

Numerical Studies of Thermochemical Nonequilibrium Flows in a DC Arcjet Thruster

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by

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Abstract

This study is concerned with the numerical simulation of high-temperature plasma flows in a low-power DC arcjet thruster. Nonequilibrium behavior of the gas and its impacts on the thruster performance are of primary interests.

By examining essential features inherent to arcjet flows, the flow field equations are constructed for gaseous flows that are in thermochemical nonequilibrium, representing the conservation of global mass, momentum, global energy, mass of each chemical species, and internal energy considered. This equation set is further coupled with Maxwell's equations that describe the electric field. Physical models associated with a series of chemical reactions, internal energy exchanges, and transport phenomena are then consistently modeled and incorporated in the computation.

These equations are discretized in space by using a newly proposed finite volume approach for axisymmetric problems and solved by applying sophisticated numerical methods developed to date. Efforts are made so as to relieve the numerical stiffness arising from strong nonlinearity of the equation system. Some strategies enhancing the convergence property of the algorithm are also proposed.

Computations are performed for a typical thruster geometry in a range of operating conditions with nitrogen as propellant. The distributions of physical properties inside the thruster are then presented for both thermally equilibrium and nonequilibrium models and the effect of nonequilibrium phenomena on the thruster performance is revealed by comparing with experimental data.

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Nomenclature

Roman Symbols

A	area vector
B	magnetic induction field vector
c	speed of sound
C	mass fraction
C_v	specific heat at constant volume
C_p	specific heat at constant pressure
C_{CFL}	CFL number
D	effective diffusion coefficient
D	electric displacement field
D	binary diffusion coefficient
Da	Damköhler number
e	energy per unit mass, electric charge
E	energy per unit volume
E	electric field vector
E_D	dissociation energy per unit mass
E_I	ionization energy per unit mass
f	velocity distribution function
F	external force
g	acceleration of gravity
h	static enthalpy per unit mass
Δh^0	enthalpy of formation
H	total enthalpy per unit volume
H	magnetic field vector
i_{max}	maximum index of ξ direction
I	current
I_{sp}	specific impulse
I_t	total impulse
j_{max}	maximum index of η direction
j	current density vector
J	Jacobian of coordinate transformation, diffusion flux
k	Boltzmann constant, reaction rate coefficient

K^{eq}	equilibrium constant
Kn	Knudsen number
L	characteristic length
m	mass
$\dot{m}$	mass flow rate
M	Mach number, molecular weight
n	number density
$neqns$	number of equations
nr	number of reactions
ns	number of species
p	static pressure
P	electric power
q	heat flux
Q	vector of conservative variable
Q_{T-e}	translation-electron energy exchange rate
Q_{R-e}	rotation-electron energy exchange rate
Q_{e-v}	electron-vibration energy exchange rate
Q_D^e	energy loss due to electron impact dissociation
Q_I^e	energy loss due to electron impact ionization
R	gas constant
$\mathbf{R}$	residual vector
$\mathfrak{R}$	universal gas constant
s	species index
S	area
S_{Joule}	Ohmic heating rate
t	time
T	thrust, temperature
u	x component of velocity
U	ξ direction contravariant velocity
v	y component of velocity
V	electric voltage, diffusion velocity, volume, η direction contravariant velocity
$\dot{w}$	mass production rate
$\mathbf{W}$	vector of source terms
x	horizontal coordinate of physical reference frame
X	mole fraction
y	vertical coordinate of physical reference frame

Greek Symbols

α	degree of ionization
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β	degree of dissociation
γ	specific heat ratio
δ	inelastic loss factor
δ_{ij}	Kronecker delta
ϵ_0	electric permittivity of free space
η	thruster efficiency, direction in computational domain
θ	angle
Θ_{vib}	characteristic vibrational temperature
λ	thermal conductivity, eigenvalue, mean free path
Λ	cut-off parameter
μ	viscosity
μ_0	magnetic permeability of free space
ν	stoichiometric coefficient, collision frequency
ξ	direction in computational domain
π	circular constant
ρ	density
ρ_e	charged density
σ	electrical conductivity
τ	viscous stress, characteristic time, relaxation time
ϕ	electric potential

