach may be applied to both continuum and particle-based gas dynamic methods. When closely coupled with a flowfield solver, the advantage of a fully three-dimensional method over the one-dimensional tangent slab approach is to account for the fact that the radiation transport is non-local. The disadvantage of this model is that the computational cost for coupling with the flow solver is more expensive than a tangent slab (TS) approximation. Therefore in preliminary analyses and design processes of simple geometries TS may be preferred compared to PMC, but, its accuracy should be calibrated.

DSMC simulations were loosely coupled with the particle-based photon Monte Carlo (p-PMC) method for Stardust reentry flow conditions.[49] To efficiently solve the radiative transport for the highly non-equilibrium gas, emission and absorption coefficient databases[35, 50] based on the NEQAIR model were generated. For Earth reentry under those conditions, atomic nitrogen and oxygen radiation are the major contributions to the total radiation.[4, 5, 49]. In DSMC-p-PMC coupled simulations[49], the influence of the radiative energy on the flowfield characteristics was considered. However, the computational load for the loosely coupled DSMC-p-PMC calculations was very high and is not easily extended to modeling the freestream conditions along a reentry trajectory. Coupled CFD-radiation simulations are also computationally intensive. Therefore, to improve the PMC radiative transport efficiency, a two-dimensional, axisymmetric finite
volume-based photon Monte Carlo (FV-PMC) method was developed for a structured body-fitted grid and coupled with a CFD solver to simulate flowfield-radiation interaction during the reentry. In the FV-PMC method, the emissive energy associated with an energy bundle is based on the cell properties rather than on computational particles. Since both the emissive energy and the absorption coefficient are based on the macroparameters of particle number density and temperature, the use of cell-based quantities is not a limitation of the method. Similarly, the absorption of a photon bundle is calculated based on the cell-averaged absorption coefficient rather than on the intersection of photon bundles with computational particles.

1.2 Objectives of This Work

The first objective of the present work is to develop efficient databasing schemes to generate spectral emission and absorption coefficients for a given flow condition. NASA air radiation codes such as LORAN code and NEQAIR code have been widely used in both equilibrium and non-equilibrium hypersonic air radiation research. However, these computational tools are not sufficiently flexible to be employed directly in a coupled flow-radiation study because they have been developed for use in stand-alone, an uncoupled radiation modeling. In addition, large computational times are required when one solves the radiative transport equation by one-dimensional TS approximation for a two or three-dimensional case. To solve the RTE using the TS method, the determination of spectral resolution also can be an important factor in obtaining an accurate spectral radiation solution independent of the spectral resolution. Therefore, new schemes for radiation calculations, which can be coupled with flow solvers accurately and efficiently,
are needed to examine the effect of radiation on the complex reentry flow physics. These new databasing schemes developed in the thesis research produce spectral emission and absorption coefficients for any given flow condition efficiently. The generated emission and absorption coefficients are used to solve the RTE using either TS approximation or PMC ray tracing schemes. The collisional-radiative modeling is used to calculate the electronic state population for the non-equilibrium gas conditions in these databasing schemes. They also provide the spectral emission and absorption coefficient values for any given wavelength or frequency, which is suitable for the random wavelength selection portion in the PMC method.

The second goal of this work is to simulate transitional hypersonic flows using DSMC coupled with a finite-volume PMC radiation approach optimized for the DSMC Cartesian-based grid. With the ability to perform coupled simulations the effect of radiation on the flow structure for different degrees of hypersonic non-equilibrium are investigated. In addition, the change in convective and radiative heat fluxes along a reentry trajectory that extends from the rarefied through the continuum flow regime using DSMC are characterized. Specifically, in this work, the Stardust Sample Return Capsule (SRC) body, the fastest human-made object to reenter, is chosen and four altitudes along the reentry trajectory: 81 km (transitional flow regime), 71.9 km, 65.4 km (near-continuum) and 61.8 km (peak heating) conditions will be considered. Since these results are the first DSMC-coupled FV-PMC simulations to be performed along a reentry trajectory, comparisons will be presented with earlier CFD results as well as semi-empirical correlations. The former results have been computed assuming that the surface is fully catalytic with respect to atomic species recombination. Therefore to
compare the DSMC simulations of the convective heat flux to these earlier results, the extension of our DSMC gas-surface interaction model to include fully catalytic surface conditions is discussed.

The radiative transport is also closely related to excitation and de-excitation mechanisms of electronic states of radiating gas species in the high temperature gas layers.\cite{25, 29, 33, 52} In addition, the radiative transport calculation is characterized as non-local because the incident radiation at a specific point is determined by the radiative intensity transferred from every other locations. Hence, the radiative transition rate, which is dependent on the incoming radiative intensity, must be adjusted after solving the RTE. To simplify this complicated coupling phenomena, the escape factor is introduced.\cite{53, 54} The definition of the escape factor can be stated as the probability that a photon emitted from a given excited state at a specific point will not be re-absorbed.\cite{29, 53} The purpose of the escape factor is to adjust the optical transition rate used in the calculation of the electronic state populations. The third goal of this work is to establish the formulation of escape factor for atomic N and O species which are strong radiators of the Stardust reentry flow condition, and to investigate its effect on the distribution of electronic state populations and the corresponding radiative heat flux.

1.3 Thesis Structure

The structure of this thesis is as follows. Chapter 2 discusses the details of DSMC modeling for hypersonic non-equilibrium ionized flows. The methodologies to describe the dissociation and ionization of molecules within the shock layers are introduced. The
chemical reactions and energy exchange model among translational and internal energy modes are discussed. The DSMC simulations of the flowfield around the Stardust SRC forebody along its Earth reentry trajectory are presented. The modeling of atom recombination at the vehicle surface in DSMC, which determines the degree of surface catalycity, is introduced and the effects of surface catalytic modeling on the convective heat flux are discussed.

Chapter 3 presents basic concepts of radiation from atoms and molecules in a high temperature gas environment. Three types of radiation from atomic species-bound-bound, bound-free continuum, and free-free continuum are introduced in detail in this chapter. In addition, for diatomic molecules, the basic relations of the Einstein transition probability with formulations of electronic and vibronic transition moments are presented. The master equation for collisional-radiative transitions among electronic states is discussed to explain the modeling of electronic state populations of atoms and molecules. Emission and absorption coefficient relations for a given macroscopic flow condition are discussed to develop the strategy of efficient databasing scheme applicable to the radiative transport calculation. The general concepts of TS and PMC method to solve the RTE are also introduced.

Chapter 4 presents the newly developed databasing schemes for generating emission and absorption coefficients to model radiation from hypersonic flows. The databasing schemes for atomic and molecular gas species are described separately. The validation of the emission and absorption coefficients calculated from new databasing schemes for a given local flow condition is performed by comparing with those from NEQAIR. The
total emission and radiative heat source term calculated from the database are also compared with those from NEQAIR for the gas conditions taken from the Stardust reentry flows computed by CFD and DSMC methods.

Chapter 5 presents the coupled DSMC simulations with finite volume PMC (FV-PMC) approach for the Stardust reentry flows. First, the ray tracing scheme of FV-PMC method combined with the wavelength selection schemes for a non-gray gas medium is discussed. For the transitional to peak-heating regimes of the reentry trajectory, the FV-PMC calculations use the flowfield data obtained from DSMC method. To validate the FV-PMC method for the DSMC cartesian macroparameter coordinates system, the results of FV-PMC for 1-D disk gas medium is compared to one-dimensional TS method. The effects of radiation on the flowfield are examined for all flow regimes and the change of translational and internal temperatures within the shock layers and convective heat flux to the surface due to the radiation are also demonstrated. Finally, a trajectory study of convective-radiative heating rates to the stagnation point of the Stardust SRC blunt body is carried out by comparing with other gas dynamic-radiation coupling calculations that used CFD and other radiation models.

Detailed approaches to calculate the escape factor and the effect of escape factor on the flowfield of Stardust SRC at 81 km altitude will be presented in Chapter 6. The DSMC simulation was performed for the entire flowfield around Stardust SRC body. To model the two-dimensional axisymmetric radiative transport, the FV-PMC method was adopted to simulate radiation. The QSS module used in the NEQAIR model was used to calculate the electronic state populations of atomic N and O species and was coupled with FV-PMC to implement the non-local collisional-radiative steady states and
the escape factor. The calculation procedure of coupled QSS-PMC is outlined and the effects of the escape factor on the electronic state populations along selected lines normal to the vehicle surface are presented. Finally, the effect of escape factor on the radiative heating rate to the surface will be discussed.

Chapter 7 summarizes the conclusions drawn from the entirety of this research.
Chapter 2

DSMC Simulation of Weakly Ionized Hypersonic Reentry Flows

2.1 Preface

The Direct Simulation Monte Carlo (DSMC) method has been widely used to simulate transitional and non-equilibrium gas flows such as rarefied hypersonic atmospheric flows, growth of thin films in material processing, plume expansion flows and microsystem applications.[55] In this chapter, numerical schemes for implementations of chemical reactions among the charged and neutral species and energy exchange model of gas species in hypersonic atmospheric reentry flows are discussed. The flowfield results of the Stardust SRC body for various freestream conditions from transitional to peak heating simulated by the DSMC method are presented. Atom recombination processes at the vehicle surface to represent a fully catalytic surface condition are implemented in DSMC and the effect of surface catalycity on the distribution of mole fraction and on the convective heating rate to the vehicle surface is investigated.

2.2 Introduction to Rarefied Flow Modeling by DSMC

The modeling of chemically reacting flows during the atmospheric entry of Earth or other planets has been studied through the continuum approach. Recently, hypersonic continuum fluid dynamics (CFD) codes with chemical reaction models have been
employed to simulate the Stardust SRC body and to investigate the impact of convective-radiative heating on the TPS with phenolic-impregnated carbon ablator (PICA) and the change of aerobrake heat shield shape.[1, 2] For a continuum model to be valid in a strong shock condition, it needs to satisfy the conditions of two parameters, the Knudsen number and breakdown parameter. The Knudsen number, $K_n$, is obtained by the ratio of the mean free path to a characteristic length. The freestream Knudsen number at 61.8 km through 81 km of the Stardust reentry are listed in Table 2.1, and at these altitudes, $K_{n,\infty}$ is less than 0.01. The continuum model breaks down with the initial symptom being that the pressure tensor becomes anisotropic if the density gradient is too high.[41] A breakdown parameter $BP$ may be calculated from the following expression

$$BP = \frac{1}{\varrho} \left| \frac{D}{Dt} \ln(\rho) \right|$$

(2.1)

where $\varrho$ is the collision rate, $\rho$ is the density and $t$ is the time. For Stardust reentry flow conditions, the continuum assumption breaks down at altitudes higher than 61.8 km.[39, 41] Therefore, to model the flow around the vehicle at these altitudes and speeds, kinetic method such as DSMC is required. The breakdown of the continuum approximation will affect the shock characteristics such as a thickness and a standing off distance as well as the modeling of thermo-chemical non-equilibrium.
2.3 DSMC Simulations for Hypersonic Reentry Flows around Stardust Sample Return Capsule Body

To model a hypersonic reentry flow a number of physical models related to the ionized, chemically reacting flow as well as the thermo-chemical non-equilibrium must be considered. Flows were simulated using the Statistical Modeling In Low-density Environment (SMILE)[56] DSMC computational tool. The majorant frequency scheme was employed for modeling the molecular collision frequency[57], and the variable hard sphere (VHS) model was used for modeling the interaction between particles.[58] The Borgnakke-Larsen (BL)[59] model with temperature-dependent rotational and vibrational relaxation numbers was used for modeling rotation-translation (R-T) and vibration-translation (V-T) energy transfer between neutral species. The Millikan and White (MW)[60] and Parker’s rates[61] were used to model V-T and R-T relaxation rates, respectively. At high temperatures, both vibrational and rotational collision numbers should converge to a similar constant number due to the strong vibration-rotation coupling. The MW vibrational collision number however implies an unrealistically large cross-section for vibrational relaxation at high temperature. Therefore, the vibrational excitation cross-section for nitrogen was adjusted to ensure that the V-T collision numbers are consistent with the rotational collision number.[24]

Chemical reactions involving both neutral and charged species were modeled using the total collision energy (TCE) model[40] with a total of 11 species (N, O, N⁺, O⁺, N₂, O₂, NO, N₂⁺, O₂⁺, NO⁺, and e⁻) modeled in 54 chemical reactions including 5 ionization processes.[25, 62] In DSMC simulation, ionization processes were considered
as chemical reactions, and thus, the TCE model is also used for these processes. The electron concentration in the flow is sufficiently low such that the computational time step is associated with molecular collisions rather than with the electron collision frequency. In our simulations, the electron movement depends on the average ion velocity per cell, and the charge neutrality assumption was used.[41] The electron velocity, or energy, is concurrently stored per simulated electron and is used to calculate the collision frequency, energy exchange, and chemical reaction rates between electrons and heavy particles. Electron-vibrational (e-V) relaxation was modeled using Lee’s relaxation model for electron collisions with N₂.[63] Finally, the gas-surface interaction was modeled using the Maxwell model with total energy and momentum accommodation. The surface wall temperature was assumed to be 3,000 K along the vehicle surface for all altitudes[4], and full charge recombination at the vehicle surface, a standard assumption in weakly ionized flows, was assumed.[64]

DSMC simulations were performed for the Stardust SRC blunt body geometry shown in Fig. 2.1 with the free stream conditions given in Table 2.1. The selection of time step, cell size, computational domain, and total number of simulated molecules was investigated to obtain results independent of these DSMC numerical parameters. Table 2.1 summarizes the number of simulated particles and collisional and macroparameter sampling cells used for the four altitude cases. The total number of time steps was about 100,000 with a time step of $2.0 \times 10^{-8}$ s used for the 81 to 65.4 km cases and $1.0 \times 10^{-8}$ s used for the 61.8 km case. Macroparameter sampling was started after 30,000 time steps, which was a sufficient time for the flowfield and heat flux to reach
steady state. In summary, heat flux values along the surface and flow macroparameters were found to be converged for these numerical parameters.

As will be shown in the next section, the flow consists mainly of atomic N and O within the shock layer of the Stardust vehicle. The collision rate between free electrons and atomic and molecular species in a cell is sufficiently high such that it can be assumed that the energy exchange between free electrons and the internal energies of heavy species is fast and completed in a single time step. Therefore, for the coupled DSMC flowfield-radiation simulations, the radiative heat source term, $\nabla \cdot q_R$, calculated by the radiation solver is re-distributed among the translational and internal energy modes of gas species in proportion to the degree of freedom of the translational, rotational, and vibrational modes[49]. The DSMC simulation employs a collisional level and a macroparameter level Cartesian grid structure. Radiative energy exchange is simulated at the collisional cell level, however, the radiative source term is obtained using the macroparameter cell values.

### 2.3.1 Flow Simulations for Stardust Forebody at 71.9 and 61.8 km altitudes

As mentioned above, the DSMC calculations were performed for the four freestream conditions given in Table 2.1. Figure 2.2 shows the profile of translational temperatures along the stagnation streamline at each altitude. It is clearly seen that the shock standoff distance increases as the altitude becomes higher because the flow rarefaction increases. A temperature overshoot is observed for altitudes below 71.9 km as the temperature profiles take on more continuum-like behavior. As we discuss below, the maximum internal temperatures are nearly 20,000 K for the lowest altitude considered. Thus as altitude
is lowered, the degree of thermal non-equilibrium decreases and the flow becomes more continuum-like. To understand the change in flow features at a more detailed level, two altitude cases, 71.9 and 61.8 km, were examined. The 71.9 km case is chosen instead of the highest altitude, 81 km, because there are a sufficient number of collisions that results in thermal excitation and ionization reactions in the stagnation region. Also, as will be discussed in Chapter 5, the radiation coupling at 81 km will be shown to be negligible.

Figures 2.3 through 2.4 show at 71.9 km the stagnation stream profiles of the flow temperatures and chemical species and contour fields in the forebody region for the electron number densities and temperatures, respectively. The degree of thermal non-equilibrium is strong with the maximum translational temperature as high as 60,000 K compared to the internal and electron temperatures being lower than 24,000 K. At this altitude, the difference among rotational, vibrational and electron temperatures is small. The simulations predict the temperature overshoot to be between \( X = -0.03 \) and \(-0.02\) m, but, the difference between the temperatures decreases to less than 10,000 K from \( X = -0.02\) to the wall. Due to the high dissociation rates, atomic neutrals followed by their ionic species are dominant in the shock and ionization occurs within \( X = -0.02\) m at this altitude. The maximum degree of ionization was found to be approximately 7 %, and the maximum electron temperature is about 22,000 K at this altitude.

The second set of DSMC calculations carried out at 61.8 km altitude correspond to peak-heating for the Stardust reentry trajectory. These computations are intensive for DSMC, but, were undertaken since the maximum radiation and heat flux to the surface occurs at this altitude. The flowfield at 61.8 km without radiation coupling along the
stagnation streamline is shown in Fig. 2.5. The difference between the translational temperature and the other internal temperatures is decreased at this altitude compared to higher altitudes, because the higher collision rate at this lower altitude brings the flow closer to thermal equilibrium. Similarly, the difference among rotational, vibrational and electron temperatures is negligibly small, and the maximum electron temperature is approximately 19,000 K. At this altitude, the overshoot phenomenon can be seen between $X = -0.02$ and $-0.015$ m, and the difference between translational and the other temperatures is less than 4,000 K between $X = -0.015$ and the wall. To compare DSMC with continuum method, DPLR flowfield results at 61.8 km in Ref. [36] were added into Fig. 2.5. It can be clearly seen that DPLR predicted a shorter shock standoff distance and lower internal temperatures than those of DSMC by a factor of two due to the difference of chemical reactions and energy exchange/relaxation modeling between DSMC and DPLR. The maximum values of atomic N and O concentrations within the shock layer are predicted nearly close to those of DSMC. Atomic N and O number densities are, however, observed to decrease near the surface because DPLR assumed the fully catalytic surface condition. Figure 2.6 shows contour plots of the electron number density and electron temperature. The regions of high electron number density and electron temperature are observed to be compressed as compared to 71.9 km altitude shown in Fig. 2.4, which produces high gradients of electron concentration and temperature. Due to the high dissociation rates, molecules are mostly dissociated inside the shock and the maximum degree of ionization is approximately 8 %.
2.3.2 Surface Catalytic Modeling in DSMC

In our previous DSMC flow modeling of the Stardust vehicle, charge recombination was assumed at the vehicle surface with no additional energy transfer to the flowfield or surface.[41, 49] This condition is also typically assumed in CFD simulations, however, for neutral atomic species collisions with the surface a surface catalycity model is usually specified. In particular, the spacecraft surface, depending on its material, can act as a catalyst to cause atomic oxygen and nitrogen recombination at the surface[4],

\[ O + O \rightarrow O_2 + 5.08 \text{ eV} \]  \hspace{1cm} (2.2)

\[ N + N \rightarrow N_2 + 9.8 \text{ eV} \]  \hspace{1cm} (2.3)

In a strong hypersonic shock layer there is a significant amount of molecular dissociation so that type of gas-surface model assumed will strongly affect the concentrations of atomic O or N, or their respective molecular diatomic species, in the boundary layer. In addition, the above recombination reactions are highly exothermic so that the convective heat flux to the surface can be significantly affected by the surface catalytic model as well. Since the DSMC simulations presented here were applied to freestream conditions close to peak heating, they will be compared with CFD simulations. In particular, the CFD simulations of Olynick et al.[1] were obtained using the common assumption of full catalytic recombination. To enable a closer comparison between the two different gas-dynamics approaches, the DSMC surface modeling was extended to include a full catalytic recombination. The assumption of a fully catalytic wall was implemented in the DSMC in the following manner. When DSMC particles representing atomic oxygen
or nitrogen atoms impact the surface, a second atomic oxygen or nitrogen atom particle is removed from that cell, the corresponding molecular species is created and introduced into the flow, and the heat of recombination is distributed among all particles within that cell and within that time step. The released energy from the atomic recombination is re-distributed among the translational, rotational and vibrational modes of all of the molecules (including those just formed during the time step). The distributions of energy among the different modes were performed assuming equi-partition. In subsequent time steps, this increased internal molecular energy due to recombination can be transferred to other species in the flow through collisions and increases the convective heat flux by gas-surface collisions.