Subscripts and Superscripts

b	backward
e	electron, exit
eq	equilibrium
ex	electronic excitation
f	forward
in	inlet
L	left
M	molecular species
n	time step
R	right
ref	reference
rot	rotational
tr	translational
vib	vibrational
1/2	cell interface
i, j, k, l, m, r	running indices

Acronyms

AMSTAT	Radio Amateur Satellite Co.
ARGOS	Advanced Global Research and Observation Satellite
AUSM	Advection Upstream Splitting Method
CE	chemical equilibrium
CFD	computational fluid dynamics
CFL	Courant, Friedrichs, and Lewy
CNE	chemical nonequilibrium
DRTS	Data Relay Test Satellite
DSMC	direct simulation Monte Carlo method
ESEX	Electric Propulsion Space Experiment
FEED	field-effect electrostatic propulsion
GE	General Electric Co.
GMRES	generalized minimal residual
IEPC	international electric propulsion conference
IHI	Ishikawa-Harima Heavy Industries Co., Ltd.
IRS	Institut für Raumfahrtsysteme
K.E.	kinetic energy
L.H.S.	left hand side
LM	Lockheed-Martin
MELCO	Mitsubishi Electric Corporation
MIT	Massachusetts Institute of Technology
MPD	magnetoplasma dynamic thruster
MUSCL	Monotone Upstream-centered Scheme for Conservation Laws
NASDA	National Space Development Agency
NSSK	north-south stationkeeping
PAC	Primex Aerospace Company
P.E.	potential energy
PPT	pulsed plasma thruster
PPU	power processor unit
RRC	Rocket Research Company
TRW	Thompson-Ramo-Wooldridge Inc.
TsNIIMash	Tsentrálny nauchno-issledvatelskiy institut mashionostroyeniya
USAF	U.S. Air Force
UTSI	University of Tennessee Space Institute
1T	one-temperature
2T	two-temperature
3T	three-temperature

Chapter 1

Introduction

1.1 DC Arcjet Thruster as an Electric Propulsion Device

The practical interest of the space development program to date has been on the near-earth activity, but recently shifting to deep-space researches including the interplanetary flights. To realize such long-range and/or long-time missions, conventional chemical rocket systems involve much disadvantages in terms of efficiency, and the use of electric propulsion has been recognized as the most reliable and promising strategy instead.

Here we define the electric propulsion as [1]

The acceleration of gases for propulsion by electrical heating and/or by electric and magnetic body forces.

The primary attraction of the application of electric propulsion for future spacecrafts lies in their possibility of highly efficient utilization of propellant mass. As will be discussed in the next chapter, it is not the thrust itself but the specific impulse that determines the efficiency and feasibility of propulsion system for a specified mission and, indeed, the specific impulse required for any interplanetary mission is readily attainable by using thrusters employing electrostatic and electromagnetic interactions.

The use of electric power for thrust has an advantage that the thruster performance is not limited by the inherent chemical properties of the propellant. In conventional chemical rockets, the thrust is obtained by nozzle expansion of a propellant previously heated by its own chemical reaction. Therefore the attainable exhaust velocity is inevitably limited by the intrinsic energy available in the chemical reaction and convertible to chamber enthalpy of the gas. This is not the case for electric propulsion since the energy is essentially supplied as volumetric heating of the electromagnetic field, which is independent of chemical properties of the

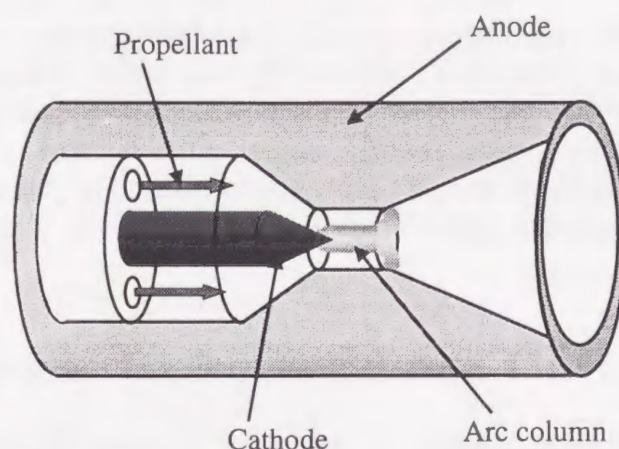


Figure 1.1: Schematic of a typical arcjet thruster

propellant itself.[†]

In general, the electric propulsion can be categorized into the following three types regarding the acceleration mechanism:

1. *Electrothermal propulsion*: the propellant gas is heated electrically and expanded in a nozzle to produce thrust.
2. *Electrostatic propulsion*: the propellant is accelerated by the application of electric body forces to ionized particles.
3. *Electromagnetic propulsion*: the ionized propellant is accelerated by electromagnetic body forces produced by interactions of external and internal magnetic fields with electric currents driven through the stream.

The arcjet thruster belongs to the electrothermal device. The schematic of a typical arcjet thruster is shown in Fig. 1.1. Arcjets utilize an arc generated between electrodes to heat the propellant gas. The propellant is injected and passed through the arc before being exhausted through a nozzle at one end of the device. Arcjets normally employ a constricted design in which the arc initiates at the tip of a cathode, extends through the constrictor (throat), attaches in the diverging section of the nozzle, which also serves as the anode. The arc core is at temperatures of more

[†]Even in this case, however, the unrecoverable energy deposition in the internal mode of the gas, referred to as *frozen loss*, can degrade the thruster performance. Quantitative estimation of this phenomenon is a main purpose of this study and will be discussed hereafter.

than 10,000 K. Therefore there is practically no flow inside the arc, which can be thought of as an effective fluid plug; this reduces the flow, without reducing the pressure integral, this leads to the high specific impulse.

Typical thruster properties for each electric propulsion system are cataloged in Table 1.1 [2]. Arcjets occupy an intermediate place in the specific impulse scale, and become advantageous for missions where there is some premium on short-burn duration (note that lower specific impulse implies higher thrust for a given power), or on thrust over only a portion of the orbit. Hence arcjet thrusters are expected to be utilized mainly as a north-south stationkeeping function for geosynchronous satellites.

1.2 Historical Background and Current Trends

Classically, the idea of using electric power for propulsion was proposed by Robert H. Goddard for the first time at the beginning of the 20th century, in 1906 [3]. After that, Herman Oberth included a chapter on electric propulsion in his classic book on rocketry and space travel in 1929 [4]. Their ideas were, of course, not realized at that time and it was after the World War II, in 1948, that the first serious feasibility studies of a space vehicle employing electric propulsion were performed [5]. In Ref. [3], Stuhlinger presents a detailed historical review of the electric propulsion development including his personal experiences.

The first study on the application of arcjets to propulsion was conducted during the late 1950's by Giannini in the United States [6]. Since then, several models of the thruster were developed for space testing around 1960 in accord with the field becoming a major component of the space industry. Many works such as the performance of correlated ground tests in large vacuum tanks, the development of suitable power supplies and power conditioning equipment, and the detailed analysis of missions appropriate to electric propulsion were required necessarily and have increased the number of research and development laboratories including the Giannini Scientific Co., Avco Co., and General Electric Co. in the United States, and many research facilities in the former USSR.