Figure 2.7 shows the sensitivity of the predicted mole fractions and heat flux profiles for atomic O and N to a non-catalytic (baseline) versus the new fully catalytic surface conditions at 71.9 km altitude. It can be seen that due to the surface catalytic recombination processes given in Eqs. (2.2) and (2.3), the mole fractions of N₂ and O₂ increase, whereas those of N and O decreases near the surface as compared to those of N and O for the non-catalytic case. Figure 2.7 also shows a comparison of the convective heat flux along the forebody surface with and without surface catalytic recombination. Since heat is released during the surface recombination processes, the DSMC predicted convective heat flux correctly increases for a fully catalytic surface as compared to a non-catalytic condition.
Table 2.1. Freestream and DSMC Numerical Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>61.8 km</th>
<th>65.4 km</th>
<th>71.9 km</th>
<th>81.0 km</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freestream:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature, K</td>
<td>235.0</td>
<td>224</td>
<td>221.42</td>
<td>217.6</td>
</tr>
<tr>
<td>Number density, molec/m$^3$</td>
<td>$4.38 \times 10^{21}$</td>
<td>$1.60 \times 10^{21}$</td>
<td>$8.65 \times 10^{20}$</td>
<td>$2.64 \times 10^{20}$</td>
</tr>
<tr>
<td>Speed, km/s</td>
<td>11.4</td>
<td>12.0</td>
<td>12.4</td>
<td>12.6</td>
</tr>
<tr>
<td>O$_2$ mole fraction, %</td>
<td>20.6</td>
<td>22.1</td>
<td>23.7</td>
<td>23.7</td>
</tr>
<tr>
<td>N$_2$ mole fraction, %</td>
<td>79.4</td>
<td>77.9</td>
<td>76.3</td>
<td>76.2</td>
</tr>
<tr>
<td>Numerical:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$K_{n,\infty}(L = 0.23$ m)</td>
<td>$6.3 \times 10^{-4}$</td>
<td>$1.2 \times 10^{-3}$</td>
<td>$3.2 \times 10^{-3}$</td>
<td>$1.0 \times 10^{-2}$</td>
</tr>
<tr>
<td>Number of simulated particles</td>
<td>34.4 million</td>
<td>11.7 million</td>
<td>6.7 million</td>
<td>2.7 million</td>
</tr>
<tr>
<td>Number of collisional cells</td>
<td>3.5 million</td>
<td>1.1 million</td>
<td>0.68 million</td>
<td>0.26 million</td>
</tr>
</tbody>
</table>
Fig. 2.1. Stardust geometric configuration.

Fig. 2.2. Variation of translational temperature along the stagnation streamline from transitional to peak heating regime.
Fig. 2.3. Distributions of temperatures (top) and number densities (bottom) along the stagnation streamline at 71.9 km altitude.
Fig. 2.4. Contours of the electron number density (top) and electron temperature (bottom) at 71.9 km altitude.
Fig. 2.5. Distributions of temperatures (top) and number densities (bottom) along the stagnation streamline at 61.8 km altitude.
Fig. 2.6. Contours of the electron number density (top) and electron temperature (bottom) at 61.8 km altitude.
Fig. 2.7. Comparison of mole fraction of atomic N and O species (top) and convective heat flux along the Stardust forebody surface (bottom) due to surface catalytic recombination at 71.9 km altitude.
Chapter 3

Theory of Spectral Radiation
Modeling in Hypersonic Reentry Flows

3.1 Preface

Hypersonic vehicles reentering into Earth’s atmosphere generate non-equilibrium flows consisting of dissociated and weakly ionized air species. These typical conditions exist behind a high Mach number shock wave leading to high temperatures that affect operational flight issues related to thermal protection system materials and radar communications. In addition, due to the high Mach number, radiation has an important role in generating heat loads to the vehicle surface, with contributions sometimes as high as 18% of the convective heat[65]. Modeling the radiative sources in hypersonic shock layers and fluxes to a spacecraft is a complex task and as summarized in the Introduction some of the important radiation models have been developed in this field prior to this work.

The Langley Optimized Radiative Nonequilibrium (LORAN) code[28] and the Nonequilibrium Air Radiation (NEQAIR) code[29] have been used extensively in many atmospheric entry radiative simulations. NEQAIR includes atomic bound-bound, bound-free, free-free transition and line-by-line models for molecular bands. The LORAN model is similar to NEQAIR, and was developed to lower the computational cost of NEQAIR by using a smeared rotational band model for the molecular species. Both NEQAIR
and LORAN use the quasi-steady-state (QSS) assumption to determine the electronic state population. More recently, Johnston developed a radiation model that applied up-to-date atomic and molecular data for both the non-Boltzmann modeling of the radiating state and spectral distributions.[66, 67] In his model, an approximate atomic collisional radiative model was developed to calculate the electronic state populations of atomic species. For molecular radiation a simplified non-Boltzmann model for the molecular electronic state populations was developed by assuming that the contribution of electron-impact dissociation and heavy particle induced excitation processes may be neglected. The smeared rotational band model was chosen to reduce the computational cost for molecular radiation. In non-equilibrium flows, the radiation field may also affect the population of electronic states to the extent that a coupled radiative transport solution is required for an exact solution. Therefore, it becomes imperative to determine emission and absorption coefficients in an efficient manner such that a large number of solutions of the radiative transfer equation (RTE) may be performed.

In this chapter, the basic mechanisms of radiation from atoms and molecules are discussed in detail. Spectral emission and absorption coefficients of atoms and molecules for a given flow condition are formulated and the meaning of terms used in each formulation and assumptions are explained. The detailed collisional-radiative model for determining the distribution of electronic excited state population for both atomic and molecular species is also discussed. Finally, the tangent slab (TS) and finite volume-photon Monte Carlo (FV-PMC) methods for solving the RTE are introduced.
3.2 Concepts of Radiation from Atomic Species

3.2.1 Basic Relations of Radiation by Atomic Species

There are three radiative mechanisms in a radiating non-scattering medium: spontaneous emission, stimulated emission and absorption. The spontaneous spectral emission coefficient is defined as \[29\]

\[
\varepsilon_\lambda = g_U N_U A_{UL} h c \frac{1}{\lambda} \frac{1}{4\pi} \tag{3.1}
\]

Stimulated emission and absorption, unlike spontaneous emission, are caused by the presence of photons in the vicinity of the emitting or absorbing species. The effective volumetric absorption coefficient is obtained in terms of the stimulated emission and absorption coefficients, as given by \[29\]

\[
\kappa_\lambda = (g_L N_L B_{LU} - g_U N_U B_{UL}) \frac{h}{\lambda} \phi_\lambda \tag{3.2}
\]

Using detailed balance \[25, 29\], \(g_L B_{LU} = g_U B_{UL}\), the absorption coefficient expression can be reduced to

\[
\kappa_\lambda = (N_L - N_U) g_U B_{UL} \frac{h}{\lambda} \phi_\lambda \tag{3.3}
\]

Normalized emission and absorption coefficients can be defined by dividing Eqs. (3.1) and (3.3) by the number density of the radiating species, \(n_a\), giving,

\[
\varepsilon^*_\lambda = \frac{\varepsilon_\lambda}{n_a} = \varepsilon^c_\lambda \left( \frac{N_U}{n_a} \right) \phi_\lambda \tag{3.4}
\]
\[ \kappa_{\lambda}^* = \kappa_{\lambda} = \kappa_{\lambda}^c \left( \frac{N_L}{n_a} - \frac{N_U}{n_a} \right) \phi_{\lambda} \] (3.5)

where \( \varepsilon_{\lambda}^c \) and \( \kappa_{\lambda}^c \) are defined as

\[ \varepsilon_{\lambda}^c = g_U A_{UL} \frac{c}{\lambda^4} \] (3.6)

\[ \kappa_{\lambda}^c = g_U B_{UL} \frac{h}{\lambda} \] (3.7)

and

\[ B_{UL} = \frac{\lambda^5}{8\pi hc} A_{UL} \] (3.8)

for all bound-bound transitions at the specific line-center wavelength[25, 29, 38]. This leads to an important result for organizing the database; i.e., \( \varepsilon_{\lambda}^c \) and \( \kappa_{\lambda}^c \) are independent of parameters, such as ion and electron number densities and temperatures.

There are two other transition mechanisms, which lead to a change of energy level by emission or absorption of a photon. Transitions from a bound to a dissociated state, known as bound-free transitions and the reverse transitions, called free-bound transitions are two such mechanisms. Also transitions between two continuum states, called free-free transitions, are possible mechanisms caused by photon-atom interactions. For atomic radiation, the bound-bound transitions are the largest contributions to the radiation compared to bound-free and free-free transitions. The bound-free radiation occurs when the upper state is in the ionized, or continuum state. In that case, the wavelength of the transition is determined by the kinetic energy of the free electron, \( E_k \),
or,

$$\lambda = \frac{1}{\Delta E} = \frac{1}{E_\infty - E_i + E_k}$$  \hspace{1cm} (3.9)$$

where $E_\infty$ is the ionization potential of the atom and $E_i$ is the energy of the $i$-th bound level. Since the electron kinetic energy, $E_k$, is continuously distributed according to a Maxwellian distribution, radiation from bound-free transitions is spectrally continuous. The bound-free absorption cross-section, $\sigma^\text{bf}_\lambda$, is defined in terms of the ionization cross-section of the hydrogen atom, $\sigma_{\lambda H}$, multiplied by a correction factor known as the Gaunt factor[68]. The hydrogenic cross-sections are defined by Kramer’s formula[69] as

$$\sigma_{\lambda H} = 7.9 \times 10^{-18} n \left( \frac{\lambda}{\lambda_n} \right)^3$$  \hspace{1cm} (3.10)$$

where the value of $\lambda_n$ is given as $\lambda_n = n^2 10^8 / I_H$, $I_H$ is the ionization potential of atomic hydrogen, 109,679 cm$^{-1}$ and $n$ is the principal quantum number. The Gaunt factor, $GF_\lambda$, is defined as

$$GF_{\lambda,i} = \frac{\sigma^\text{bf}_{\lambda,i}}{\sigma_{\lambda H}}$$  \hspace{1cm} (3.11)$$

The Gaunt factor is determined by comparing the cross-sections with those of Peach[68]. Note that for a specific electronic state $\sigma^\text{bf}_\lambda$ is only a function of wavelength. Finally, the bound-free absorption coefficient for each energy level is obtained by the bound-free cross-section multiplied by the electronic state population as

$$\kappa^\text{bf}_\lambda = \sum_{i=1}^{l} (\sigma^\text{bf}_{\lambda,i} N_i)$$  \hspace{1cm} (3.12)$$
where \( l \) stands for the number of electronic states modeled in the NEQAIR database. For atomic O and N, there are \( l=15 \) out of the total 19 states and 14 out of 22, respectively. The remaining levels do not contribute to the sum because they are assumed to be quasinon-bound or existing in the continuum. The bound-free emission is calculated from Eq. (3.12) using relations given by[29],

\[
\varepsilon_{\lambda}^{bf} = \sum_{i=1}^{l} \left( \sigma_{\lambda,i}^{bf} \frac{2\hbar c^2}{\lambda^5} (N_i/N_U - 1) \right)
\]  

(3.13)

where \( N_U \) is chosen as the population at the ionization limit given by,

\[
N_U = 2.07 \times 10^{-16} \frac{n_+ n_e}{Q^e T_1.5} \exp \left( -\frac{\hbar c}{k_B T_e} \right)
\]

(3.14)

The value of \( 2.07 \times 10^{-16} \) is calculated from the expression of \( \left( \frac{h^2}{(2\pi m_e k_B)} \right)^{3/2} / 2 \) given by Ref. [29]. Free-free transition occurs when an electron in the vicinity of an ion or an atom is decelerated and emits radiation to conserve energy. The free-free absorption coefficient divided by the atomic number density, employing the hydrogenic free-free cross-section, \( \sigma_{\lambda H}^{ff} \), is calculated as[29]

\[
\frac{\kappa_{\lambda}^{ff}}{n_a} = \frac{n_+ n_e}{n_a} \sigma_{\lambda H}^{ff} (1 + d_{ff})
\]

(3.15)

where \( d_{ff} \) is a correction factor for the free-free cross-section of non-hydrogenic atomic species[68]. The free-free emission is calculated using the blackbody function given
by [29],

$$
\varepsilon_\lambda^{ff} = k_\lambda \lambda^5 \left[ \exp\left( \frac{2hc^2}{\lambda k_BT_e} \right) - 1 \right]
$$

(3.16)

### 3.2.2 Calculation of Atomic Electronic Excited State Populations - Quasi Steady State Assumption

Under non-equilibrium flow conditions, the atomic electronic states are excited and de-excited by collisional and radiative processes. When an atom collides with other atoms, molecules, or electrons, the electronic states potentially become excited. Collision induced electronic transitions in an atomic or molecular system are particularly effective when the collider is an electron. Specifically, when a free electron with large energy collides with an atom in a bound state, the energy of the free electron can be transferred to the atom in the form of electronic state excitation. In this case, the excitation rate from the initial state \( i \) to the final state \( j \) is \( K^e(i,j)N_i n_e \). In non-equilibrium flow conditions, radiative transitions also have an important role in determining the electronic state of neutral species. A summary of the excitation/de-excitation processes of atoms may be written as,

\[
O(i) + e^- \xrightarrow{K^e(i,j)} O(j) + e^- \quad (3.17)
\]

\[
O(i) + e^- \xrightarrow{K(i,c)} O^+ + 2e^- \quad (3.18)
\]

\[
O(i) \xrightarrow{A(i,j)} O(j) + h\nu \quad (3.19)
\]

\[
O(i) + h\nu \xrightarrow{A(i,c)} O^+ + e^- \quad (3.20)
\]
where \( \text{O}(i) \) and \( \text{O}^+ \) represent an atomic species of electronic energy level \( i \) and its ion, respectively. Under non-equilibrium flow conditions, there are not enough collisions to describe the electronic states by a Boltzmann distribution and, therefore, a rate equation approach must be needed to calculate the electronic state populations\[25\]. The time rate of change of number density \( N_i \) is given by the difference between the sum of the rates of all collisional and radiative transitions that populate and depopulate state \( i \),

\[
\frac{\partial N_i}{\partial t} = \text{formation} - \text{removal} \tag{3.21}
\]

where the population and the depopulation of the \( i \)-th state may be expressed as

\[
\text{formation} = \sum_{j=1}^{l} K^e(j, i)N_j n_e + K(c, i)n_+ n_e^2 + \sum_{j=1}^{l} A(j, i)N_j + A(c, i)n_+ n_e \tag{3.22}
\]

\[
\text{removal} = \sum_{j=1}^{l} K^e(i, j)N_i n_e + K(i, c)N_i n_e + \sum_{j=1}^{l} A(i, j)N_i + A(i, c)N_i \tag{3.23}
\]

When the rate of change of \( N_i \) on the left-hand side is much smaller than both the sum of all population rates and all depopulation rates on the right-hand side, the quasi-steady-state (QSS) condition holds. For this condition, the left hand side is set to zero and the system of differential equations can be rewritten as a set of algebraic equations as follows,
\[
\begin{bmatrix}
\sum_{j=1}^{l} K^e(i,j) + K(i,c) + \frac{\sum_{j=1}^{l} A(i,j) + A(i,c)}{n_e}\\
\end{bmatrix} \rho_i - \sum_{j=1}^{l} \left[ K^e(i,j) + \frac{N_{jE} A(j,i)}{N_{iE} n_e} \right] \rho_j
= K(i,c) + A(c,i) \frac{n_+}{N_{iE}} \tag{3.24}
\]

where

\[
K^e(i,j)N_{iE} = K^e(j,i)N_{jE}
\]

\[
K(i,c)N_{iE} = K(c,i)n_+n_e \tag{3.25}
\]

\[
\rho_i = \frac{N_i}{N_{iE}} \tag{3.26}
\]

and \(N_{iE}\) is the number density of the \(i\)-th state in equilibrium. The symbols \(n_+\), \(n_e\), \(n_a\) and \(T_e\) are the ion, electron, atom number densities and the electron temperature, respectively. Since the sum over all \(N_i\) must be equal to the total number density of the atomic species, or,

\[
\sum_{i=1}^{l} \frac{N_{iE}}{n_e} \rho_i = \chi \frac{N_{aE}}{n_e} \tag{3.27}
\]

Equations (3.24) and (3.27) can be rewritten in the matrix form of

\[
M \ddot{\rho} = \ddot{C} + \dot{D} \frac{n_a}{N_{aE}} \tag{3.28}
\]
where $\chi = n_a/N_{aE}$ and $N_{aE} = \sum_{i=1}^{l} N_{iE}$ and the matrix $M$ and vectors $\bar{C}$ and $\bar{D}$ are functions of only $T_e$ and $n_e$.\[25]\) Finally, the normalized population can be expressed as

$$\frac{N_i}{n_a} = F_i(T_e,n_e)\frac{n_+}{n_a} + G_i(T_e,n_e)$$

(3.29)

where

$$F_i(T_e,n_e) = M^{-1}\bar{C}\frac{N_{iE}}{n_+}$$

$$G_i(T_e,n_e) = M^{-1}\bar{D}\frac{N_{iE}}{N_{aE}}$$

(3.30)

The two functions, $F_i$ and $G_i$, contain the effects of both collisional and radiative transitions for the excitation of atoms in the $i$-th electronic energy state.

### 3.3 Concepts of Radiation from Diatomic Species

#### 3.3.1 Basic Relations of Radiation by Diatomic Species

Modeling of molecular radiation is more complex than for atomic species because in addition to electronic transitions, rotational and vibrational transitions must also be considered. The large number of rotational lines in a diatomic band system makes the task of determining the Einstein coefficients for each line from the NEQAIR database complicated. In NEQAIR, the transition probabilities are calculated from a number of parameters. The expression for the Einstein $A$ coefficient, $A_{UL}$, is given by\[29]\)

$$A_{UL} = \left(\frac{64\pi^4\nu_{UL}^3}{3h}\right) (e\alpha_0)^2 R^2 q_{UL}^2 S_{J_U} S_{J_L} / (2J_U + 1)$$

(3.31)
where
\[ \tilde{\nu}_{UL} = \frac{1}{\lambda_c} = T_{eU} - T_{eL} + [G(V_U) - G(V_L)] + [F(J_U) - F(J_L)] \] (3.32)

By using Eqs. (3.1) and (3.31), the spontaneous emission coefficient can be written as[70]
\[ \epsilon_\lambda = \frac{16\pi^3 \tilde{\nu}_{UL}^4 c}{3(2J_U + 1)} (ea_0)^2 N_U g_U \text{Re}^2 q_{V_U} q_{V_L} S_{J_U J_L} \phi_\lambda \] (3.33)

where \( \phi_\lambda \) is again the line shape function and \( N_U \) is the upper state population in a given vibrational rotational state. The normalized emission and absorption coefficients can be defined in a manner similar to the atomic cases given in Eqs. (3.4) and (3.5).