The primary focus of the arcjet thruster development in the United States was on providing primary propulsion on major NASA missions and started in the mid-1950's. Most of the effort at that time was focussed on the development of devices that operated at the 30 kW power level and used hydrogen as the propellant. This is because the programs in this period planned to utilize the space-based nuclear power systems and cryogenic hydrogen storage. Some of the resources were directed toward the 2 kW range and these efforts resulted in the fabrication of a 1 kW flight system designed which was expected to be accepted for the Space Electric Rocket Test (SERT) program. Unfortunately, ground tests of this unit encountered design problems and the system was shelved. Other propellants including ammonia were tried using hardware from the 1 kW program with little success and, after all, the

Table 1.1: Typical electric thruster features [2]

Thruster type	Resistojet	Arcjet	MPD	Ion	Hall	PPT	FEEP
Propellant	N ₂ H ₄	N ₂ H ₄	NH ₃ , H ₂	Xe	Xe	Teflon	Cs
Power range (W)	500-1,500	300-2,000	1-100 K	200-4,000	300-6,000	1-200	10 ⁻⁵ – 1
I_{sp} (s)	300	500-600	2,000-5,000	2,800	1,600	1,000	6,000
η	0.8	0.35	0.3	0.65	0.5	0.07	0.8
Peak voltage (volt)	28	100	200	900	300	1,000-2,000	6,000
Thruster mass (kg/kW)	1-2	0.7	–	3-6	2-3	120	–
PPU mass (kg/kW)	1	2.5	–	6-10	6-10	110	–
Lifetime (h)	500	>1,000	–	10,000	>7,000	> 10 ⁷ (pulses)	–

Table 1.2: Application of arcjet to operational/experimental flight [2]

Launch	Vehicle type/Experiment	Propellant	Kilowatts	Sponsor/builder
1987	Shadow	Cs	1.5	TsNIIMash
1993	Telstar-4	N ₂ H ₄	1.8	LM/OAC
1996	GE-1	N ₂ H ₄	2.0	LM/OAC
1998	AMSAT	NH ₄	0.7	AMSAT/IRS
1999	ARGOS/ESEX	NH ₄	26.0	USAF/TRW + Primex
2000*	DRTS	N ₂ H ₄	1.8	MELCO/NASDA

* Planned date

program was terminated in the mid-1960s. These progress were reported by Wallner and Czika in 1965 [7].

The advantage and the feasibility of arcjet systems were, however, recognized again after the evolution of commercial communication satellites. Since the 1980's, low power arcjet research efforts have been directed worldwide toward the development of a system to replace the state-of-art resistojet and bi-propellant systems in use for north-south stationkeeping on geosynchronous communications satellites. In fact, some efforts have resulted in actual application for practical satellites or experiments as listed in Table 1.2. A more detailed account can be found in Ref. [8]. In the United States, high power arcjet propulsion technology was demonstrated in the Air Force-sponsored Electric Propulsion Space Experiment (ESEX), and the 26 kW ammonia arcjet system was launched as part of ARGOS on February 23, 1999 [9]. Major ESEX experiment objectives were to demonstrate the performance of the arcjet in space, to identify any impacts of the operation arcjet on spacecraft systems, and to collect data necessary for comparison to ground results. The thruster performed as expected in flight (787 seconds specific impulse and 1.93 N thrust).

On the other hand, in Japan, the National Space Development Agency (NASDA) has a plan to launch an arcjet-onboard satellites named Data Relay Test Satellite (DRTS) [10]. 1.8 kW and 250 mN class hydrazine arcjet thrusters were delivered from Primex Aerospace Company (PAC) in the U.S. to Mitsubishi Electric Corporation (MELCO) for integration into the DRTS. Work is presently underway as well in Ishikawajima-Harima Heavy Industries Co., Ltd. (IHI) to develop a 1 kW DC arcjet system [11]. A 100 hours firing test was conducted successfully using the engineering model of thruster, gas generator, power processor and domestic hydrazine. A flight type system of the 1 kW DC arcjet has been designed and manufactured by reflecting the test result.

From these trends, it can be confirmed that arcjet thrusters are now in the midst of a rapid transition from experimental to practical device.

1.3 Review of Arcjet Modeling

As outlined in the previous section, studies on electric propulsion have been performed for many years. This is also evident from the fact that the international electric propulsion conference (IEPC) has been held since the late 1960's and is already 26th in 1999. However, basic development of the arcjet system was associated with experimental works at the beginning and theoretical and analytical approach gave few guidelines to designers.[†] This is because reproduction of basic physics inside the thruster, interaction of the fluid motion, chemical reactions, transport phenomena, and electromagnetic effect, are extremely difficult to perform, but indispensable to predict the thruster performance correctly. Thus until recently, there was little hope of being able to construct comprehensive models of the complete device and the design process was inevitably forced to be empirical and intuitive.

The situation is now rapidly changing owing to the combination of highly developed computational resources and the accumulation of plasma information via a new generation of plasma diagnostics. This leads to a possibility that the thruster development by means of experimental efforts can be replaced by more sophisticated approaches including the numerical prediction of thruster performance by using the computational fluid dynamics (CFD).

Since the late-1980's, many attempts have been made to model and simulate the plasma flow inside the arcjet thruster. The main issues of the arcjet modeling published in the past are listed in Table 1.3 and discussed in detail by the following. This review is basically coincident with the excellent report of Martinez-Sanchez and Miller [12], but includes additional literatures published recently and limited to two-dimensional computations.

One of the first two-dimensional arcjet calculation was that of Okamoto and Nishida [13], [14]. They performed a computation for a 1 kW class thruster with argon as propellant. Viscosity, heat conduction, and finite rate chemistry were consistently modeled and incorporated. Fairly good thrust and efficiency predictions were obtained in comparison to experiment.

In Ref. [15], King and Butler developed a numerical code called KARNAC (Kinetic Arc Nonequilibrium Analysis Code), that can deal with hydrogen, nitrogen or mixtures. Their code is based on the Arbitrary Lagrangian-Eulerian (ALE) method, so that computations are advanced in time by two phases, namely Lagrangian phase and Eulerian phase. The advantages of this method are threefold: 1) the solution can withstand steep gradients and extreme transients; 2) the method is independent of the Mach number regime; 3) separate modules can be developed to simulate specific physical processes. Results showed qualitative agreement with experimental data, but severely overpredicted the input power and specific impulse.

[†] "Like many other practical devices, arcjets for space propulsion have evolved largely on the basis of a series of intuition-guided empirical developments, with theory providing at best a general background, and very little detailed help to the designer." [12]

Table 1.3: Examples of numerical analysis

Author	Affiliation/Country	Model	References
Okamoto and Nishida	Kyushu Univ./Japan	1T, CNE	[13], [14]
King and Butler	RRC/USA	1T, CNE	[15]
Rhodes and Keefer	UTSI/USA	1T/2T, CE	[16], [17]
Ciucci et al.	CENTROSPAZIO/Italy	1T, CNE	[18]
Babu et al.	Ohio State Univ./USA	1T, CNE	[19]
Miller and Martinez-Sanchez	MIT/USA	2T, CNE	[20], [21]
Fujita and Arakawa	Univ. Tokyo/Japan	1T/2T, CNE	[22], [23], [24]
Megli et al.	Univ. Illinois/USA	2T, CE/CNE	[25], [26], [27]
Auweter-Kurtz et al.	IRS/Germany	3T, CNE	[30]
Boyd	Cornell Univ./USA	3T*, CNE	[28], [29]

* DSMC calculations

The computation of Rhodes and Keefer employed the SIMPLE (Semi-Implicit Method for Pressure-Linked Equation) algorithm as a flow field solver. In Ref. [16], they assumed chemical equilibrium and this led to severe underprediction of electron outside the arc, requiring an artificially elevated value for electrical conductivity, sometimes referred to as conductivity floor, to maintain discharge. This work was later extended to thermochemical nonequilibrium flow field [17], and the results underpredicted the thruster performance compared to experimental data.