Here, \( \epsilon^c_\lambda \) and \( \kappa^c_\lambda \) for molecules are defined as
\[ \epsilon^c_\lambda = \frac{16\pi^3 \tilde{\nu}_{UL}^4 c}{3(2J_U + 1)} (ea_0)^2 g_U \text{Re}^2 q_{V_U} q_{V_L} S_{J_U J_L} \] (3.34)
\[ \kappa^c_\lambda = \epsilon^c_\lambda \frac{\lambda^5_c}{2hc^2} \] (3.35)

To database \( \epsilon^c_\lambda \) and \( \kappa^c_\lambda \) we need to determine the dependency of the quantities in Eqs. (3.34) and (3.35) on the flowfield variables. Since an electronic transition in a molecule takes place much more rapidly than a vibrational transition, in a vibronic transition, the nuclei have very nearly the same position and velocity before and after the transition.[71]

A transition moment between two vibrational quantum numbers, \( V_U \) and \( V_L \) of different electronic states can, therefore, be approximated by[71]
\[ R_{V_U V_L} = \text{Re} \int \Psi_{V_U} \Psi_{V_L} dr_c \] (3.36)
where $\text{Re}$ is an averaged value of the electronic transition moment. The transition probability is directly proportional to $R_{V_U,V_L}^2$ or $\left| \int \Psi_{V_U} \Psi_{V_L} d\tau \right|^2$, where the vibrational overlap integral, $q_{V_U,V_L} = \left| \int \Psi_{V_U} \Psi_{V_L} d\tau \right|^2$, is called the Franck Condon factor and does not depend on species concentrations or temperatures.[71]. The line strength factor, $S_{J_U,J_L}$, depends on the type of electronic transition and the spin multiplicity as well as rotational quantum number. Using standard spectroscopic relationships it can be shown that the upper state population, $N_U$, is given by:

$$N_U = \frac{N_U^e}{(Q_{VR})_U} (2J_U + 1) \exp \left[ -\frac{\hbar c}{k_B} \left( \frac{G(V_U)}{T_{vib}} + \frac{F(J_U)}{T_{rot}} \right) \right] \quad (3.37)$$

where $N_U^e$ and $(Q_{VR})_U$ are the electronic upper state population and upper state total partition function respectively. Using the above relationships, the population ratio, $N_L/N_U$, is given by

$$\frac{N_L}{N_U} = \frac{N_L^e}{N_U^e (Q_{VR})_L} \frac{2J_L + 1}{2J_U + 1} \exp \left[ \frac{\hbar c}{k_B} \left( \frac{G(V_U) - G(V_L)}{T_{vib}} + \frac{F(J_U) - F(J_L)}{T_{rot}} \right) \right] \quad (3.38)$$

where the upper state total partition function, $Q_{VR}$, is given as[70]

$$(Q_{VR})_U = \sum_{V_U=0}^{\max} \left[ \sum_{J_U=0}^{\max} (2J_U + 1) \exp \left( -B_{V_U} J_U (J_U + 1) \frac{\hbar c}{k_B T_{rot}} \right) \right] \exp \left( -G(V_U) \frac{\hbar c}{k_B T_{vib}} \right) \quad (3.39)$$
3.3.2 Calculation of Excited Electronic State Population for Diatomic Species

In this section, derivation of the excited electronic state populations, \( N^e_U \), for diatomic species using the QSS assumption is discussed. The baseline excitation/de-excitation processes for diatomic species are modeled as

\[
\begin{align*}
Z + U + W & \underset{K_{Wi}}{\overset{K_{Wj}}{\rightleftharpoons}} ZU(i) + W \quad (3.40) \\
e^- + ZU^+ + e^- & \underset{K_{ci}}{\overset{K^e_{ci}}{\rightleftharpoons}} ZU(i) + e^- \quad (3.41) \\
ZU(i) + W & \underset{K_{W(i,j)}}{\overset{K^W_{(i,j)}}{\rightleftharpoons}} ZU(j) + W \quad (3.42) \\
e^- + ZU(i) & \underset{K^e_{(i,j)}}{\overset{K_e(i,j)}{\rightleftharpoons}} ZU(j) + e^- \quad (3.43) \\
ZU(i) & \overset{A_{(i,j)}}{\longleftrightarrow} ZU(j) + h\nu \quad (3.44)
\end{align*}
\]

where \( Z \) and \( U \) represent atomic species and \( W \) and \( e^- \) represent a heavy particle and an electron, respectively. Equations (3.40) - (3.44) represent heavy particle and electron induced recombination, heavy particle and electron induced excitation, and spontaneous emission, respectively[72]. The time rate of change of normalized number density, \( \rho_i = \frac{N_i}{N_{iE}} \), is given by the difference between the incoming rates and outgoing rates[25, 72],

\[
\frac{1}{n_e} \frac{\partial \rho_i}{\partial t} = \left[ -\sum_{j=1}^{m} \left[ K^e_{(i,j)} + K^W_{(i,j)} \frac{N_W}{n_e} + \frac{A_{(i,j)}}{n_e} \right] + K_{ic}^e + K_{iW} \frac{N_W}{n_e} \right] \rho_i \\
+ \sum_{j=1}^{m} \left[ K^e_{(i,j)} + K^W_{(i,j)} \frac{N_W}{n_e} + \frac{A_{(j,i)}}{n_e} \frac{N_{jE}}{N_{iE}} \right] \rho_j \\
+ \left[ K_{ic}^e + K_{iW} \frac{N_W}{n_e} \right] \quad (3.45)
\]
where $K^e(i,j)$ is the electron-impact excitation rate coefficient between two electronic states of a molecule, $K^W(i,j)$ is the excitation rate coefficient by neutral impact between two electronic states and $K_{iW}$ and $K_{ic}^e$ represent dissociation rate coefficients due to heavy particle collision and electron impact, respectively. Note that the reversal of indices such as, “$iW$” to “$Wi$” changes the rate coefficient from collisionally induced dissociation to a recombination mechanism. Under the QSS condition, the left hand side is set to zero and the system of differential equations becomes a matrix equation of the form,

$$M_m\bar{\rho} = \bar{C}_m + \bar{D}_m \frac{N_m}{N Z}$$

(3.46)

where $N_m = \sum_{i=1}^{l_m} N_i$ and the matrix $M_m$ and vectors $\bar{C}_m$ and $\bar{D}_m$ are assembled by excitation and dissociation rate coefficients. The final form of the diatomic QSS relation is given as

$$\bar{\rho} = \frac{N_i}{N_{iE}} = M_m^{-1}(\bar{C}_m + \bar{D}_m \frac{N_m}{N Z})$$

(3.47)

The upper and lower electronic state populations, $N^e_L$ and $N^e_U$, are solved by a $4 \times 4$ matrix inversion.

3.4 The One-Dimensional Tangent Slab Approximation, a Method for Radiative Transport

Radiative intensity, $I_\lambda$, is used to describe radiative properties and defined as radiative energy flow per unit solid angle and unit area normal to the intensity rays. This intensity can be attenuated and augmented through emitting and absorbing media. It can be described in differential form of the one-dimensional equation of radiative
transfer as given by

$$\frac{dI_\lambda(\theta)}{dx} = -\kappa_\lambda I_\lambda(\theta) + \varepsilon_\lambda$$  \hspace{1cm} (3.48)$$

where $\varepsilon_\lambda$ and $\kappa_\lambda$ are the emission and absorption coefficients, respectively. The tangent slab (TS) approximation is one of the basic methods to solve a radiative transport equation (RTE) for one-dimensional gas media. The spectral radiative heat flux, $q_R(\tau_\lambda)$, which is of interest for heat transfer applications, is written as[38]

$$q_R(\tau_\lambda) = \int_0^{2\pi} \int_0^\pi I_\lambda(\theta) \cos \theta \sin \theta d\theta d\psi$$  \hspace{1cm} (3.49)$$

where $\tau_\lambda = \int_0^l \kappa_\lambda ds$ is the optical thickness. The final form to solve Eq. (3.49) may be written in terms of the second and third order exponential integrals.

$$q_R(\tau_\lambda) = 2\pi [I_{b1} E_3(\tau_\lambda) - I_{b2} E_3(\tau_{\lambda L} - \tau_\lambda)]$$

$$+ 2\pi \left[ \int_0^{\tau_\lambda} S_c(\tau_\lambda') E_2(\tau_\lambda - \tau_\lambda') d\tau_\lambda' - \int_{\tau_\lambda}^{\tau_{\lambda L}} S_c(\tau_\lambda') E_2(\tau_\lambda' - \tau_\lambda) d\tau_\lambda' \right]$$  \hspace{1cm} (3.50)$$

where $I_{b1}$ and $I_{b2}$ are the blackbody intensities leaving two wall boundaries. Detailed derivations to solve the radiative heat flux ($q_R$) and the incident radiative intensity ($G_\lambda = \int_4^\pi I_\lambda d\Omega$) for the parallel plate media are introduced in Ref.[38]. In equilibrium conditions without scattering the source term, $S_c$, is defined as the blackbody function. However, for non-equilibrium conditions, local emission and absorption coefficients must be calculated individually for each cell condition, leading to $S_{c,\lambda} = \varepsilon_\lambda/\kappa_\lambda$. The radiative
energy change in a cell is then calculated by

\[ \nabla \cdot \mathbf{q}_R(\tau_\lambda) = \frac{\Delta q_R(\tau_\lambda)}{\Delta x}. \quad (3.51) \]

where \( \Delta x \) is the cell thickness.

### 3.5 The Photon Monte Carlo (PMC) Ray Tracing Scheme, the Second Method for Radiative Transport

A two-dimensional axisymmetric finite volume based PMC (FV-PMC) code was developed using the same macroparameter grid structure of the DSMC code and the same physical model and principles as in the PMC three-dimensional model. The FV-PMC method was initially developed to use the body-fitted structured grid system which has been used in CFD[51]. In this work, the portion of ray-tracing of photon bundles at each cell was optimized for a structured-square type cells used in DSMC flow simulation. The mathematical formula to calculate the distance which the photon bundle travels through each cell and searching procedures for finding the cell face intersected with photon bundles in the DSMC cell become simpler than the original ones used in the body-fitted grid system. The FV-PMC method simulates radiation by tracing photon bundles from an emission point to a termination location. The locations and directions of the emitting photon bundles in each cell are determined using random number relations. The direction of each ray is selected randomly by,

\[ \psi = 2\pi R_{\psi}. \quad (3.52) \]
\[ \theta = \cos^{-1}(1 - 2R_\theta) \] (3.53)

where \( R_\psi \) and \( R_\theta \) are uniformly distributed random numbers from 0 to 1.

The finite volume based PMC (FV-PMC) tracing scheme uses the energy partitioning method[51], which traces a photon bundle and calculates the fraction of energy absorbed by each cell that the bundle passes through. To accomplish this, the distance \( (S_d) \) which the bundle travels as it passes through the cell and to the particular cell face with which it intersects has to be determined. That distance is used to calculate the quantity of energy absorbed, and the intersection coordinates on the cell face of the photon bundle become the new initial location of the ray tracing in the next cell. The following equations give the cell face intersection coordinates in terms of the emission location coordinates and directional vectors of a photon ray. The intersection point is written as

\[
\begin{align*}
x_i &= x_e + S_d s_x \\
y_i &= y_e + S_d s_y \\
z_i &= S_d s_z
\end{align*}
\] (3.54) (3.55) (3.56)

where \( x_i, y_i \) and \( z_i \) are the intersection coordinates with the cell face in the \( x, y \) and \( z \) directions, respectively, \( S_d \) is the distance traveled through the cell, \( x_e \) and \( y_e \) is the emission location in the cell, and \( \vec{s} \) are the unit directional vectors. Figure 3.1 shows a schematic diagram of the method used to determine the intersected cell face in a single cell. The four face conditions for ray tracing in a 2-D axisymmetric PMC on the DSMC
macroparameter grid are defined as follows:

\begin{align*}
\text{face 1: } & \ x_1 < x < x_2, \ r = y_1 \\ 
\text{face 2: } & \ x = x_2, \ y_1 < r < y_2 \\ 
\text{face 3: } & \ x_1 < x < x_2, \ r = y_2 \\ 
\text{face 4: } & \ x = x_1, \ y_1 < r < y_2
\end{align*} 

The procedure to determine which face will be intersected by the photon bundle begins with testing whether face 1 or 3 satisfies the criteria for a valid intersection. The distance traveled by a photon bundle through the cell \( S_d \) and the radial distance \( r \) are calculated by assuming that the photon bundle will intersect either face 1 or 3, or, 

\[ l_{1,2} = -B \pm \sqrt{B^2 - C} \tag{3.61} \]

where

\[ B = \frac{s_y y_e}{(1 - s_x^2)} \tag{3.62} \]

\[ C = \frac{(y_e^2 - y_{2or1}^2)}{(1 - s_x^2)} \tag{3.63} \]

There are two solutions to Eq. (3.61) for \( l \), but, the valid intersection must be \( l_1 \) or \( l_2 > 0 \) and \( x_1 < x_i < x_2 \). If \( l_1 \) or \( l_2 \) satisfies these conditions, then \( S_d \) is set to that \( l \) value. If face 1 or 3 is found not to be a valid intersection face, then faces 2 and 4 are examined.
by calculating the quantities,

\[ S_d = \frac{x_2 (\text{or } x_1) - x_e}{s_x} \quad (3.64) \]

\[ r = \sqrt{(S_d s_y + y_e)^2 + (S_d s_z)^2} \quad (3.65) \]

Likewise, if the two conditions that \( S_d > 0 \) and \( y_1 < r < y_2 \) are satisfied, then either face 2 or 4 is a valid intersected face, and the intersection point, \((x_i, y_i)\), becomes the new emission location, \((x_e, y_e)\), of the next cell.

After determining the intersection point and the corresponding distance traveled, the intersection point must be transformed back into the original X-Y plane in order to keep the computation two-dimensional. Also the direction of the photon bundle must be adjusted to reflect this rotation back into the original plane (bottom portion of Fig. 3.1). This new azimuthal angle of the photon bundle is calculated using \( \psi - \varphi \) (azimuthal angle, face intersection angle) where

\[ \psi = \tan^{-1}\left(\frac{s_y}{s_x}\right) \quad (3.66) \]
\[ \varphi = \tan^{-1}\left(\frac{s_i}{y_i}\right) \quad (3.67) \]

As the photon travels through the computational domain, the energy associated with the photon bundle is decreased due to the absorptivity of the traversed cell. The optical length traveled through the cell can be calculated as,

\[ \alpha = 1 - e^{-\kappa \lambda S_d} \quad (3.68) \]
where $\kappa\lambda$ denotes the cell absorption coefficient. The amount of energy absorbed by the cell, $E_{abs}$, and the energy carried by the photon bundle, $E_{trans}$, can be calculated as,

$$E_{abs} = \alpha E_{bundle} \quad (3.69)$$

$$E_{trans} = E_{bundle} - E_{abs} \quad (3.70)$$

The next cell which the ray will enter is also determined by Eqs. (3.54) through (3.65). The absorbed energy ($E_{abs}$) is calculated by tracing a large number of bundles using the random number relations (Eqs. (3.52)-(3.53)) and Eqs. (3.54)-(3.65). Therefore, as the number of photon bundles increases the standard deviation in each cell is reduced. For a non-gray medium, a ray is randomly assigned a wavelength using an emission random number database (ERND) for the cell species, as is discussed in the next chapter.

Finally, the divergence of the radiative heat flux ($\nabla \cdot q_R$) term is calculated as the difference between the emission and absorption energy for each cell by,

$$\left( \nabla \cdot q_R \right)_{i,j} = \left( \frac{E_{emis} - E_{abs}}{V_{cell}} \right)_{i,j} \quad (3.71)$$

where $i$ and $j$ are cell indices and $V_{cell}$ denotes a cell volume.

Generally, the number of rays emitted from an individual cell is determined according to the fraction of emissive cell energy to total emissive energy as follows,

$$N_{rays\ per\ cell} = N_{total\ rays} \times \frac{E_{cell}}{E_{total}} \quad (3.72)$$
where $N_{\text{rays per cell}}$ and $E_{\text{cell}}$ are the number of rays emitted from a cell and the corresponding total emission energy of the cell, and $N_{\text{total rays}}$ is an initial number of rays specified by the user and $E_{\text{total}}$ is the total emission energy in the entire domain, which can be obtained by summing the emission energy of each cell, $E_{\text{cell}}$. Since the emission energy of each cell ($E_{\text{cell}}$) is proportional to the cell volume, the number of rays emitted from cells located along the symmetry axis is very small. Hence, the statistical deviation in the net radiative heat flux near the symmetry axis is higher than that of in the outer cells, but, the former is usually the main region of interest. In order to avoid a large statistical variation near the symmetry axis, the number of rays per cell is re-defined based on the cell cross-sectional area instead of the cell volume[51], and is expressed as,

$$N_{\text{rays per cell}} = N_{\text{total rays}} \times \frac{E_{\text{cell cross section}}}{E_{\text{total cross section}}} \quad (3.73)$$

where $E_{\text{cell cross section}}$ is the emission per volume times the cell area, and $E_{\text{total cross section}}$ is a summation of $E_{\text{cell cross section}}$ values over the entire domain. Use of this relationship helps us to obtain roughly an equal number of photon rays per cell, which in turn, causes the high emission rate per volume near the symmetry axis to generate a large number of photon bundles and improve the symmetry axis statistics. Even though the number of photon rays are specified based on the cell area, the emission energy per ray is determined by dividing the cell emissive power by the number of photon rays. Hence, compared to the volume weighted scheme, cells near the symmetry axis will emit a larger number of weaker photon rays, whereas, cells further away from the symmetry axis will
emit fewer photon rays. Therefore for those cells off of the symmetry axis, each photon ray will be stronger than the corresponding ones emitted in the volume weighted scheme.
Fig. 3.1. Schematic diagram of ray tracing in one cell on X-Y (top) and Y-Z plane (bottom).
Chapter 4

Development of Databasing Schemes for Efficient Radiation Calculations of Hypersonic Reentry Flows

4.1 Preface

In this chapter, an efficient databasing scheme for generating spectral emission and absorption coefficients using the NEQAIR code is discussed. In contrast to the models mentioned in Chapter 3, assembled parameters, extracted directly from NEQAIR, to calculate spectral line strengths were used. One of the main challenges in developing the databasing scheme is to incorporate the QSS procedure, which includes the calculation of about forty electronically excited states for atomic oxygen and nitrogen. Also because the line broadening effect due to the electron collision may be important for the reentry flows, to maintain accuracy in computing the radiative heat loads, the databasing procedure has to incorporate the Voigt line shape. The accuracy and efficiency of atomic and diatomic emission and absorption coefficients obtained from the new database is examined for a flow condition close to peak heating along the Stardust reentry trajectory. In the final section, the accuracy of the databasing scheme is examined by comparing the divergence of radiative heat fluxes using the database with those obtained directly from NEQAIR. The efficiency of the databasing scheme is quantified and the radiative heat generation using the new database is calculated for a Stardust reentry flowfield.
4.2 Strategy for Generating Databases of Atomic Spectral Quantities

For bound-bound transitions, the line strength factors $\varepsilon^c_\lambda$ and $\kappa^c_\lambda$ for the emission and absorption coefficients given by Eqs. (3.6) and (3.7), respectively, are obtained from NEQAIR[29]. The line center wavelengths at which the bound-bound transitions occur and the potential upper and lower electronic states for each bound-bound transition are also obtained from NEQAIR. Tables 4.1 and 4.2 show the first five line strength factors $\varepsilon^c_\lambda$ and $\kappa^c_\lambda$, the line center wavelength, and the upper and lower electronic energy levels for each bound-bound transition for atomic O and N, respectively. The normalized electronic state populations calculated using the QSS assumption are given by Eq. (3.29).

In this equation, since the ion and atomic number densities will be obtained from the flowfield solution directly, one needs to database values of $F_i(T_e, n_e)$ and $G_i(T_e, n_e)$ at various values of $T_e$ and $n_e$ to calculate the normalized electronic state populations for each electronic state $i$. Cubic spline interpolation of $F_i$ and $G_i$ at arbitrary $T_e$ and $n_e$ values may then be used. The data sets for $F_i(T_e, n_e)$ and $G_i(T_e, n_e)$ are defined at 50 $n_e$ values and 70 $T_e$ values, with $n_e$ varying from $10^{13}$ to $4 \times 10^{16}$ cm$^{-3}$ and $T_e$ ranging from 1,000 to 28,000 K, with a equal spacing given by

$$H_j = (H_{init}^{0.1} + (j - 1)\Delta H^{0.1})^{10}$$

(4.1)

where $\Delta H^{0.1} = (H_{end}^{0.1} - H_{init}^{0.1})/(P - 1)$. Here, $P$ is the number of data points, 50 for $n_e$ and 70 for $T_e$, and $j$ denotes the data point index, $1 \leq j \leq P$. The form of Eq. (4.1) reduces the computation time for interpolation of $F_i$ and $G_i$ at any $n_e$ and $T_e$ conditions because searching for a desired point is faster using equally spaced rather
than non-equally spaced data points. The total size of the database of $F_i(T_e, n_e)$ and $G_i(T_e, n_e)$ of each atomic species O and N is about 6.2 MBytes. This approach allows us to incorporate all of the models developed over many years in NEQAIR for the QSS model as well as permit the efficient recalculation of the database as the QSS model evolves.

To complete the database formulation, we need to specify the line shape. The Voigt line shape function is selected because it is the most general form of line broadening. It considers both thermal and collisional broadening effects, as required to properly simulate line broadening under non-equilibrium flow conditions. The approximate formula of Whiting[73] is given as,

$$
\phi_\lambda = \left[ (1 - w_l/w_v) \exp(-2.772(\Delta \lambda/w_v)^2) + (w_l/w_v)/\{1 + 4(\Delta \lambda/w_v)^2\} \right.
+ 0.016(w_l/w_v)(1 - w_l/w_v)(\exp\{-0.4(\Delta \lambda/w_v)^{0.25}\} - 10/\{10 + (\Delta \lambda/w_v)^{2.25}\})
/ [w_v\{1.065 + 0.447(w_l/w_v) + 0.058(w_l/w_v)^2\}] \right] \times (w_l + w_g) (4.2)
$$

where $w_l$ and $w_v$ denote the Lorentzian and Voigt widths, respectively, and $\Delta \lambda$ is given by,

$$
\Delta \lambda = \lambda - \lambda_c \quad (4.3)
$$

The Voigt width is calculated from the following approximation[74]

$$
w_v = [1 - 0.18121 \times (1 - d^2) - (0.023665 \exp(0.6d) + 0.00418 \exp(-1.9d) \times \sin(\pi d))] \times (w_l + w_g) \quad (4.4)
$$
where \( d = (w_l - w_g)/(w_l + w_g) \) and \( w_g \) is Gaussian or Doppler width. The main contribution to the Lorentzian width for hypersonic flow conditions is due to Stark broadening caused by high energy electron collisions with atoms. The Stark line broadening widths, \( w_s \), at half line center peak height are calculated for each individual line by the following equation\[75, 76\]
\[
w_s = w_{s,0} \left( \frac{T_e}{10,000 K} \right)^b \left( \frac{n_e}{1 \times 10^{16} \text{cm}^{-3}} \right)
\]
(4.5)
where the reference Stark width, \( w_{s,0} \), and the exponent, \( b \), are stored in the database for each atomic line. The Doppler line half-width, \( D_w \), for the Gaussian broadening is given by\[38\]
\[
D_w = \frac{\lambda_c}{c} \sqrt{\frac{2k_B T_{trn}}{m} \ln 2}
\]
(4.6)
where \( T_{trn} \) is the translational temperature and \( m \) is the mass of the radiating species.

The Voigt line shape function of Eq. (4.2) is a function of two parameters, \( w_l/w_v \) and \( \Delta \lambda/w_v \). Therefore, to calculate the spectral emission and absorption coefficients broadened by the Voigt profile at any wavelength or flow condition, values of \( w_l/w_v \) from 0 to 1 and \( \Delta \lambda/w_v \) from 0 to 200 are pre-stored at increments for \( w_l/w_v \) and \( \Delta \lambda/w_v \) of 0.002 and 0.025, respectively. During the RTE calculation the line-shape can be calculated using a bi-linear interpolation of these stored database parameters. Figure 4.1 shows the required cutoff range, \( \Delta \lambda/w_v \), for the half-width of the full line shape that satisfies 99.9 % of the integrated emission as a function of the ratio of the Lorentzian to Voigt width for all possible \( n_e \) and \( T_e \) values. It can be seen that the cutoff range rapidly increases as the ratio of \( w_l/w_v \) increases to \( 2.4 \times 10^{-2} \) and then remains constant. If the ratio is greater than \( 2.4 \times 10^{-2} \), the cutoff range, \( \Delta \lambda/w_v \), should be greater than
200 to capture 99.9% emission for each atomic line. However, our database for the Voigt profile considered 200 times the Voigt width as the maximum cutoff range, when the ratio of the Lorentzian to Voigt width is greater than $2.4 \times 10^{-2}$, the cutoff limit for a single line is set to be 200. In a thermo-chemical non-equilibrium flowfield the widths of different atomic lines can be vary by orders of magnitude because the change in electron number density and electron temperature in the hypersonic shock layer is large. Since this large variation in the line width can lead to different line broadening shapes for individual atomic lines, an efficient approach to determine the proper cutoff wavelength for each atomic line is needed to accurately model emission and absorption of radiative energy in the radiative heat transport calculation. This approach is particularly important in radiative transport for the optically thick hypersonic flows considered here because transport through the line wings cannot be neglected. In the present work, the cutoff wavelength that guarantees that the emission integrated over the line-shape gives 99.9% of the total line emission is stored for each line as a function of the ratio of the Lorentzian to Voigt width.

With the atomic line shape defined, the normalized emission and absorption coefficients given by Eqs. (3.4) and (3.5) are calculated for any given density, temperature, and wavelength. For the bound-free case, the normalized bound-free absorption coefficients are calculated using the bound-free cross-sections, Eq. (3.12), and the normalized electronic state populations, $N_i/n_a$, which are already calculated for the bound-bound radiation. Lastly, the normalized free-free absorption coefficients are obtained by Eq. (3.15) and computed using the density values from the flowfield solution and physical parameter datasets available from NEQAIR.
4.3 Strategy for Creating Databases of Spectral Quantities for Diatomic Emitters

In this section, databasing schemes for diatomic gas species will be introduced. First, the diatomic line strength factors $\varepsilon^c_\lambda$ given by Eq. (3.34) are extracted from NEQAIR and stored with line center wavelengths. Since the vibrational term energy, $G(V)$, and rotational term energy, $F(J)$, are not dependent on gas concentration or temperature, these energy terms, which are needed to calculate the upper and lower state populations, will also be stored with the corresponding line center wavelength. In this work, the assembled line strength factor, line center wavelength and vibrational rotational term energy of $N_2^+$, NO, $N_2$, $O_2$ are extracted from NEQAIR and stored in the database. Table 4.3 shows the types of electronic transitions for $N_2^+$, NO, $N_2$, $O_2$ considered in NEQAIR and Table 4.4 presents the first 5 rows of the $N_2^+$ 1st negative transition dataset. The electronic state populations are obtained from the QSS assumption and then the final forms of emission and absorption coefficients are constructed combining the line center dataset with the electronic state populations. Similar to the atomic case, a Voigt or Doppler line shape function is assumed for each vibrational and rotational line-center.
4.4 Application of Radiation Databases to Reentry Flow Cases

4.4.1 Investigation of the Accuracy of Spectral Coefficients Generated using the Database

Before considering the radiation from specific reentry flows, we discuss the accuracy of the new databasing schemes by comparing the emission and absorption coefficients with those obtained from NEQAIR. Figures 4.2 and 4.3 show comparisons between the database and NEQAIR of the emission and absorption coefficients of atomic O for the wavelength range from 500 to 2,000 Å with a wavelength increment of 0.003 Å and from 2,000 to 7,000 Å with 0.005 Å steps. For this comparison the database and NEQAIR utilize the Voigt line shape function. The density and temperature conditions were obtained from the flowfield solution of the Stardust vehicle with a speed of 12 km/s at 81 km altitude, calculated using the direct simulation Monte Carlo (DSMC) method. The conditions represent the location in the flow where high radiation occurs due to the high electron temperature. The difference in the emission and absorption coefficients is defined as,

\[
\text{Difference} (%) = \left( \frac{|X_{i,\text{data}} - X_{i,\text{NEQ}}|}{|X_{i,\text{NEQ}}|} \right) \times 100
\]  

(4.7)

where \(X_{i,\text{data}}\) and \(X_{i,\text{NEQ}}\) are the emission or absorption coefficients from the database and NEQAIR at the \(i\)-th wavelength data point, respectively. In this comparison, most of the differences between the database and NEQAIR are observed to be smaller than 1\% except for the continuum radiation below 800 Å and the bound-bound transitions at 5,331 and 6,158 Å. The difference at 5,331 Å is due to the overlap of the line-shape functions in the wings of each of the three atomic oxygen transitions, all closely located
at 5,330.46, 5,331.07 and 5,332.14 Å. The difference observed at 6,158 Å is due to a similar problem. The continuum spectral coefficients for both bound-free and free-free transitions are linearly interpolated using the precalculated values stored in increments of 1 Å. As discussed in the previous section, bound-free transitions occur in spectral regions with sharp wavelength start and stop intervals. Because there is a delta-function like cutoff, the linear interpolation error can be larger due to large gradients in the emission and absorption lines with respect to wavelength. Figures 4.4 and 4.5 show the comparisons of the emission and absorption coefficients for atomic N between the database and NEQAIR for the range from 500 to 7,000 Å. Again the difference in the emission and absorption coefficients of atomic N are below 5.0 %.

Now we compare the bound-bound line strengths and continuum spectral coefficients of atomic species generated from the database with those from NEQAIR for the entire range of $n_e$ and $T_e$ conditions. The bound-bound emission line strengths and continuum spectral coefficients at three interior points between two successive data points of $n_e$ and $T_e$ were generated and compared with NEQAIR. The maximum difference in the bound-bound emission line strength of atomic O and N was found to be within 0.12 % for the entire range of $n_e$ and $T_e$ conditions as shown in the top portion of Fig. 4.6. Since the emission line strength is proportional to the upper state electronic population, the comparison shows that the electronic state populations of atomic O and N are well predicted by the database and interpolation schemes. For the absorption bound-bound line strength, it was observed that below 10,000 K there are some absorption line strength differences greater than 3% as shown in the bottom portion of Fig. 4.6, but, this was the largest discrepancy observed. Since the absorption line strength is proportional to the
difference of the lower and upper electronic state populations, the error in the difference may be larger than the error in the upper electronic state population. However, there are only 1,702 absorption line strengths that have differences of over 3% out of a total of 15,904,000 cases (200 for \( n_e \) points \( \times \) 280 for \( T_e \) points \( \times \) 284 for lines for N and O). Since the ratio of absorption line strengths with difference greater than 3% to the maximum absorption line strength is within \( 10^{-4} \), this larger difference of 3% does not affect the radiation calculation.

The average difference in the continuum emission and absorption coefficients was also investigated. Since the absorption and emission coefficients of the bound-free transition are related to the electronic state population as given by Eqs. (3.12) and (3.13), respectively, the accuracy of the bound-free spectral coefficients depends on the error of the electronic state populations. As discussed earlier in the bound-bound line strength comparisons, the electronic state populations calculated from the database agree well with those from NEQAIR, and thus the bound-free spectral coefficients obtained from the database are expected to be in a good agreement with those of NEQAIR. The free-free absorption and emission coefficients are calculated directly in terms of number density and electron temperature, as given by Eqs. (3.15) and (3.16), respectively. Therefore the only difference between the continuum spectral coefficients obtained from the database and NEQAIR can occur from the bound-free transitions. The difference in the continuum spectral coefficient was investigated for a range of 500 to 10,500 Å with a 0.2 Å wavelength increment. The same number of \( n_e \) and \( T_e \) conditions used in the bound-bound line strength comparisons (200 for \( n_e \) points \( \times \) 280 for \( T_e \) points) were considered, again, to cover all possible flow conditions. Finally, the average difference in the continuum
emission and absorption coefficients was found to be less than 0.05 % and 0.03 % as shown in the top and bottom portion of Fig. 4.7, respectively.

With respect to radiation from molecular species, Figs. 4.8 through 4.11 show the emission and absorption coefficients from NEQAIR and the absolute difference of coefficients between the database and NEQAIR for the $N_2^+$, NO, $N_2$ and $O_2$ molecular systems, respectively. There are small differences between the databasing scheme and NEQAIR mainly due to the difference in the implementation of the Voigt line shape. NEQAIR uses an approximate approach to define the Voigt line shape for each rotational line. In our databasing scheme we use a more accurate procedure to apply the Voigt line shape with no additional computational cost. A summary of the differences in the procedures is as follows. In NEQAIR, the Voigt width is assumed to be constant for a given vibrational band whereas, in the present databasing scheme, the Voigt line width is calculated at the center line wavelength of each vibrational-rotational line. NEQAIR prepares a template for the Voigt line shape for a single rotational line in the vibrational-rotational transition. The same template is then copied to all the lines in that particular vibrational band. In the databasing scheme, different line shapes are used for each vibrational-rotational line center. The value of line shape function is not calculated exactly at the desired spectral point in NEQAIR. Rather it is assumed that some of the spectral points coincide with the center line wavelength. The line shape function is thus approximated by the value at a wavelength fixed a distance away from the center line wavelength. In the databasing scheme, the line shape function is calculated at the exact wavelength position. In NEQAIR, whether the contribution from a line is important or not is determined by a cutoff limit based on the emission line strength whereas, in the
database, we specify two separate cutoff limits on emission and absorption line strength. The absorption limit is specified as a fixed value and the emission cutoff limit is related to the absorption cutoff limit according to the following relation,

$$
\varepsilon_{\text{min}} = \kappa_{\text{min}} \frac{2hc^2}{\lambda_c^5 \left[ \exp(hc/\lambda_c k_B T_e) - 1 \right]}
$$

(4.8)

The emission cutoff limit changes each line differently. In the database scheme we are interested in retaining some of the lines which are not important from an emission point-of-view but are important from the absorption point-of-view and vice versa.

To verify the accuracy of the new databasing schemes for diatomic species, the emission and absorption coefficients from the database and NEQAIR are compared using the same Voigt line distribution method for both the database and NEQAIR. The accuracy of the databasing scheme is temporarily degraded in order to compare as closely as possible with the NEQAIR approach. In this comparison the four methods for the distribution of Voigt line shape function are applied to the database and NEQAIR. Voigt widths are determined at the vibrational band center. The line center wavelength in Eq. (4.3) is defined for each different vibrational-rotational transition. Emission and absorption coefficients at a given wavelength are approximated using the nearest spectral data point in NEQAIR. The emission and absorption coefficients are also directly calculated in the database using the same approach. The emission cutoff limit is used as a single value, given by NEQAIR, for the entire spectral region. Figures 4.8 through 4.11 also show the absolute difference of spectral coefficients between the database and NEQAIR calculated under the same Voigt line distribution method. It can be seen that
there is excellent agreement between the emission and absorption coefficients predicted by the temporarily degraded database and NEQAIR.

4.4.2 Investigation of Databasing Scheme Efficiencies

The objective of this work is to create a database that can be used in calculating the spectral coefficients efficiently. This is essential for the coupled study of radiation heat transfer in hypersonic non-equilibrium flow fields. These databasing schemes provide an efficient way for calculating the spectral coefficients for full as well as narrow wavelength ranges. For molecular band calculation, all the rotation-vibration lines that contribute to the spectral coefficients at each given wavelength, are stored in the database. The spectral coefficients for a given narrow band can be efficiently generated using this information. Note that the basic database, example shown in Table 4.4, is read only once and the actual computational time of the database is much less than that of NEQAIR because it is not needed to repeat many arithmetical operations to calculate the basic radiation parameters. The CPU times on dual 2.4 GHz AMD Opteron processors shown in Tables 4.6 and 4.7 clearly demonstrate that by using our new database scheme spectral coefficients can be generated more efficiently both for a large wavelength range and for small narrow bands than by the present procedure in NEQAIR. In this CPU time study, the wavelength increment is 0.05 Å, and 20 gas cells were considered from the stagnation streamline flow condition of Stardust at the 68.9 km altitude calculated by DSMC. In these gas cells, the electron temperature varies from 5,252 to 19,846 K. Atomic N and O bound-bound, bound-free and free-free transitions and six molecular bands (1st negative for $\text{N}_2^+$, 1st and 2nd positive for $\text{N}_2$, $\beta$ and $\gamma$ for NO and Schumann-Runge for $\text{O}_2$)
were considered in this example. Because we use an efficient interpolation scheme for generating atomic spectral coefficients, there is large saving on computational time for the atomic calculations. The data interpolation scheme provides an efficient and accurate means for generating spectral coefficients for atomic bound-bound, bound-free and free-free transitions.

The efficiency of applying a variable cutoff range in the atomic radiation calculation was also examined. Atomic O and N bound-bound radiation was considered, and 40 gas layers were used from the stagnation streamline flow of a Stardust flowfield at the 68.9 km altitude simulated by DSMC method. The wavelength range from 100 to 20,000 Å was assumed to capture emission far from the line center for all the lines and the spectral resolution was 0.0025 Å. The difference in the total emission energy, \( E_{emis} = 4\pi \int_{\lambda} \epsilon_\lambda d\lambda \), between the integrated emission obtained using a variable and a fixed cutoff range compared with the summation of the line strengths of all atomic lines is shown in Fig. 4.12 for each cell along the stagnation streamline. A value of 121.2 was chosen as the fixed value for all atomic bound-bound transitions because it captures 99.9% of the total emission energy for ratios of Lorentzian to Voigt widths which are less than 0.024. From the figure it can be seen that the variable cutoff range satisfies 99.9% total emission energy. The variable cutoff range scheme leads to a reduction of computational time because the unnecessarily large cutoff range is not applied to all atomic lines. The CPU time for the calculation using the variable range is 16.4 s, whereas using the fixed cutoff range it was found to be 20.72 s. Most of the atomic lines in the spectral region below 2,000 Å need to use a value of 121.2 as the cutoff range to satisfy the 99.9% total emission energy criterion, under the high electron number density and electron
temperature gas conditions. Therefore, only a reduction of about 20% in computational time was achieved. However, when iterative calculations are used, such as in the PMC RTE, and in highly optically thick conditions [49], this reduction of the computational time without loss of accuracy will be important.

4.4.3 Application of Databasing Schemes to Radiation Calculations

In the previous section, we have shown that the database procedure calculates emission and absorption coefficients accurately for a single flowfield condition. As the final verification of our databasing scheme, we have used it to demonstrate the calculation of radiative heat generation rates along the stagnation streamline and a flow field condition close to the shoulder line of the Stardust vehicle. For non-equilibrium gas conditions, calculations of radiative heat generation require data for both the emission and absorption coefficients. Thus, the objective of this work is to verify the reliability of the emission and absorption coefficients through the radiative heat generation computation for all possible flow conditions. In this work, flowfield solutions for three freestream conditions were used to provide species concentrations and temperatures in each cell. The radiation computation was performed using the tangent slab approximation and radiative results obtained from the new databasing schemes were compared with those of NEQAIR. Due to the fact that diatomic species contribute much less to the radiative heat flux compared to atomic emitters, it is not necessary to use a fine wavelength resolution for the entire wavelength range. Hence, a variable wavelength increment in this calculation was used as follows: $\Delta \lambda = 0.005 \, \text{Å}$ for 500 to 5,000 Å, $\Delta \lambda = 0.01 \, \text{Å}$ for 5,000 to 14,000 Å.
Radiative transfer calculations were performed along two lines - the stagnation streamline and one of the lines normal to the vehicle shoulder body. The flowfield solutions are obtained from the Data Parallel Line Relaxation (DPLR) CFD code[27, 36] and Direct Simulation Monte Carlo (DSMC) method[41]. The freestream conditions of each flow solver are listed in Table 4.8. These flow solvers include chemical reaction processes of 11 species such as N, O, N\(^+\), O\(^+\), N\(_2\), O\(_2\), NO, N\(_2\)\(^+\), O\(_2\)\(^+\), NO\(^+\) and e\(^-\).

Figure 4.13 shows the locations of the stagnation streamline and shoulder line for the Stardust vehicle. For the two locations, the radiative heat generation per unit volume was calculated using the database and compared with the results of NEQAIR. The spatial distribution of number densities of the six radiating species such as N, O, N\(_2\)\(^+\), NO, N\(_2\), O\(_2\) and e\(^-\) and the temperature along the stagnation streamline and the shoulder line of DPLR flowfield are shown in Figs. 4.14 and 4.15, respectively. It can be seen that atomic species such as N and O are dominant in the shock layer due to the strong dissociation of the molecular species. The figure also shows that the electron number density is high in the shock layer due to ionization processes.