Other works associated with the thermal equilibrium assumption include that of Ref. [18] and Ref. [19].

The most successful computation with respect to performance prediction may be the work of Miller and Martinez-Sanchez [20], [21]. They abandoned the single-temperature assumption and separated the electron temperature from the heavy particle temperature (two-temperature model). This requires solving electron energy equation separately from the total energy equation, and enables us to describe the rates of ionization and recombination, ambipolar diffusion, and ultimately current attachment path outside the arc core more accurately. Hydrogen was employed as propellant, and the predictive accuracy of their model is excellent: the discharge voltage calculated is within 1-10 % of experimental measurements, and predicted specific impulse is within 5-10 %.

The two-temperature computations were also performed by Fujita and Arakawa [22], [23], [24], and Megli et al. [25], [26], [27]. In Ref. [23], Fujita developed an electrode sheath model to evaluate the voltage drops at anode and cathode. The calculated electron and heavy particle temperatures were similar in magnitude and distribution to those of Ref. [21], but the predicted voltage was consistently low compared to experimental data. Martinez-Sanchez [12] attributes this trend to the assumption of equi-potential anode, which is expected to shift the arc attachment area more upstream.

In turn, Megli et al. developed a numerical model for nitrogen/hydrogen mix-

tures. The flow field equations are solved using a compressible form of the pressure-based pressure implicit with splitting of operators (PISO) algorithm. They assumed chemical equilibrium at first [25], and then extended to chemical nonequilibrium [26]. An important thing to note is, for calculations including nitrogen, the use of low inelastic loss factor δ (see following chapter) leads to increase electron temperature excessively near the anode, which results in severe underprediction of voltage. Furthermore, in Ref. [27], they evaluated the δ by solving the Boltzmann transport equation and incorporated into their model. The results confirmed the strong energy dependent of δ , which, unfortunately, led to predict much lower voltage compared to experimental data in turn. This implies the difficulty of estimating intermolecular effects on computations assuming thermal nonequilibrium.

The most complicated computations employing the three-temperature (3T) model is presently underway by the working group of Institut für Raumfahrtsysteme (IRS) in Germany [30]. Unlike 2T computations, their 3T model further splits the heavy particle temperature into translational-rotational and vibrational temperatures. This requires additional modeling of the equation representing vibrational energy conservation and accompanying physical phenomena. Although involving a number of computation burden, they succeeded to reproduce the plasma flow inside the high-power hydrogen arcjet thruster named HIPARC-R.

The computational challenge also goes to the field of rarefied gas dynamics. In Refs. [28] and [29], Boyd developed a numerical method to model the nozzle and plume flows of a hydrogen arcjet by using the direct simulation Monte Carlo (DSMC) technique. Starting from a continuum solution of the flow just downstream the constrictor, computations were performed with nonequilibrium chemistry, thermal relaxation, and Ohmic heating taken into consideration. The results were compared with measurements and quite good agreement was obtained for thruster performance, indicating the Monte Carlo method becoming a viable approach to simulate arcjet flow fields.

1.4 Motivation and Scope of the Present Study

The limitations of ground-based experimental facilities and the rapid improvements of digital computers and numerical solution algorithms have meant that computational fluid dynamics has been becoming a useful design tool for electric propulsion developments. In fact, computational codes for the solution of supersonic and hypersonic flow are now in routine use in the field of aeroplane or spacecraft design processes. Adding this, accumulated information of the physical properties including finite-rate dissociation/ionization rates, collision frequencies required to evaluate the transport properties, and thermal relaxation rates have brought us to construct more accurate and reliable models which describe high temperature plasma gases.