Figure 4.16 shows comparison of the total emission and radiative heat generation per unit volume from the aforementioned six radiating species calculated using the database and NEQAIR. The horizontal axis in Fig. 4.16 indicates the distance from the vehicle wall. In these calculations, all three types of transitions for the two atomic species and 26 electronic band systems of the four diatomic species were considered. Since electron temperature is not calculated directly in the DPLR CFD flow solver, it is assumed to be equal to translational temperature for radiation calculation using the database and NEQAIR. In order to confirm the accuracy of the emission coefficients from the
database, total emission along the two lines was compared with NEQAIR results. Due to the fact that radiation from atomic species is dependent on electron temperature, location of the maximum peak heat generation coincides with that of the maximum electron temperature. Good agreement of radiative heat generation and total emission between the new database and NEQAIR is obtained with errors below 0.5% in the peak heating region. Figures 4.17 through 4.21 show number densities and temperature profiles along the stagnation streamline and shoulder line obtained from the DSMC flowfield at 68.9 km and 81 km altitudes, respectively. Figures 4.19 through 4.22 show that the new database and NEQAIR predict the same amount and spatial dependency for radiative heat generation and total emission along the stagnation streamline and shoulder line of the Stardust blunt body at 68.9 km and 81 km altitudes, respectively. In the DSMC method, the electron temperature can be directly calculated and is predicted to be lower than the total averaged translational temperature in the shock layer for both 68.9 km and 81 km altitudes. From the figures, it can be seen that the database and NEQAIR predict that there is significant heat generation and total emission created in the high electron number density and electron temperature region. This result is reasonable because radiation from atomic species is strongly dependent on electron number density and temperature. Finally for the stagnation streamline and shoulder line, it is found that the radiative heat generation calculated using the spectral data from the database is in good agreement with NEQAIR with an error below 1% in the high radiative heating region.
Table 4.1. Datasets for $\varepsilon^c_\lambda$ and $\kappa^c_\lambda$ of atomic O

<table>
<thead>
<tr>
<th>Wavelength(Å)</th>
<th>$\varepsilon^c_\lambda$ (W/sr)</th>
<th>$\kappa^c_\lambda$ (cm$^3$)</th>
<th>Upper (NEQAIR Indices)</th>
<th>Lower Indices</th>
</tr>
</thead>
<tbody>
<tr>
<td>807.365</td>
<td>$1.374 \times 10^{-10}$</td>
<td>$3.957 \times 10^{-24}$</td>
<td>19</td>
<td>1</td>
</tr>
<tr>
<td>879.450</td>
<td>$7.007 \times 10^{-11}$</td>
<td>$3.095 \times 10^{-24}$</td>
<td>19</td>
<td>1</td>
</tr>
<tr>
<td>879.538</td>
<td>$2.156 \times 10^{-10}$</td>
<td>$9.526 \times 10^{-24}$</td>
<td>19</td>
<td>1</td>
</tr>
<tr>
<td>880.599</td>
<td>$5.742 \times 10^{-11}$</td>
<td>$2.553 \times 10^{-24}$</td>
<td>19</td>
<td>1</td>
</tr>
<tr>
<td>880.648</td>
<td>$4.252 \times 10^{-11}$</td>
<td>$1.891 \times 10^{-24}$</td>
<td>19</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 4.2. Datasets for $\varepsilon^c_\lambda$ and $\kappa^c_\lambda$ of atomic N

<table>
<thead>
<tr>
<th>Wavelength(Å)</th>
<th>$\varepsilon^c_\lambda$ (W/sr)</th>
<th>$\kappa^c_\lambda$ (cm$^3$)</th>
<th>Upper (NEQAIR Indices)</th>
<th>Lower Indices</th>
</tr>
</thead>
<tbody>
<tr>
<td>1101.276</td>
<td>$2.841 \times 10^{-11}$</td>
<td>$3.8633 \times 10^{-24}$</td>
<td>12</td>
<td>2</td>
</tr>
<tr>
<td>1134.725</td>
<td>$6.962 \times 10^{-11}$</td>
<td>$1.0966 \times 10^{-23}$</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>1134.975</td>
<td>$1.392 \times 10^{-10}$</td>
<td>$2.2012 \times 10^{-23}$</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>1135.535</td>
<td>$1.837 \times 10^{-10}$</td>
<td>$2.9113 \times 10^{-23}$</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>1164.412</td>
<td>$2.605 \times 10^{-13}$</td>
<td>$4.6820 \times 10^{-25}$</td>
<td>10</td>
<td>2</td>
</tr>
</tbody>
</table>
Table 4.3. Electronic transitions of diatomic species in NEQAIR

<table>
<thead>
<tr>
<th>Molec.</th>
<th>Name</th>
<th>Spectral Range (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2^+$</td>
<td>1$^-$ (1st negative)</td>
<td>2,547 $\sim$ 25,759</td>
</tr>
<tr>
<td>$N_2^+$</td>
<td>Meinel</td>
<td>2,749 $\sim$</td>
</tr>
<tr>
<td>$N_2$</td>
<td>1$^+$ (1st positive)</td>
<td>4,125 $\sim$</td>
</tr>
<tr>
<td>$N_2$</td>
<td>2$^+$ (2nd positive)</td>
<td>2,602 $\sim$ 7,229</td>
</tr>
<tr>
<td>$N_2$</td>
<td>Birge-Hopfield</td>
<td>870 $\sim$ 1,568</td>
</tr>
<tr>
<td>$N_2$</td>
<td>Birge-Hopfield 2</td>
<td>827 $\sim$ 1,889</td>
</tr>
<tr>
<td>$N_2$</td>
<td>Carrol-Yoshino</td>
<td>845 $\sim$ 1,240</td>
</tr>
<tr>
<td>$O_2$</td>
<td>Schumann Runge</td>
<td>1,763 $\sim$ 5,919</td>
</tr>
<tr>
<td>NO</td>
<td>Beta</td>
<td>1,681 $\sim$ 9,210</td>
</tr>
<tr>
<td>NO</td>
<td>Gamma</td>
<td>1,653 $\sim$ 5,403</td>
</tr>
<tr>
<td>NO</td>
<td>Delta</td>
<td>1,553 $\sim$ 3,519</td>
</tr>
<tr>
<td>NO</td>
<td>Epsilon</td>
<td>1,532 $\sim$ 4,130</td>
</tr>
<tr>
<td>NO</td>
<td>Beta prime</td>
<td>1,479 $\sim$ 2,913</td>
</tr>
<tr>
<td>NO</td>
<td>Gamma prime</td>
<td>1,395 $\sim$ 2,229</td>
</tr>
<tr>
<td>NO</td>
<td>(C-A)</td>
<td>5,700 $\sim$</td>
</tr>
<tr>
<td>NO</td>
<td>(D-A)</td>
<td>6,436 $\sim$ 47,484</td>
</tr>
<tr>
<td>NO</td>
<td>B'-B</td>
<td>4,777 $\sim$ 57,779</td>
</tr>
<tr>
<td>NO</td>
<td>E-C</td>
<td>5,186 $\sim$ 70,955</td>
</tr>
<tr>
<td>NO</td>
<td>F-C(3)</td>
<td>6,087 $\sim$ 129,110</td>
</tr>
<tr>
<td>NO</td>
<td>H-C</td>
<td>5,689 $\sim$ 110,131</td>
</tr>
<tr>
<td>NO</td>
<td>H'-C</td>
<td>5,845 $\sim$ 82,550</td>
</tr>
<tr>
<td>NO</td>
<td>E-D(5)</td>
<td>6,870 $\sim$ 38,754</td>
</tr>
<tr>
<td>NO</td>
<td>F-D(3)</td>
<td>6,447 $\sim$ 36,623</td>
</tr>
<tr>
<td>NO</td>
<td>H-D</td>
<td>7,019 $\sim$ 24,737</td>
</tr>
<tr>
<td>NO</td>
<td>H'-D(5)</td>
<td>6,940 $\sim$ 14,439</td>
</tr>
<tr>
<td>NO</td>
<td>IR</td>
<td>2,986 $\sim$ 178,078</td>
</tr>
</tbody>
</table>

Table 4.4. Dataset example for $N_2^+$ 1st negative transition

<table>
<thead>
<tr>
<th>Wavelength(Å)</th>
<th>$\varepsilon_x^f$ (W/sr)</th>
<th>$-\frac{hc}{k_B} G(V_U)$ (K)</th>
<th>$-\frac{hc}{k_B} F(J_U)$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2547.335</td>
<td>$1.149 \times 10^{-15}$</td>
<td>$-3.486 \times 10^4$</td>
<td>$-1.265 \times 10^2$</td>
</tr>
<tr>
<td>2547.340</td>
<td>$9.848 \times 10^{-16}$</td>
<td>$-3.486 \times 10^4$</td>
<td>$-9.488 \times 10^1$</td>
</tr>
<tr>
<td>2547.353</td>
<td>$1.149 \times 10^{-15}$</td>
<td>$-3.486 \times 10^4$</td>
<td>$-1.265 \times 10^2$</td>
</tr>
<tr>
<td>2547.355</td>
<td>$9.847 \times 10^{-16}$</td>
<td>$-3.486 \times 10^4$</td>
<td>$-9.487 \times 10^1$</td>
</tr>
<tr>
<td>2547.364</td>
<td>$1.313 \times 10^{-15}$</td>
<td>$-3.486 \times 10^4$</td>
<td>$-1.626 \times 10^2$</td>
</tr>
</tbody>
</table>
Table 4.5. Dataset example for $N_2^+$ 1st negative transition-Continued

<table>
<thead>
<tr>
<th>Wavelength(Å)</th>
<th>$\frac{hc}{k_B}(G(V_L) - G(V_U))$ (K)</th>
<th>$\frac{hc}{k_B}(F(J_L) - F(J_U))$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2547.335</td>
<td>1.968×10^4</td>
<td>16.318</td>
</tr>
<tr>
<td>2547.340</td>
<td>1.968×10^4</td>
<td>16.210</td>
</tr>
<tr>
<td>2547.353</td>
<td>1.968×10^4</td>
<td>15.915</td>
</tr>
<tr>
<td>2547.355</td>
<td>1.968×10^4</td>
<td>15.865</td>
</tr>
<tr>
<td>2547.364</td>
<td>1.968×10^4</td>
<td>15.679</td>
</tr>
</tbody>
</table>

Table 4.6. Comparison of computation time for narrow spectral region from 500 to 2,000 Å

<table>
<thead>
<tr>
<th>Species</th>
<th>NEQAIR</th>
<th>DATABASE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic Species</td>
<td>5.33 s</td>
<td>0.36 s</td>
</tr>
<tr>
<td>Diatomic Species</td>
<td>12.15 s</td>
<td>3.86 s</td>
</tr>
<tr>
<td>All Species</td>
<td>17.27 s</td>
<td>3.55 s</td>
</tr>
</tbody>
</table>

Table 4.7. Comparison of computation time for wide spectral region from 500 to 10,000 Å

<table>
<thead>
<tr>
<th>Species</th>
<th>NEQAIR</th>
<th>DATABASE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic Species</td>
<td>48.65 s</td>
<td>2.13 s</td>
</tr>
<tr>
<td>Diatomic Species</td>
<td>230.33 s</td>
<td>75.41 s</td>
</tr>
<tr>
<td>All Species</td>
<td>279.90 s</td>
<td>79.05 s</td>
</tr>
</tbody>
</table>
Table 4.8. Freestream conditions of Stardust reentry flow

<table>
<thead>
<tr>
<th></th>
<th>DPLR</th>
<th>DSMC (1)</th>
<th>DSMC (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Altitude (km)</td>
<td>61.76</td>
<td>68.9</td>
<td>81.0</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>10.871</td>
<td>11,902</td>
<td>12,600</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>234.95</td>
<td>224.0</td>
<td>217.6</td>
</tr>
<tr>
<td>Number density (m(^{-3}))</td>
<td>(4.407\times10^{21})</td>
<td>(1.603\times10^{21})</td>
<td>(2.639\times10^{20})</td>
</tr>
</tbody>
</table>

Fig. 4.1. Cutoff range of the Voigt line shape to satisfy 99.9\% integrated line for atomic line with respect to the ratio of Lorentzian to Voigt width which is less than 0.024.
Fig. 4.2. Comparison of emission (top) and absorption (bottom) coefficients of atomic O from 500 to 2,000 Å between the database and NEQAIR for $n_a = 1.1513 \times 10^{15}$ cm$^{-3}$, $n_+ = 3.8214 \times 10^{12}$ cm$^{-3}$, $n_{e} = 1.2667 \times 10^{14}$ cm$^{-3}$, $T_{trn} = 24,187$ K and $T_{e} = 17,485$ K.
Fig. 4.3. Comparison of emission (top) and absorption (bottom) coefficients of atomic O from 2,000 to 7,000 Å between the database and NEQAIR for $n_a = 1.1513 \times 10^{15}$ cm$^{-3}$, $n_+ = 3.8214 \times 10^{12}$ cm$^{-3}$, $n_e = 1.2667 \times 10^{14}$ cm$^{-3}$, $T_{trn} = 24,187$ K and $T_e = 17,485$ K.
Fig. 4.4. Comparison of emission (top) and absorption (bottom) coefficients of atomic N from 500 to 2,000 Å between the database and NEQAIR for \(n_a = 3.1609 \times 10^{15} \text{ cm}^{-3}\), \(n_+ = 5.5472 \times 10^{12} \text{ cm}^{-3}\), \(n_e = 1.2667 \times 10^{14} \text{ cm}^{-3}\), \(T_{trn} = 24,187 \text{ K}\) and \(T_e = 17,485 \text{ K}\).
Fig. 4.5. Comparison of emission (top) and absorption (bottom) coefficients of atomic N from 2,000 to 7,000 Å between the database and NEQAIR for $n_a = 3.1609 \times 10^{15}$ cm$^{-3}$, $n_+ = 5.5472 \times 10^{12}$ cm$^{-3}$, $n_e = 1.2667 \times 10^{14}$ cm$^{-3}$, $T_{trn} = 24,187$ K and $T_e = 17,485$ K.
Fig. 4.6. Maximum difference of emission (top) and absorption (bottom) bound-bound line strength of atomic N and O between the database and NEQAIR for the entire $n_e$ and $T_e$ conditions.
Fig. 4.7. Averaged difference of bound-free emission (top) and absorption (bottom) coefficient of atomic N and O between the database and NEQAIR for the entire $n_e$ and $T_e$ conditions.
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Chapter 5

Coupled DSMC-Photon Monte Carlo Radiation Simulations

5.1 Preface

To perform spectrally accurate radiation simulations with the FV-PMC method, a wavelength selection scheme is required to be developed and integrated with the FV-PMC code. The emission random number database (ERND) and schemes to efficiently select the wavelength of emitted photon bundle were successfully implemented and validated.[50] DSMC simulations coupled with the FV-PMC method were performed for the reentry trajectory of the Stardust SRC body from the transitional (81 km) to the peak heating (61.8 km) flow regime. The effect of radiation on the flow properties such as translational and internal temperatures and the convective heating rate to the surface is investigated and compared with the baseline flow solution that neglected the effects of radiation. The stagnation-point convective and radiative heating rates with respect to the freestream conditions for all altitudes calculated from the coupled DSMC-FV-PMC simulations are compared to those from the former gas-dynamics coupled with radiation research using CFD and one-dimensional radiative transport modeling.
5.2 Finite Volume Photon Monte Carlo Method for Non-Gray Radiation

5.2.1 Wavelength Selection in the FV-PMC Procedure

The emitting species for a given ray is selected, based on the ratio of the emitting energies for each species to the total emission. For a given photon bundle, a wavelength is selected by comparing a random number, $R_\lambda$, to the ratio of the partially integrated emission to the total integrated emission, $R_\lambda = \frac{Q_{emis,\lambda}}{Q_{emis}} = \frac{\int_{\lambda_{min}}^{\lambda} \varepsilon_\lambda d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} \varepsilon_\lambda d\lambda}$ (5.1)

where $\lambda$ is the corresponding wavelength of a photon bundle, and $R_\lambda$ is a random number uniformly distributed from 0 to 1. A bi-section method is used to select the value of wavelength between $\lambda_{min}$ and $\lambda_{max}$ as it needed to evaluate Eq. (5.1). An emission random number databases (ERND) was developed for conditions that occur in non-equilibrium flows,[50], based on NEQAIR-based emission and absorption coefficient database discussed in the Chapter 4.

In the aforementioned atomic database, the electronic excited population is calculated using the quasi steady state (QSS) model as a function of electron temperature $T_e$, electron number density $n_e$, and the ratio of ion to neutral number density, $n_+/n_a$. Emission and absorption coefficients are calculated as a function of $T_e$, $n_e$, $n_+/n_a$, and translational temperature $T_{trn}$. For N and O, 170 and 86 atomic lines are included in
the databases, respectively and the atomic lines are sorted in order of increasing wave-
length. Based on investigations of hypersonic reentry flowfields[36, 41], the important
range of the electron temperature, $T_e$, has been identified as 1,000-28,000 K, and simi-
larly for electron number densities, $n_e$, as $1 \times 10^{13} - 4 \times 10^{16}$ cm$^{-3}$. For each atomic line,
normalized accumulated emission coefficients have been databased for equidistant values
of $T_e^{0.1}$ (70 points) and $[\log(n_e)]^{0.1}$ (50 points). For bound-free transitions, partially
integrated emission is stored as a function of $\lambda$ for each $T_e$, $n_e$, and $n_+/n_a$ condition.
For continuum transitions, the considered wavelength range is from 500 to 6000 Å with
a resolution of 10 Å.

Once the emission and absorption coefficient database is available, separate ERND
bound-bound, bound-free, and free-free continuum transition databases are constructed.
Note that, however, for the Stardust reentry cases considered here, the contribution
of free-free transitions is negligible and are not considered further. For bound-bound
transitions, the line-center wavelength $\lambda_k$ (Å) and the normalized accumulated emission
coefficient, $Q_{emis,k}^*(T_e, n_e, n_+/n_a)$, are stored. The normalized accumulated emission
coefficient is calculated as

$$Q_{emis,k}^* = \sum_{i=1}^{k} \varepsilon_i^*(T_e, n_e, n_+/n_a),$$

(5.2)
where $\varepsilon_i^*(T_e, n_e, n_+/n_a)$ is a normalized emission line strength, $\varepsilon_i$, which is normalized by $n_a$. Also, the partially integrated emission is calculated as

$$Q_{emis, \lambda}^* = \int_{\lambda_{min}}^{\lambda} \varepsilon_i^*(T_e, n_e, n_+/n_a, T_{trn}) d\lambda$$

$$= \sum_{i \leq k_1} \varepsilon_i^*(T_e, n_e, n_+/n_a) + \sum_{k_1 < i \leq k_2} \int_{\lambda-b_{hw,max}}^{\lambda} \varepsilon_{\lambda,i}^*(T_e, n_e, n_+/n_a, T_{trn}) d\lambda$$

$$= Q_{emis,k_1}^*(T_e, n_e, n_+/n_a) + \sum_{k_1 < i \leq k_2} \varepsilon_i^* \int_{\lambda-b_{hw,max}}^{\lambda} \phi_\lambda d\lambda, \quad (5.3)$$

where $\phi_\lambda$ is the line broadening function. In Eq. (5.3), the first line index $k_1$ corresponds to the maximum integer and is selected by determining whether $\lambda_{k_1} < \lambda - b_{hw,max}$ where $b_{hw,max}$ is the maximum half-width for the type of line broadening that is assumed. Since we assume that the line shape is a Voigt profile, we use a constant value of $b_{hw,max} = 50.0$ Å, a value adequate to cover the half-width for hypersonic flow conditions. The second line index $k_2$ is the maximum integer selected by $\lambda_{k_2} < \lambda + b_{hw,max}$. The wavelength selection process is the most time-consuming portion of the PMC procedure. To select a wavelength, a bi-section method is used following Eq. (5.1). In the spectral module, $k_1$ and $k_2$ are thus efficiently found, and the partially integrated emissions are calculated effectively. Additional details of the wavelength selection procedure and the ERND can be found in Ref. [50].
5.2.2 Validation

To validate the DSMC FV-PMC approach, a series of 1-D disks were constructed using the Stardust stagnation streamline flow conditions obtained from the DSMC solution at 71.9 km. Figure 5.1 (top) shows a comparison of the radiative source term ($\nabla \cdot q_R$) obtained from the DSMC-PMC with an exact tangent-slab simulation. In both calculations, atomic N and O radiation including bound-bound and bound-free transitions are considered. For this flow condition, the emitted energy of the photon rays are highly absorbed by the medium because the flow is optically thick. The magnitude of the net radiative heat source is small compared to the emission energy, e.g., at $X=-0.0105$ m the fraction of the divergence of the radiative heat flux to the emission energy is approximately 1.8 %. As is shown in Fig. 5.1 (top), good agreement is achieved between the PMC and TS calculations and the small differences in the radiative heat source term may be attributed to the small variation in flow properties in the direction normal to the surface. The highest statistical error in the divergence of the heat flux in the stagnation region was found to be less than 5 %. The FV-PMC code is parallelized by assigning “columns” of cells orthogonal to the surface to each processor. Then each processor traces photons emitted from its “column” of cells until they are absorbed or leave the domain. Even though a single photon-bundle is emitted from a specified cell assigned on a processor, the tracing of this photon bundle is performed on that processor for the entire computational domain. After the tracing is completed by multiple processors, in parallel, the main processor gathers the information of the tracing results (absorbed energy) from each processors to compute the radiative source term. Two hundred million
photon bundles were traced through the entire domain, taking about 10 CPU hours with 16 processors. Note that when the volume-based weighting method given in Eq. (3.72) was used more than five hundred million photon bundles were required to obtain about a 5% statistical error near the symmetry axis. The same level of accuracy was obtained using the cross-section based method to determine the number of photon rays per cell given in Eq. (3.73) at about a CPU time savings of more than a factor of two. The same validation case was performed for the lower altitude of 61.8 km and is shown in the bottom portion of Fig. 5.1. Similar to the results of higher altitude case, the agreement between the radiative heat fluxes predicted by the 1-D PMC disk and TS methods is good. Again the emitted energy of the photon rays is highly absorbed by the medium due to the fact that flow is optically thick. Hence the magnitude of the net radiative heat source term is as small as 1.2% compared to the total emission energy at $X=-0.0155$ m.

5.3 Coupled DSMC-PMC Simulation Results

5.3.1 Coupled DSMC Calculations with PMC at 81, 71.9 and 65.4 km altitudes

First the effect of radiation coupling on the shock layer flowfield at 81 km altitude is considered. At 81 km altitude, coupling effect of radiation on the flowfield was found to be negligible. Figure 5.2 shows a comparison of distributions of the translational, rotational, vibrational and electron temperatures along the stagnation streamline between two simulations with and without radiation at 81 km. It is seen that there is no significant change of temperatures due to the radiation. The convective heat flux was not
changed due to the radiation as shown in the top portion of Fig. 5.3. Without radiation coupling, the convective heat flux at the stagnation point was approximately $1.8 \times 10^6$ W/m$^2$ and, thus, the heating on the surface is not as crucial as for lower altitude cases. With radiation coupling, the convective heat flux at the stagnation point is decreased by only 5%, and the radiative heat flux contributes to the total heat flux is about 16% at 81 km. Total of three iterations of DSMC-PMC coupled calculation were performed until the convergence of both flowfield and radiation was achieved as shown in the bottom of Fig. 5.3. By seeing this figure it is also verified that there is no change of convective heat flux with respect to the coupling iteration due to the small effect of radiation at 81 km. The radiative heating is unchanged with respect to the coupling iteration due to no significant change of flowfield.

Figure 5.4 shows a comparison of distributions of the translational, rotational, vibrational and electron temperatures along the stagnation streamline between two simulations with and without radiation at 71.9 km. The simulation results shown with radiation coupling are those obtained after the final coupling iteration. Along the stagnation streamline, the peak in the radiation profile was found to be located at $X=-0.015$ m (not shown). It can be seen that the temperature profile remains the same upstream of this location, but, from $X=-0.015$ m to the surface, the effect of radiative cooling on the temperature profile can be observed. After two coupling iterations, the maximum decrease in the translational and internal temperatures was approximately 8,000 and 5,500 K, respectively, as energy was removed from the flow in the form of radiation. However, in the third iteration, radiative energy was added back to the flow because the amount of energy removed due to the radiation cooling effect was overestimated in the first two
iterations. This over-correction causes the gas temperatures to increase after the third coupling iteration. As the coupling is repeated, it is found that the translational and internal temperatures converge. Finally, after the fifth iteration of DSMC-PMC coupling, the translational and internal temperatures were observed to drop by about 5,000 and 3,500 K, respectively.

Now we turn to the quantities and profiles of heat flux. Figure 5.5 (top) shows a comparison of the convective heat flux and the radiative heat flux without and with the final converged value of radiation to the surface at 71.9 km. Due to the radiative cooling effect, the convective heat flux along the surface from the stagnation point to the shoulder decreases. The maxima in the radiative heat flux are observed to be in both the stagnation region as well as the shoulder because of the high electron number densities and temperatures, as can also be seen in Fig. 2.4. Figure 5.5 (Bottom) presents the convective and radiative heat flux to the stagnation point as a function of coupling iterations. The results show that after about four iterations both convective and radiative heat fluxes are converged within 5 % and that the convective heat flux decreases when coupled to the radiation. The convective heat flux was found to be affected by radiation heat coupling and decreased by 23 % after two iterations and 14 % after the final coupling iteration. The contribution of radiative heat flux to the total heat flux is about 43 % at this altitude. Since the DSMC simulations assumed a non-catalytic surface condition for this case, the convective heating rate is lower than CFD results, which are usually reported for fully catalytic surface conditions.[1] For this reason, the contribution of the radiative flux to the total heat flux is higher than usually shown. However, there are large uncertainties in the degree of catalyticity and in cases where a wall material
warrants a non-catalytic model, the results show that the effect of the radiative heating to the total heat flux is not negligible.

At 65.4 km altitude, the convective heat flux to the surface is decreased by 16% due to the radiation, and the translational and internal temperatures drop by 3,500 and 2,500 K, respectively. The converged radiative heat flux to the stagnation point is \(3.07 \times 10^6\) W/m\(^2\), which is 47% of total heat flux assuming a non-catalytic surface condition in DSMC. The converged DSMC-PMC coupled results within 5% convergence criterion are achieved after the five iterations.

### 5.3.2 Coupled DSMC Calculations with PMC at 61.8 km

At peak heating we first consider the effect of radiation on the flowfield and then the importance of radiative coupling on the heat fluxes. Figure 5.6 shows a comparison of distributions of the translational, rotational, vibrational and electron temperatures along the stagnation streamline between cases without and with (final iteration) radiation cooling at 61.8 km altitude. The DSMC-PMC calculations were iterated until both the flow macroparameters and radiation are converged within 5% criterion, which at this altitude occurred after three iterations. Along the stagnation streamline, the radiation peak is located near \(X=-0.015\) m, and the effect of radiative cooling on the flow along the stagnation streamline can be seen between \(X=-0.015\) m and the surface in the figure. Translational and internal temperatures decreased by a maximum of approximately 2,000 and 1,500 K, respectively, due to the high radiative energy in this region after one iteration of DSMC-PMC coupling. At this altitude, after the first iteration,
the temperature profiles did not change significantly as additional coupling calculations were performed.

The convective and radiative heat fluxes to the vehicle surface were also calculated and compared for cases with and without radiation at 61.8 km in Fig. 5.7. The convective heat flux spatial distribution is similar to that at the higher altitude of 71.9 km, but, in this case, the peak radiative heat flux is at the stagnation point. The radiative heat flux spatial dependence is consistent with the electron number density and temperature contours shown in Fig. 2.6 where both parameters are seen to have maximum values in the stagnation region only. It is also observed that the convective heat flux along the surface is reduced by the effect of radiation cooling. Figure 5.7 (bottom) presents the convective and radiative heat flux to the stagnation point with respect to the coupling iterations. The figure shows that both the convective and radiative heat fluxes are nearly converged after the first iteration. It can be seen that surface convective heat flux after the first coupling iteration decreases by 21% due to radiation. However, with further coupled iterations, the convective heat flux obtained from the third iteration is not significantly different from the second iteration result, and finally, the convective heat flux after three iterations is reduced by 13%. The behavior in the change of the convective heat flux as a function of iteration at the stagnation point is also consistent with the small change in the translational temperature profiles shown in the top portion of Fig. 5.6. The contribution of the radiative heat flux to the total heat flux is approximately 46% at this altitude. Since there is no additional heat at the surface due to atomic recombination using the non-catalytic surface condition, the convective heating rate to the surface is
not much higher than the radiative heating. Thus, the effect of radiative heating to the non-catalytic surface must be considered at the vehicle design stage.

In summary, the net effect of radiation on the flowfield temperatures and heat fluxes are similar at both 71.9 and 61.8 km altitudes. However, the detailed convergence of the flow-radiation coupling is different. At the lower altitude, the radiative energy does not influence the distribution of energy modes in the gas because the flow is sufficiently dense to be closer to thermo-chemical equilibrium. This is consistent with the fact that the QSS solution of the electronic state populations are dominated by electron impact collisions. Thus, the temperatures and convective heat flux are not changed after even the first iteration. In contrast, at the higher altitude it was found that flow noticeably changes after the first and second radiation coupling iterations, but the flow change is overestimated. Further iterations are required to obtain converged temperature and convective heat flux.

5.3.3 Uncertainty Estimation of Radiative Heat Flux due to the Statistical Deviation of Flow Properties in DSMC

Since the DSMC is a statistical particle method, the finite sample size (related to numbers of particles and collisions) will affect the uncertainty in the radiation predictions. The PMC approach for modeling the RTE is also a statistical approach and its uncertainty levels are related to the number of photon bundles selected. The selection of the two different sets of numerical parameters for each method are completely independent, suggesting that we can estimate the total uncertainty in the radiative heat flux by taking the square root of the sum of squares of the individual uncertainties in
DSMC and PMC. The PMC simulations in this work used a number of photon bundles that generally corresponded to an uncertainty of 1% or less, as listed in the first row of Table 5.1. It will be seen that PMC uncertainties are smaller than DSMC so that the major contribution to the uncertainty in the radiative heat flux is due to the noise in DSMC implied by the finite numbers of particles and cells listed in the last two rows of Table 2.1.

The most thorough analysis would use multiple DSMC flows based on the standard deviation of the different macroparameters as input to a number of separate PMC simulations. The average and standard deviation of the radiation computed using the PMC simulation would then illustrate the effect of the DSMC uncertainties on the PMC radiation calculation. Unfortunately, running the PMC over such a highly multidimensional parameter space would be difficult. For this reason we made two reasonable approximations to make the assessment feasible. First we used the much faster tangent slab approximation to the RTE which is as accurate as the PMC at the stagnation point, the location where the uncertainty estimation is being performed. Then we assumed that the spread in DSMC values in each cell along the stagnation streamline of electron temperature and number density, the two macroparameters which are the important properties to compute radiation, could be represented by different normal distributions, each with a confidence level of 95 %. Note that when we repeated the entire analysis of the uncertainty in the stagnation-point radiative heat flux assuming a confidence level of 99% to define the macroparameter normal distribution functions, there was no significant difference in the mean and standard deviation of the stagnation-point radiative heat
flux. The neutral atom number densities and translational temperature are also important factors to calculate radiation, however, the noise in these parameters is negligibly small and was neglected in this analysis. The statistical parameters of the mean value and the standard deviation of the DSMC two aforementioned flow macroparameters were calculated using 30,000 sampling steps in each cell along the stagnation streamline. The minimum and maximum value of the ratio of the standard deviation to the mean value for the two macroparameters in the approximately 25 cells along the stagnation streamline are given for each altitude in the second and third row of Table 5.1. It can be seen that the standard deviations are largest for the higher altitude of 81 km, consistent with the smaller number of DSMC particles. The maximum uncertainty values presented in the second and third row correspond to values in the freestream and therefore will have little effect on the radiation uncertainty because the emission is orders of magnitude lower than the peak values in the shock.

With the macroparameter distributions so prepared we then sampled the electron number density and temperature values using the acceptance-rejection method[40] which is based on the assumption that flow properties follow a normal distribution function with a confidence level of 95 %. For each sample, the stagnation-point radiative heat flux was calculated using this flow sampled data in the TS approximation. This procedure was repeated 1,000 times, a value that was determined to be sufficient such that both the averaged and standard deviation values of the stagnation-point radiative heat flux remained unchanged.

The uncertainties in the radiative heat flux to the stagnation point at each altitude are summarized in the fourth row of Table 5.1. It can be seen that the DSMC-TS
uncertainty is higher than the pure uncertainty in the PMC method at all altitudes. Both the pure PMC and DSMC-TS uncertainties at 81 km are higher than at the lower altitudes because the number of simulated particles and photon bundles used in that case was less than for the lower altitudes, which in turn, leads to the higher statistical variation in both DSMC and PMC. It can clearly be seen, however, that the total uncertainty in the DSMC-TS and PMC simulations is sufficiently small such that the DSMC and the PMC predictions of the variation of the radiative heat flux with altitude are much greater than the statistical uncertainties. Hence the coupled DSMC-PMC simulations can be used to understand the dependence of heat flux with altitude for a reentry trajectory, as will be discussed in the next subsection.

5.3.4 Discussion of Convective-Radiative Heating during the Stardust Reentry Trajectory

In this section, a comparison of the stagnation-point convective and radiative heat fluxes for the Stardust vehicle along the reentry trajectory obtained from the coupled DSMC/FV-PMC method with previous results is discussed. Figure 5.8 shows a comparison of convective heat flux to the stagnation point with and without radiation coupling as a function of the product of the square root of the freestream mass density and the freestream velocity raised to the cubic power. The latter is chosen for the abscissa of the figure based on the correlation of convective heat flux with freestream conditions suggested by Sutton[77] and discussed further in Anderson[78]. Also shown is a comparison of our DSMC results with the previous CFD calculations performed by Olynick et al. [1]. First it can be seen that both CFD and DSMC predict a linear dependence
of convective heat flux with the freestream correlation. It can also be seen that the DSMC-PMC coupled convective fluxes have a very similar dependence with altitude to the DSMC without radiation values. The difference in magnitudes between these two cases is small, but some decrease in the convective heat flux occurs when radiative cooling is taken into account. Both set of results are consistent with the results presented earlier in Sec. 5.3. The difference in the DSMC results with those of Olynick et al.[1] is a factor of two to three and is due to the use of the fully catalytic surface condition in the CFD simulations. This conclusion was validated by performing DSMC simulations with a catalytic surface condition using the implementation discussed in Chapter 2. The DSMC simulations are not coupled with the PMC radiation, however, and the effect of radiation coupling on the convective heat flux is much smaller than the gas-surface interaction model. Given the very different numerical approaches, the CFD and DSMC convective heat flux dependence with freestream conditions are believed to be in good agreement and the difference is within 20%.

The radiative heat flux to the stagnation point at the same four altitudes is shown in Fig. 5.9. In this figure, two PMC radiation results, which use Doppler and Voigt line shapes, are compared to Olynick’s results and the radiative heat flux correlation suggested by Tauber and Sutton.[79] In the correlation of Tauber and Sutton[79] stagnation-point radiative heating relations for Earth and Mars entries were developed using an equilibrium radiation model coupled with an inviscid flowfield code that assumed thermo-chemical equilibrium conditions. Their relationship[79] used tabulated radiative heating velocity functions and a linear interpolation to calculate the stagnation-point radiative heating rate. The radiative heating is not quite linearly related to the freestream
velocity and density. We obtained the correlation of $\rho_\infty^{1.22} V_\infty^3$ as our independent variable on the X-axis of Fig. 5.9 by trial and error. The power of the freestream number density is given by the Tauber and Sutton correlation, but, the freestream velocity power dependence was selected such that the radiative heat flux should vary linearly with it. This freestream correlation used above to calculate the abscissa for the convective heat flux is used again in Fig. 5.9.

Two important conclusions can be drawn from Fig. 5.9, i.e., the DSMC, CFD, and Tauber-Sutton correlation have different magnitudes and altitude dependence. The agreement, however, between the CFD and the correlation is not better than the DSMC-CFD agreement because the flow and radiation model used in the correlation are different from Olynicks CFD calculation. In Tauber and Suttons work, thermo-chemical equilibrium and non-ablation are assumed throughout. The differences in flow modeling between the two continuum approaches also have a large influence on the radiative heating and has been shown by Hash et al\cite{34}, even when different continuum flow models predict similar convective heating, the radiative heating rates can be significantly different.

With respect to the DSMC-PMC coupled simulations we see that using the Doppler line shape predicts a different freestream dependence compared to that obtained using the Voigt line shape. In addition, the stagnation-point radiative heating calculated from the DSMC-PMC with the Doppler line shape is not linearly related to the freestream correlation. Since Doppler line broadening is only dependent on the translational temperature, the wings of narrow atomic lines are not sufficiently broadened compared to the Voigt line shape so that the net radiatively transferred energy is
almost re-absorbed near the line-center wavelength. However, for the high electron concentration flows discussed here, electron collisions are an important mechanism for line broadening. By using the Voigt line shape, the combination of Gaussian and Lorentzian line broadening components, the wings of a line extend further from the line-center allowing the transport of strong spectral radiative flux in the line wings. When the Voigt line shape is used in DSMC-PMC coupling calculations, the peak radiative heating occurs near 61.8 km altitude and the stagnation-point radiative heating rate is proportional to the freestream correlation, similar to the CFD results.

In addition, the question remains why the DSMC-PMC simulations that use the Voigt line-shape predict a radiative heat flux about a factor of two higher than the CFD results of Olynick. In Olynick's calculations the NOVAR radiation model, which was developed from the LORAN code was used. This model calculates atomic line and continuum and molecular radiation using a one-dimensional TS approximation. However, differences in the radiation approaches used in the DSMC and CFD results presented here are not assessed to be the main reason for the discrepancies in the radiative heat flux. Our previous comparisons with CFD simulations for Stardust as well as the DSMC simulations of others find that the electron temperature in DSMC is predicted to be nearly twice as high as the internal temperatures in continuum flow models.[39, 80] Since the population of the upper electronic levels for strong atomic emitters is strongly dependent on the electron temperature, this discrepancy between the CFD and DSMC simulations has a significant impact on the radiative heat flux. This discrepancy could probably be reduced by using similar thermo-chemical models in the two different gas
dynamic approaches\[34\] and should be strongly considered for reentry flows into highly non-equilibrium atmospheric conditions.
Table 5.1. Uncertainty in stagnation-point radiative heat flux due to the statistical variation of DSMC flows.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>81.0 km</th>
<th>71.9 km</th>
<th>65.4 km</th>
<th>61.8 km</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMC (%)</td>
<td>1.3</td>
<td>0.6</td>
<td>0.6</td>
<td>0.7</td>
</tr>
<tr>
<td>Min-Max ratio for $T_e$ (%)</td>
<td>1.3 - 59.6</td>
<td>1.2 - 39.0</td>
<td>0.6 - 15.3</td>
<td>0.4 - 29.5</td>
</tr>
<tr>
<td>Min-Max ratio for $n_e$ (%)</td>
<td>2.5 - 34.4</td>
<td>2.6 - 29.1</td>
<td>2.3 - 16.1</td>
<td>0.8 - 34.8</td>
</tr>
<tr>
<td>DSMC - TS Analyses (%)</td>
<td>5.2</td>
<td>2.4</td>
<td>2.4</td>
<td>1.4</td>
</tr>
<tr>
<td>Total $((\text{DSMC-TS Analyses}^2 + \text{PMC}^2)^{0.5}, %)$</td>
<td>5.4</td>
<td>2.5</td>
<td>2.5</td>
<td>1.6</td>
</tr>
</tbody>
</table>
Fig. 5.1. Comparison of $\nabla \cdot q_R$ along the stagnation streamline among the PMC 1-D disk, PMC Stardust geometry and 1D-TS at 71.9 km (top) and 61.8 km (bottom) altitudes.
Fig. 5.2. Comparison of distributions of the translational (top) and rotational, vibrational, electron (bottom) temperatures along the stagnation streamline between cases with and without radiation at 81 km altitude.
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Fig. 5.4. Comparison of distributions of the translational (top) and rotational, vibrational, electron (bottom) temperatures along the stagnation streamline between cases with and without radiation at 71.9 km altitude.
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Chapter 6

Effect of Non-Local Vacuum UltraViolet (VUV) Radiation on a Hypersonic Non-equilibrium Flow

6.1 Preface

In this chapter, the formulation of the escape factor for atomic N and O VUV radiative transitions, which are strong radiators of the Stardust reentry flow condition, is discussed, and its effect on the distribution of electronic state populations and the corresponding radiative heat transfer at 81 km altitude are investigated. Since there are insufficient collisions in the flow to ensure that the electronic states of the radiating species are in a Boltzmann distribution, a rate equation approach that includes collisional excitation/de-excitation and radiative transitions must be formulated. For altitudes lower than 81 km, the flow becomes continuum-like in nature and the electron concentration as well as those of neutrals and ions increases significantly.[41] Under these high number density flow conditions, the electronic excitation/de-excitation processes due to electron or heavy particle impact will dominate in determining the electronic state population. However, since the contribution of radiative transitions to electronic excitation/de-excitation processes becomes large at the 81 km altitude regime, the 81 km altitude flow condition is chosen to fully investigate the effect of non-local radiation. This condition corresponds to Knudsen numbers of transitional to rarefied non-equilibrium flows.
6.2 Entire Flowfield Simulation of Stardust SRC at 81 km in DSMC

The DSMC calculation was performed over the entire Stardust SRC body at 81 km altitude. The time step, cell size, computational domain, and total number of simulated molecules were selected to obtain flow results independent of these DSMC numerical parameters. Table 6.1 summarizes the number of simulated particles and collisional and macro parameter sampling cells. The total number of time steps was about 120,000 with a time step of $5.0 \times 10^{-8} \text{s}$ used for this case. Macro parameter sampling was started after 40,000 time steps, which was a sufficient time for the flowfield and heat flux to reach steady state. In summary, heat flux values along the surface and flow macro parameters were found to be converged for these numerical parameters.

Figure 6.1 shows the distribution of Mach number and streamlines around the Stardust SRC body at 81 km altitude. It is observed that the strong detached bow shock occurs in front of the vehicle body. It is also seen that flows are compressed at the forebody surface and expanded around the shoulder of the vehicle. In the backplate region, a re-circulation of flows occur, which was also shown in Ref. [81, 82].

Due to the strong dissociation of N$_2$ and O$_2$ molecules within the shock layer, atomic N and O species are dominant behind the shock as shown in Figs. 6.2 and 6.3. As was shown in Ref. [49] and Chapter 5, radiation is mainly generated by atomic N and O. Two other important factors that determine the strength of radiation are the electron number density and electron temperature distribution.[25] Figure 6.4 shows the distribution of electron number density about the Stardust SRC body. The maximum electron concentration was found to be in the region of the vehicle shoulder as well as near
the stagnation region. A similar distribution pattern of electron temperature was also observed, as shown in Fig. 6.5. The reason why the peak in the electron number density and electron temperature occurs near the shoulder region is that the majority of the gas particles pass through a strong shock wave and travel around the blunt body without being cooled by collisions with the surface. Since particles travel a longer distance through the shock layer than those particles traveling along the stagnation streamline, they experience more collisions which results in high degree of thermal excitation and chemical reactions[41]. It can be estimated that the highest radiative energy will be generated near the stagnation and shoulder region where both electron number density and temperature are high.

In the flow expanding region, it was found that there is a multiple spatial distribution of the electron temperature as shown in Fig. 6.5. Note that the multiple structure in the electron temperature is not observed in the spatial distribution of the electron number density shown in Fig. 6.4. In order to investigate the mechanisms responsible for generating such phenomena, only one ionization reaction (N+O → NO⁺ + e) of total five ionization reactions, which is the most important initiation process for a production of electrons[41], was considered. Although only one ionization reaction was used in the DSMC simulation, the spatial distribution of the electron temperature and its maximum values were not changed, whereas the electron number density decreased by about 50 %. Since the multiple maxima structure in the electron temperature in the flow expanding region might be dependent on the characteristics of flow properties formed near the shoulder and the side of the vehicle, flow properties along a normal line to the vehicle side (line (2) of Fig. 6.5) were investigated.
The calculation of the electron temperature in the DSMC simulation is dependent on the colliding cross-section model for collisions with other particles and the energy exchange/relaxation model with internal energy modes of molecules and ionization reaction processes. To examine the temperature distribution of the newly created electrons by the ionization process (N+O → NO\(^+\) + e) in the shoulder region, the velocity distribution functions of the electrons produced by the ionization reaction were obtained and the temperature of the newly produced electrons was then calculated. Figure 6.6 shows the profile of the translational temperature of atomic nitrogen, of the newly produced electrons from the ionization reaction (N+O → NO\(^+\) + e), and the steady state of final electron temperature, all along the line (2) of Fig. 6.5. The steady state profile of the electron temperature is obtained by the combination of electrons coming from the forebody region where the electron temperature is high and the newly created electrons by the ionization process. Since the atomic N is the dominant species, as shown in Fig. 6.7, collisions between the steady state electrons and atomic N species are a major process to determine the steady state electron temperature. Among the many factors related to the electron temperature, energy exchange and relaxation model between the electrons and molecular nitrogen are important in determining the vibrational and electron temperatures in the ionizing flow regime.[41, 63] However, due to the low concentration of N\(_2\), the contribution of energy exchange between electrons and N\(_2\) vibrational energy mode (e-V) to the steady state electron temperature is not significant. Figure 6.8 shows the steady state electron temperature profiles with and without the e-V relaxation model along the line (2) of Fig. 6.5. It is found that there is no significant difference of the steady state electron temperature. Therefore, the newly produced electrons gain energy by colliding
with atomic N species and the electron temperature is not significantly decreased as the
gas flow expands in the afterbody region. When surface reactions, such as the recombina-
tion of atomic N and O, or chemical ablation were considered, the double structure of
electron temperature in the afterbody disappeared because the atomic N was consumed
near the surface and the electron temperature near the side surface of the vehicle thus
decreases. Figure 6.9 shows the comparison of the electron temperature and atomic N
number density with and without the surface recombination of atomic N species along
the line (2). It can be seen that the electron temperature and atomic N concentration
near the surface decreases due to the consumption of N atoms during the surface re-
combination. Figure 6.10 also shows that the double structure of electron temperature
in the afterbody is removed when the surface recombination is employed. Figure 6.11
shows the electron temperature along the vertical lines from the vehicle surface located
at different horizontal locations. It is seen that the multiple structure of electron tem-
perature created near the side of the vehicle is developed in the flow expanding region
as shown in Fig. 6.11, which influences the spatial distribution of the radiative emission
as shown in Figs. 6.13 through 6.15. The radiative transport in the PMC method and
radiative energy distribution about the Stardust SRC body are discussed next.
6.3 Derivation of the Escape Factor for Non-local Collisional-Radiative Modeling of N and O

6.3.1 Master equation for electronic state populations

Under non-equilibrium flow conditions, there are not enough collisions to describe the electronic states by a Boltzmann distribution and, therefore, a rate equation approach is needed to calculate electronic state populations[25]. In non-equilibrium flow conditions, radiative transitions also have an important role in determining the electronic state of neutral species. A summary of the excitation/de-excitation processes of atoms was presented in Eqs. (3.17) through (3.20). The time rate of change of the number density of an electronically excited state, \( N_i \), is given by the difference between the sum of the rates of all collisional and radiative transitions that populate and depopulate state \( i \). The simple form for the rate equation of a specified transition from upper state \( i \) to lower state \( j \) can be written as,

\[
\frac{\partial N_i}{\partial t} = -K^e(i,j)N_in_e + K^e(j,i)N_jn_e - (\frac{\partial N_i}{\partial t})^{rad}_{ij} + (\frac{\partial N_i}{\partial t})^{rad}_{ji} + K(c,i)n_+n_e^2 - K(i,c)N_in_e + A(c,i)n_+n_e - A(i,c)N_i
\]  

(6.1)

The change of radiative energy per unit time, per unit area, distance and per unit solid angle is[38]

\[
h \frac{c}{\lambda} \frac{d}{d\Omega} \left( \frac{\partial N_i}{\partial t} \right)^{rad}_{ij} = (N_jB(j,i) - N_iB(i,j)) \frac{h}{\lambda} I_{\lambda}
\]  

(6.2)
Since the radiative transition occurs across a wavelength interval, Eq.(6.2) becomes

\[ \frac{d}{d\Omega} \left( \frac{\partial N_j}{\partial t} \right)_{ji} = \int_{\lambda_1}^{\lambda_2} \frac{(N_j B(j,i) - N_i B(i,j)) h \phi_{\lambda} I_{\lambda}}{hc/\lambda} d\lambda \]  

(6.3)

which becomes

\[ = \int_{\lambda_1}^{\lambda_2} \frac{\kappa_{\lambda} I_{\lambda}}{hc/\lambda} d\lambda \]  

(6.4)

where \( \kappa_{\lambda} \) is the absorption coefficient given by Ref. [29, 38] and \( I_{\lambda} \) and \( \phi_{\lambda} \) are the incident radiative intensity and the line broadening function, respectively. By integrating Eq.(6.4) over all directions, the fourth term in Eq.(6.1) is expressed as

\[ \left( \frac{\partial N_j}{\partial t} \right)_{ji}^{rad} = \int_{\lambda_1}^{\lambda_2} \frac{\kappa_{\lambda} \int_{4\pi} I_{\lambda} d\Omega}{hc/\lambda} d\lambda \]  

(6.5)

where \( G_{\lambda} = \int_{4\pi} I_{\lambda} d\Omega \) is the integrated incident radiative intensity from over all directions. The final form of the rate equation can be written as,

\[ \left( \frac{\partial N_j}{\partial t} \right) = -K^c(i,j)N_i n_e + K^c(j,i)N_j n_e - A(i,j)N_i + \int_{\lambda_1}^{\lambda_2} \frac{\kappa_{\lambda} G_{\lambda}}{hc/\lambda} d\lambda + K(c,i)n_+ n_e^2 - K(i,c)N_i n_e + A(c,i)n_+ n_e - A(i,c)N_i \]  

(6.6)

where the third term on the right hand side comes from the standard definition of the Einstein transition coefficient for spontaneous emission. The fourth term in Eq. (6.6) represents the number of transitions from a lower to an upper electronic state due to the absorption of incoming radiative intensity where \( G_{\lambda} \) is defined as the spectral incoming intensity transferred from every other points in the flowfield. In Eq. (6.5), the fraction
of the incoming intensity that contributes to the absorption from a lower to a higher electronic state may be obtained by multiplying the incoming intensity by an absorption coefficient $\kappa_\lambda$. The escape factor, $\rho_{ij}$, the ratio of the number of transitions from a lower to an upper electronic state to the number of transitions leaving the upper electronic state due to spontaneous emission is determined by subtracting this ratio from unity, i.e.,

$$\rho_{ij} = 1 - \frac{\int_{\lambda_1}^{\lambda_2} \frac{\kappa_\lambda G_\lambda d\lambda}{hc/\lambda}}{A(i,j)N_i}$$  \hspace{1cm} (6.7)

This form is consistent with earlier formulations in the literature of Ref. [33] and [52].

When Eq. (6.7) is substituted into Eq. (6.1), we obtain,

$$\left( \frac{\partial N_i}{\partial t} \right) = -K^e(i,j)N_in_e + K^e(j,i)N_jn_e - \rho_{ij}A(i,j)N_i$$

$$+ K(c,i)n_+n_e^2 - K(i,c)N_in_e + A(c,i)n_+n_e - A(i,c)N_i$$  \hspace{1cm} (6.8)

Finally, in the QSS assumption the left hand side of Eq. (6.8) is set to be zero because electronic transitions in the VUV occur at a much faster time scale than the gas dynamic residence time in hypersonic shocks. As the escape factor goes to unity, which means that the flow is optically thin, the emitted photons from a specific upper electronic state all escape from the vicinity and, as can be seen from Eq. (6.8), the population of the upper electronic state decreases. However, when the escape factor approaches zero, indicating that the flow is optically thick, the emitted photons are re-absorbed during the transition from a lower to an upper electronic state and the corresponding upper electronic state density is re-populated. In high density flows, the collision rate
is much greater than the radiative transition rate and the distribution of electronic state populations becomes close to the Boltzmann distribution regardless of the value of the escape factor. Thus, the escape factor is insignificant in such collision-dominated flow. In the rarefied, non-equilibrium gas regime, however, the contribution of collisional transitions to excitation/de-excitation processes is low. Thus, the radiative transition rates associated with the escape factor are important in determining the population densities of electronic states for highly non-equilibrium conditions.

6.3.2 Calculation of escape factor coupled with non-local radiative transport

As discussed in the previous section, the escape factor for a specific transition given in Eq. (6.7) is not known a priori and must be calculated by solving the RTE to obtain the non-local incoming intensity over all directions $G_\lambda$. Either the tangent slab (TS) approximation[36, 38] or the photon Monte Carlo (PMC) method[51, 83] can be used to calculate the incoming intensity and then be iteratively coupled with the collisional-radiative population modeling to obtain the converged distribution of electronic state populations.[33, 52] In this work, both the PMC and TS methods are used to solve the RTE and are coupled with the QSS modeling of the electronic state populations. In this manner we can assess the importance of three-dimensionality coupled with optical thickness. Figure 6.12 shows the procedure for the iterative RTE calculation coupled with the QSS model to obtain the converged electronic state population data.

To calculate the initial distribution of electronic state populations and the corresponding spectral emission and absorption coefficients, the initial value of the escape factor is
assumed to be one (optically thin). In the next iteration, the new escape factor is calculated by solving the RTE with the PMC method (or TS) and is then substituted into the QSS model again to obtain the new electronic state populations. The escape factor corresponding to the new distribution of electronic state population is then re-calculated. This procedure is performed iteratively until converged electronic state populations are obtained. The converged distribution of electronic state populations ensures that we have converged emission and absorption coefficients for each cell in the entire domain. Thus, the radiative intensity or heat flux is also finally converged.

The non-local escape factor calculation could potentially be computationally expensive due to slow convergence. To avoid the complexity of a non-local escape factor calculation, an approximate local escape factor approach has been suggested.[29] This approximate method assumes that the photon escaping phenomena occurs in a small spherical homogeneous radiating gas medium that is governed by the local source function.[54, 84] In other words, the absorption of the radiative energy carried by photons due to the incident radiative intensity from other gas cells can be neglected. The approximate form of escape factor introduced in Ref. [54] is identical to the form used in NEQAIR[29] expressed as,

\[
\rho_{ij} = \frac{\int_{\lambda_1}^{\lambda_2} \varepsilon_{\lambda} \exp(-\kappa_{\lambda} D) d\lambda}{\int_{\lambda_1}^{\lambda_2} \varepsilon_{\lambda} d\lambda} \tag{6.9}
\]

where \(D\) is the distance that a photon travels through a homogeneous gas before being re-absorbed. Note that there is no established criteria for selecting this value, but, in NEQAIR, a value of \(D = 1.0\) cm is recommended for calculating the local escape
factor given by Eq. (6.9). This approximation will be compared with the exact non-local approach in the section 6.7.

6.4 Comparison of Radiative Transport between PMC and TS Method

The TS method has been widely used to solve the RTE in many applications of hypersonic flight regime, but this method is limited to one-dimensional radiative transport. To fully model the three-dimensional nature of radiative transport the PMC method is adopted. The PMC is an excellent approach, but it can be computationally expensive when one wants to reduce the statistical uncertainty and the number of simulated photon rays must be carefully determined to calculate the radiative transport with low statistical uncertainty. A two-dimensional axisymmetric FV-PMC simulation was performed using the DSMC flowfield around the Stardust SRC body and assuming an escape factor of unity. The spatial distribution of the two-dimensional radiative heat flux contour is shown in the top portion of Fig. 6.13. Both the bound-bound electronic transitions from atomic N and O and the corresponding electron impact continuum transitions were considered in the PMC modeling. The macroparameter sampling cells of the DSMC simulation were used in the FV-PMC simulation to calculate the radiation. Five hundred million photon rays were traced to obtain the averaged divergence of radiative heat flux $(\nabla \cdot q_R)$ with a total volumetric standard deviation of less than 5% using 16 processors.

Figure 6.13 shows that there is a significant variation in the spatial distribution of the radiative heat source$(\nabla \cdot q_R)$. Due to the fact that both the electron number density and temperature are high in the forebody region, the radiative heat source is predicted to be much greater than in the afterbody region. In the center of the flow
expansion region, it was found that there is a low $\nabla \cdot q_R$ area near point C in the top portion of Fig. 6.13. To understand this phenomena one needs to consider the distribution of electron temperature and species concentrations. Figure 6.14 shows the electron temperature and number densities of electron and atomic N and O species along a line normal to the surface, which passes through the center of flow expansion region shown in the top portion of Fig. 6.13. Along the four intervals along this line labeled it can be seen that electron temperature at B and D in Fig. 6.14 are higher than those at A and C. The number densities of atomic N and O increase within 10% along the line from the surface to the outer region and also increase near the surface due to the charge recombination at the surface. Since the local emission is proportional to electron number density and is even more strongly influenced by the electron temperature, the emission at B and D can be expected to be greater than the emission at A and C. Figure 6.15 shows profiles of the emission and the divergence of radiative heat flux ($\nabla \cdot q_R$) along this line. It can be seen that the emission behavior along the line is consistent with the electron temperature behavior. The upper electronic state populations and the local emission increase due to the fact that high electron temperatures at B and D, compared to A and C, which was discussed in Sec. 6.2, causes an increase of the electron impact excitation rate. Since the flow is still optically thick, most of emission energy is re-absorbed, i.e., the amount of $\nabla \cdot q_R$ is approximately less than 10% of the local emission. Specifically, at the location where the highest emission occurs, the ratio of $\nabla \cdot q_R$ to the local emission is about 3.5%. Since the ground state number density is essentially constant, the pattern of $\nabla \cdot q_R$ profile is similar to the emission pattern along the line as shown in Fig. 6.15, and the values of $\nabla \cdot q_R$ at C are lower than those at B and D.
To compare the PMC and TS the radiative heat source was also calculated using the TS method. A total of 76 lines of sight normal to the surface were extracted by interpolation from the DSMC flowfield and 60 cells were used to ensure spatial resolution of the high flow gradients along each line. The flooded contours of the percentage difference of $\nabla \cdot q_R$ between the PMC and TS methods are shown in the bottom portion of Fig. 6.13 where it is assumed that PMC is the reference calculation. Interpolation errors can occur when the DSMC flowfield data are interpolated to form the lines-of-sights normal to the surface for the TS calculations. Also in the regions downstream of the forebody the DSMC simulated electron temperature and number densities drop and the native advantage of the PMC smoothing of the DSMC noise is not present in the TS simulations. Nevertheless, it is clearly seen that the TS result is predicted to be close to the PMC in the forebody region as expected because the gradient of flow properties along the normal direction to the surface is much greater than along the tangential direction to the surface. For the downstream region beyond the shoulder, the species concentrations and temperature significantly decrease so that the gradients from one line-of-sight to the next are too large for the TS method to be used to solve the two-dimensional radiative transport. Finally it is found that there is greater than a 50 % difference of $\nabla \cdot q_R$ in the afterbody flow region. In this region, the radiative transport must be considered as three-dimensional and the PMC method is thus required to calculate the radiative heat source and absorbed radiative energy regardless of the escape factor value.
6.5 Coupled PMC - QSS Simulations using the Escape Factor

The effect of the escape factor on the distribution of electronic state populations of atomic N and O species obtained by coupling the PMC with the QSS model at four locations around the capsule body (stagnation streamline and the three locations indicated in Fig. 6.5 will be discussed in this section for the Stardust SRC at 81 km altitude. First, we investigate the effect of the escape factor on the collisional-radiative model of atomic N and O along the stagnation streamline. As was explained in the previous section, the escape factor is determined by solving Eq. (6.7) during the PMC simulation. The QSS method is used to calculate the electronic state population and the electron impact and radiative transition rate coefficients are obtained from the NEQAIR model. The NEQAIR model uses 22 and 19 electronic energy levels for atomic N and O[25], respectively, and assumes the escape factor is only required for strong radiative transitions in the vacuum ultra violet (VUV) spectral region. The corresponding line center wavelengths of atomic N and O radiative transitions at which photons are re-absorbed are tabulated in Table 6.2. To obtain the initial distribution of the electronic state populations for the first radiative transport calculation, the escape factor is initially set to be unity. The new escape factor is then calculated using Eq. (6.7) and substituted into the QSS module. The QSS module again generates a new distribution of electronic state populations and a new escape factor and the PMC coupled with the QSS module solves the RTE. The convergence of the electronic state populations is examined to ensure that non-local collisional-radiative modeling is implemented in the coupled PMC-QSS
method. This process is iterated until both the escape factor and the electronic state populations are converged.

Figure 6.16 shows the change of the electronic state population of atomic N and O coupled with the iterative escape factor calculations along the stagnation streamline for the 4th, 5th and 10th states of N and the 5th electronic state population for O. (See Table 6.2.) During the iterative process, all electronic state populations tabulated in Table 6.2 are converged, which indicates that emission is also converged because the emission depends on the upper electronic state population as indicated in Eq. (3.1) It can be seen that only one iteration is required to obtain a converged population distribution for all cases. After one iteration the upper electronic state populations for each cell are changed due to the newly calculated escape factor and the corresponding emission is also changed. The figure shows that the fourth electronic state population of atomic N increases after the first iteration compared to its initial value obtained with the escape factor of unity. Since photons are re-absorbed between the ground and fourth electronic state, the escape factor decreases and the upper state is re-populated by a factor of three. Within the shock layer the new calculated escape factor for this transition is less than 0.02 as shown in Fig. 6.17, which means that the flow is optically thick. The 5th and 10th electronic state of atomic N and the 5th state for atomic O are also re-populated due to the new escape factor. The 5th and 10th electronic state populations increase by less than a factor of two as the escape factor for the atomic N transitions from the 5th to 3rd and 2nd states become less than 0.17 and 0.05, respectively, in Fig. 6.17. The escape factor of the atomic N 10th to 3rd transition is set to be zero because the absorption rate is greater than emission rate. Figure 6.17 also shows that the escape factor of the 5th
electronic state of atomic O is less than 0.17 within the shock layer. Due to the fact that the strongest VUV radiation for the given flow condition occurs for the transition from the 4th to ground state of atomic N, the change of total emission is mainly governed by the change of 4th electronic state population associated with the new escape factor that is less than 0.02.

Figure 6.18 shows that the change of number of transitions by the non-local absorption from the ground to the 4th electronic state of atomic N (top) and from the ground to the 5th electronic state of atomic O (bottom) along the stagnation streamline. It can be seen that there are no significant changes of the number of transitions by the non-local absorption after one iteration for both N and O case, which indicates that the absorbed radiative intensity (numerator of Eq. (6.7)) is not affected by the escape factor after one iteration. However, due to the fact that the number of transitions by the non-local absorption is nearly identical to the number of transitions by emission, the standard deviation of the escape factor in Eq. (6.7) may be high compared to the its mean value for highly optically thick gas medium even though the standard deviation of the number of transitions due to the non-local absorption calculated by the PMC method is very small. Therefore, there may still exist the statistical uncertainty of the escape factor after one iteration. Note that the escape factor after only one iteration decreased to the small value less than 0.2 from the unity and the contribution of net radiative transition rates to the rate equation become negligibly small compared to the electron impact collisional transition rates. Thus, the collisional processes in the rate equation become dominant and there is no significant change of electronic state populations after one iteration.
Figure 6.19 shows the iterative electronic state populations coupled with the escape factor calculation along the normal line to the surface near the vehicle shoulder, i.e., line (1) shown in Fig. 6.5. At 81 km altitude, strong radiation occurs in this region because the electron number density and electron temperature are predicted to be as high as in the forebody stagnation region. Similar to the stagnation streamline, the 4th, 5th and 10th electronic state populations of atomic N are all converged after one iteration and increase by about a factor of two. The 5th electronic state of atomic O also increases due to the change of the escape factor. Along this line, the values of the escape factor for atomic N and O are less than 0.1 and 0.07, respectively, as shown in Fig. 6.20 which indicates that the flow is still optically thick downstream of the stagnation region.

The change of electronic state populations at the rear-side region (lines (2) and (3)) where the electron temperature and electron number density are low compared to the forebody is potentially more affected by the escape factor than at the forebody region because radiative transitions are competitive with electron impact excitation/de-excitation mechanisms. Figure 6.21 shows the effect of the escape factor on the upper electronic state populations of atomic N and O species along a line normal to the side surface of the Stardust vehicle, line (2). Similar to the case of the stagnation and shoulder lines, upper electronic state populations of the 4th, 5th and 10th levels for N and the 5th for O are all converged after only one iteration with the escape factor coupling. However, the degree of upper electronic state population change due to the escape factor on the side of vehicle becomes greater than in the forebody region. As discussed previously, radiative transitions become dominant compared to excitation/de-excitation processes for populating the electronic states compared to the electron or
heavy particle impact transitions in the flow region where the electron number density and electron temperature are low. Along the line normal to the vehicle side, the values of the escape factor of atomic N and O are less than 0.2 and 0.1, respectively, which leads to the increase of the upper state populations. The effect of escape factor on the electronic state populations are also examined along the line normal to the backplate of the vehicle, line (3), as shown in Fig. 6.22. In this region, there is some noise in the flowfield due to fewer numbers of DSMC particles. Since the electron concentration and electron temperature are low, spontaneous emission is also low compared to the forebody and side regions. Furthermore, since the absorption rate due to the incoming radiative intensity from the flow expansion region is high compared to the local spontaneous emission rate, the escape factor is set to zero. The zero values of escape factor cause the electronic state populations in the backplate region to be re-populated. The 4th and 5th electronic state populations of atomic N increase approximately by one order of magnitude and the 10th electronic state population increases by about a factor of two. Likewise, the new escape factor of atomic O is also calculated to be zero and the 5th electronic state population associated with the full re-absorption of emitted photons from the 5th energy level increases by about one order of magnitude.

Figure 6.23 shows the distributions of the escape factor for the strongest transitions for atomic N and O around the Stardust SRC body. It is seen that the escape factor for the atomic N transition from the 4th to the ground state (Top portion of Fig. 6.23) is less than 0.2 for the entire domain. This low value of the escape factor for the strongest atomic transition in VUV spectrum causes the re-population of the 4th electronic state population and the corresponding radiative energy from the 4th energy
level for the entire flowfield around the vehicle body. The escape factor for the strongest atomic O transition from the 5th to the ground state is found to be less than 0.2 for the region of the forebody shock layer and the expanding flow as shown in the bottom portion of Fig. 6.23. Similar to the atomic N transition, the density of the 5th electronic energy level and the corresponding emissive energy of atomic O increases due to the fact that the escape factor is small. In the backplate region the local spontaneous emission rate is small compared to the absorption rate because the VUV radiative intensity coming from the expanding region is absorbed. In other words, the number of transitions from the lower to upper state exceeds those from the upper to lower states, which gives negative values of the escape factor. Because the negative values of the escape factor can cause artificial population inversion of the electronic levels and these negative values in the backplate region do not affect radiation behavior in other portions of the vehicle since the emitted radiative intensity from that region is negligibly small, we set the escape factor to be zero. For cells where the electron temperature is less than 1,000 K, the escape factor is also artificially set to zero because the QSS assumptions do not describe properly the distribution of electronic state populations due to the low electron temperature. In this region the escape factor is not calculated by Eq. (6.7) during the PMC-QSS coupled iteration.

6.6 Effect of the Escape Factor on Radiative Heating to the Surface

Having verified that the interactions between the non-local radiative transport and the collisional-radiative excitation/de-excitation processes in the high altitude regime of the Stardust reentry flow can be implemented, we turn now to consider the effect of
the coupling or the radiative heat flux to the surface. Due to the newly calculated escape factor being less than 0.2, the upper excited state densities increase, which leads to higher emission. The population ratio of the lower to upper electronic state, which determines the absorption coefficient, is also changed. The absorption coefficient is, however, not as sensitive to the escape factor because the number density of the lower level electronic state such as the ground, 2nd and 3rd states are much greater than the upper electronic energy levels. Thus, the net radiative flux obtained with the non-local escape factor calculations is expected to be larger than the case of the unit escape factor of our previous work.

Figure 6.24 shows a comparison of the radiative heat flux to the Stardust surface using the new escape factor versus the original escape factor of unity. The radiative heat flux to the surface in the case of the new escape factor is approximately twice as large as the original radiative heat flux obtained with the escape factor of unity. Comparisons are also provided using the two RTE methods of TS and PMC. Due to the high electron number density and electron temperature in the region near the vehicle shoulder (shown in Figs. 6.4 and 6.5), the maximum radiative heat flux occurs in this region. The radiative heat flux from the TS method is close to PMC results near the stagnation region because the gradient of flow along the tangential direction to the vehicle surface is quite small. However, the difference in the radiative heat flux between PMC and TS begins to increase in the region near shoulder (S=0.42) because the flowfield becomes two-dimensional.

The convective heating rate is calculated in DSMC under the assumption of a non-catalytic surface condition. As expected, the maximum value of the convective heating rate is observed in Fig. 6.24 to be at the stagnation point. In the stagnation region,
the convective heating is over three times greater than the radiative heating, however, the radiative heating rate to the surface near the shoulder region becomes as important as the convective heating rate. In fact, note that the radiative heating to the surface obtained by inclusion of the escape factor exceeds the convective heating in this region. Under the highly non-equilibrium and low density flow conditions, the effect of the escape factor on the radiative heating is an important considerations in the TPS design process.

6.7 Simplifications to the Non-Local Escape Factor

As mentioned in Sec. 6.3, approximations to the non-local escape factor have previously been considered. Figure 6.25 compares the escape factor and the corresponding 4th electronic state population of atomic N for the transition from the 4th to ground state along the stagnation streamline calculated using the approximate Eq. (6.9) versus the exact non-local approach of Eq. (6.7). The values of the escape factor and electronic state populations in this figure are shown after one iteration. In both cases the full QSS model is used to calculate the upper electronic state population. The values of the local escape factor within the shock layer are less about 0.02, which leads to an increase of the 4th electronic energy level population. It can be seen that there are no significant differences in the 4th electronic state populations calculated either by the local or non-local way. Even though the spatial distributions of the escape factors are different, it is also found that the local escape factor decreases as the gas flows from the freestream to the stagnation point. The value of the local escape factor in the freestream is one because there is no absorption. However, the degree of self-absorption increases dramatically within the shock layer, which means that the gas medium is very optically
thick. Hence, the local escape factor within the shock layer decreases. For the other VUV transitions of atomic N and O, the electronic state populations calculated with the local escape factor are as small as those calculated by the non-local escape factor. Even though there are large differences in the local and non-local escape factors in the region near the freestream, these values do not affect the distribution of the electronic state populations within the shock layer, which mainly dominates the radiative emission and heat source. Similar to Fig. 6.23, the actual value of the non-local escape factor is less than zero in the freestream because the local spontaneous emission rate is small compared to the absorption rate because the strong VUV radiative intensity coming from the shock layer is absorbed. Due to the lack of significant difference in electronic state population between the local and non-local way of the escape factor calculation, the radiative heat flux coupled with the local escape factor calculation is expected to be similar to that computed with the non-local escape factor. A PMC simulation using Eq. (6.9) to calculate the local escape factor was also performed and, as expected, the radiative heat flux along the surface with the local escape factor was not significantly different from that coupled with the non-local escape factor.

As explained in Section 6.5, the values of the escape factor in the strongest transition of atomic N species predicted by the non-local way are less than 0.2 for the entire flowfield around the Stardust blunt body. If the escape factor is set to be zero and the electron impact ionization / recombination processes are neglected, only electron impact excitation / de-excitation processes among the bound electronic states remain in QSS
and Eq. (6.8) reduces to,

\[ \sum_{j=1}^{l} K^e(j, i)N_j - \sum_{j=1}^{l} K^e(i, j)N_i = 0 \] (6.10)

The solution of Eq. (6.10) is

\[ \frac{N_i}{N_j} = \frac{K^e(i, j)}{K^e(j, i)} \] (6.11)

and since the ratio of the electron impact excitation coefficient, \( K^e(i, j)/K^e(j, i) \), can be written in terms of partition functions[25],

\[ \frac{K^e(i, j)}{K^e(j, i)} = \frac{Q_i}{Q_j} \] (6.12)

where the partition function for state \( i \), \( Q_i \), is written as

\[ Q_i = g_i \exp(-E_i/k_B T_e) \] (6.13)

and \( g_i \) is the degeneracy of the \( i \)-th electronic state and \( k_B \) is a Boltzmann constant. Since the summation of each electronic state population is equal to the species number density, \( n_a \), the final form of the population of electronic state \( i \) can be expressed as,

\[ N_i = \frac{n_a g_i}{Q_a} \exp \left( \frac{-E_i}{k_B T_e} \right) \] (6.14)
where $Q_\alpha = \sum_{i=1}^{l} Q_i$ is the total partition function. Therefore, in the case of complete optical thickness for bound-bound transitions only, the QSS formulation is reduced to a Boltzmann distribution. To investigate the effect of the net radiative transition and the electron impact ionization in the QSS model, the 4th electronic state populations of atomic N, which is the most important energy level in determining radiation, coupled with the non-local escape factor were compared with those calculated by the Boltzmann distribution. Figure 6.26 shows three distributions of the 4th electronic state population of atomic N along the shoulder line shown in Fig. 6.5, calculated using the non-local escape factor, a value of zero for the escape factor, and the Boltzmann distribution. Due to the fact that the non-local escape factor for the atomic N transition from the 4th to the ground state along the shoulder line is calculated to have values less than 0.01 as indicated in the top portion of Fig. 6.20, there are no significant differences of the 4th electronic state population between the non-local and zero escape factor cases. However, the populations calculated by the Boltzmann distribution are higher predicted than the others because the rate of electron impact ionization / recombination processes are still important in determining the electronic state population in the QSS for the conditions along the shoulder line where both electron concentrations and temperatures are high. When the electron impact ionization / recombination processes are neglected in QSS, the population distribution for all three cases was found to be identical.

Another comparison was performed in the flow expansion region where the electron number density and temperatures are low as compared to the forebody region. Figure 6.27 shows the distribution of the 4th electronic state population of atomic N species obtained by the aforementioned three ways along the line normal to the side
surface as indicated in Fig. 6.13. It is seen that the population distribution with the zero escape factor is very close to that predicted by the Boltzmann distribution. Since the rate of electron impact ionization / recombination is negligibly small due to the low electron temperatures along this side line, the populations produced by only the collision mechanism in QSS are distributed nearly identical to the Boltzmann populations. There are differences in the population distribution between the non-local and the zero escape factor because the effect of radiative transition on the collisional-radiative modeling is more significant in this region of low electron number density and temperatures that shown in Fig. 6.26.
Table 6.1. DSMC Numerical Parameters for the entire flowfield around Stardust blunt body at 81 km

<table>
<thead>
<tr>
<th>$K_{n,\infty}(L = 0.23\ m)$</th>
<th>$1.04 \times 10^{-2}$</th>
</tr>
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<tbody>
<tr>
<td>Number of simulated particles</td>
<td>26 million</td>
</tr>
<tr>
<td>Number of collisional cells</td>
<td>3 million</td>
</tr>
<tr>
<td>Number of macroparameter cells</td>
<td>$300 \times 200$</td>
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Table 6.2. Electronic transitions affected by escape factor

<table>
<thead>
<tr>
<th>Species</th>
<th>Wavelength (Å)</th>
<th>Upper (NEQAIR)</th>
<th>Lower Indices</th>
</tr>
</thead>
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<tr>
<td>$N\ (^4P_{5/2} \rightarrow ^3S_{3/2})$</td>
<td>1200.0789</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>$N\ (^4P_{3/2} \rightarrow ^4S_{3/2})$</td>
<td>1200.7487</td>
<td>4</td>
<td>1</td>
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<tr>
<td>$N\ (^4P_{1/2} \rightarrow ^4S_{3/2})$</td>
<td>1201.2385</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>$N\ (^2D_{5/2} \rightarrow ^2P_{3/2})$</td>
<td>1311.0453</td>
<td>10</td>
<td>3</td>
</tr>
<tr>
<td>$N\ (^2D_{3/2} \rightarrow ^2P_{3/2})$</td>
<td>1311.4752</td>
<td>10</td>
<td>3</td>
</tr>
<tr>
<td>$N\ (^2P_{1/2} \rightarrow ^2P_{3/2})$</td>
<td>1319.5440</td>
<td>10</td>
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</tr>
<tr>
<td>$N\ (^2P_{3/2} \rightarrow ^2P_{3/2})$</td>
<td>1320.2238</td>
<td>10</td>
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</tr>
<tr>
<td>$N\ (^2P_{3/2} \rightarrow ^2D_{5/2})$</td>
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<td>2</td>
</tr>
<tr>
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<td>$N\ (^2P_{1/2} \rightarrow ^2D_{3/2})$</td>
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<td>$N\ (^2P_{3/2} \rightarrow ^2P_{1/2})$</td>
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<td>5</td>
<td>3</td>
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<td>$N\ (^2P_{3/2} \rightarrow ^2P_{3/2})$</td>
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<tr>
<td>$N\ (^2P_{1/2} \rightarrow ^2P_{3/2})$</td>
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<td>1</td>
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<tr>
<td>$O\ (^3S_1 \rightarrow ^3P_0)$</td>
<td>1306.5461</td>
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Fig. 6.1. Mach number distribution and streamlines around Stardust SRC body at 81 km.
Fig. 6.2. Mole fractions of atomic N (top) and O (bottom) at 81 km altitude.

Fig. 6.3. Mole fractions of N\(_2\), O\(_2\), N and O along the stagnation streamline at 81 km altitude.
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Fig. 6.19. Upper electronic state populations of atomic N and O during the iterative coupling process with the escape factor calculations along the line normal to the shoulder surface. (line (1) of Fig. 6.5)
Fig. 6.20. Escape factor of atomic N (Top) and O (Bottom) during the iterative coupling process along the line normal to the shoulder surface. (line (1) of Fig. 6.5)
Fig. 6.21. Upper electronic state populations of atomic N and O during the iterative coupling process with the escape factor calculations along the line normal to the side surface. (line (2) of Fig. 6.5)
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Fig. 6.26. Distribution of the 4th electronic state population along the shoulder line (line (1) of Fig. 6.5) calculated by using non-local escape factor and zero escape factor and Boltzmann relation.

Fig. 6.27. Distribution of the 4th electronic state population along the line normal to the side face (a line of Fig. 6.13) calculated by using non-local escape factor and zero escape factor and Boltzmann relation.
Chapter 7

Conclusions

New databasing schemes have been developed for advanced radiation calculations of hypersonic non-equilibrium reentry flows. Due to the non-equilibrium flow conditions, the quasi-steady-state assumption was used for generating the electronic state populations of atomic and diatomic gas species. A Voigt line broadening function was used to describe the line shape of bound-bound spectral lines. The emission and absorption coefficients for any given flow condition and wavelength range were accurately and efficiently calculated using new database and its associated interpolation schemes. Comparisons of the emission and absorption coefficients for atomic O and N between the database and NEQAIR were performed to validate the accuracy of the databases and good agreement within 1% error was observed. For diatomic species \( N_2^+ \), NO, \( N_2 \) and \( O_2 \), there are some differences of results between the database and NEQAIR. This is because the broadening method as implemented in NEQAIR is different from the one used in the database presented here. It was also found that there is excellent agreement for spectral coefficients when the same broadening method was applied to both the database and NEQAIR. Radiative heat generation for the Stardust reentry for two different flow fields computed using CFD and DSMC methods, was calculated using the database. The radiative heat
production from the databasing schemes predicts the same magnitude and spatial distribution as NEQAIR but more efficiently. The improved computational method will have a significant impact for coupled radiation-gas dynamic calculations.

Coupled DSMC flowfield FV-PMC radiation simulations were performed for the Stardust reentry trajectory from transitional to continuum peak heating conditions to examine the effect of radiation on high-Mach number flows. The dissertation presented the first such simulations performed using the high-fidelity DSMC kinetic method. Building on previous Stardust modeling, the DSMC simulations employed a chemistry model that included ionization as well as high-energy relaxation models. To enable a direct comparison with CFD results at peak heating, a fully catalytic surface condition was implemented in the DSMC simulations. Using this surface boundary condition, the DSMC and CFD convective heat fluxes were found to be in good agreement, considering the very different gas dynamic approaches. A two-dimensional/axisymmetric version of the FV-PMC RTE method was implemented for direct use in the DSMC macroparameter sampling grid and using a photon weighting scheme that improves the photon bundle statistics along the axis of symmetry.

Using this newly developed approach, coupled DSMC-radiative transfer simulations were performed at four altitudes corresponding to a Stardust reentry trajectory. The flowfield internal energy was found to be reduced when coupled to the radiative transport, which in turn lowered the radiative heat flux. Convergence in the convective and radiative heat fluxes was typically obtained within three to four iterations. For the range of conditions considered the radiative heat flux was found to be about 40% of the total heat flux, highlighting the non-equilibrium nature of the Stardust reentry flow.
The DSMC results were found to more closely follow the Tauber-Sutton correlations for radiative heat transfer when the Voigt line shape was used. The differences of radiative heat flux obtained in the DSMC versus the CFD can be understood in terms of the different thermo-chemical models employed. Since the Tauber-Sutton correlations are based on CFD results, it is not surprising that they and the DSMC results do not have the same dependence on freestream parameters. For the non-equilibrium conditions of the Stardust reentry these discrepancies are important and should be resolved.

The effect of the escape factor on radiation for the hypersonic non-equilibrium flow conditions was discussed. The non-equilibrium and transitional flow of the Stardust SRC at 81 km altitude was simulated using DSMC. Due to the strong dissociation of $N_2$ and $O_2$ molecules within the shock layer, atomic N and O species are dominant in the whole domain, which indicates that the majority of gas radiation is generated from the electronic excited atoms. The QSS model of NEQAIR was used to estimate the electronic state populations of N and O in the 22 and 19 levels, respectively. The escape factor was chosen to efficiently describe the phenomena of photon escaping among the electronic levels in the excitation/de-excitation process of electronic states. To calculate the non-local escape factor and couple it with the QSS modeling, the PMC method was adopted to obtain the radiative intensity. It was further verified that the PMC is required for the after regions of the flows by comparing the divergence of radiative heat flux calculated by PMC with TS.

The effect of the escape factor on the electronic state population distribution of atomic N and O species and radiation was investigated using PMC. The non-local approach to estimate the escape factor was derived and iteratively coupled with the QSS
method used in NEQAIR until the converged population distribution was achieved. It was found that only one iteration was required to converge the upper electronic state populations and that when non-local radiation was accounted for the upper electronic state populations increased by about a factor of two for a given flow condition. The converged values of escape factor were close to zero, which indicates that the flow is optically very thick. Due to the increase of the electronic state population distribution predicted by the coupled PMC-QSS calculations, the radiative heating rates to the surface of the Stardust SRC were increased by about a factor of two. Furthermore, the radiative heating to the surface of vehicle shoulder region and afterbody may exceed the non-catalytic convective heating when the effect of non-local, three-dimensional radiative transport is considered.
References


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