The motivation of the present study stems from some long term goals to develop a suitable numerical algorithm and associated computer code for the prediction of

thruster performance and ultimately to complete the CFD code as a tool for the design of practical arcjet thrusters. This dissertation follows the numerical works reviewed in the previous section to a certain extent, but do supply deeper insight for both physical and computational aspects.

It is now evident that we need to construct equation systems that describe the flow field with at least two-dimensional assumption: the radial flow structure is extremely nonuniform so that one-dimensional models must have serious limitations concerning the details of the gas physics and flow dynamics. Furthermore, it is inevitable to employ quite complicated physical models to describe plasma properties. Arcjet thrusters are electrothermal devices, and the flow structure is maintained by complicated physics including a series of chemical reactions. This is in contrast to hypersonic computations such as blunt-body flows with strong shock wave, where the flow structure is basically determined by fluid dynamics itself and so-called real gas effects[†] play supplementary roles.

One of the main purpose of the present study is to investigate the effect of thermochemical nonequilibrium phenomena on the prediction of thruster performance. This is because accurate evaluation of flow chemistry in the nozzle is of particular importance. It is well known that the latent chemical energy contained in the exit flow is a main cause of thruster degradation, which is referred to as *frozen loss*. Thus an analysis that includes thermochemical nonequilibrium is required to accurately predict this phenomena. This requires high-resolution, robust, and efficient CFD algorithms capable of solving large systems of conservation laws with very stiff source terms. Computational difficulties inherent in the arcjet physics such as Ohmic heating, convergence deterioration subject to low Mach number region, and very diffusive nature of the flow field must be overcome as well. Therefore a first step toward achieving the stated long term goals includes the development of sophisticated, reliable, and accurate solution algorithms that enable us to obtain converged data within allowable computational time.

1.5 Organization of the Thesis

The outline of the thesis is as follows. Basic theories on electric propulsion, key features of physics inherent in the arcjet flow, and expected numerical problems are discussed as a general discussion in the next chapter, **Chapter 2**.

In **Chapter 3**, the basic governing equations are constructed for both flow field and electric field by combining existing theories on the assumptions introduced. Expressions for convective and viscous flux, transport properties, and the terms

[†]Here we use the term *real gas effects* as a meaning of high temperature effects including dissociation, ionization, vibrational excitation, etc. This sometimes leads to confusion with the case where the so-called Van der Waals force becomes important. Hence, to what follows, the term *high temperature effects* is used instead [31].

representing interactions among various energy modes are then consistently modeled. Physical boundary conditions introduced are discussed in detail as well.

Chapter 4 is concerned with providing complete and comprehensive descriptions of the numerical algorithms employed and the expression of their practical implementations. Key issues include: 1) the newly proposed finite volume formulation for axisymmetric problems, 2) the construction of approximate Riemann flux combined with monotonous reconstruction of physical properties, 3) time-integration algorithms including the treatment of stiff thermochemical source terms, and 4) an efficient algorithm to solve elliptic equation for electric field by using the generalized minimal residual (GMRES) method.

Computations are performed in a range of operating conditions employed in the previously conducted experiments with nitrogen as propellant. Computational results are then presented and compared with the experimental data in **Chapter 5**. The effect of thermal and chemical nonequilibrium on the thruster performance are cleared and discussed therein.

Finally, **Chapter 6** includes a few conclusions for the results obtained and some recommendations for future work.

Chapter 2

General Discussion

2.1 Definitions and Fundamental Argument

As expected, rigorous demonstration of potentialities on the use of electric propulsion requires a number of detailed analysis for specific missions, which is difficult to perform. The essential concept, however, can be illustrated by the following basic dynamical arguments. Generally the flight of a space vehicle is described simply by the differential equation of motion in one-dimensional manner as [1], [32]

$$m\dot{u} = \dot{m}u_e \quad (2.1)$$

where $\dot{u}$ and $\dot{m}$ denote the rate of change of rocket speed (i.e. acceleration) and that of mass by propellant exhaustion (i.e. *mass flow rate*), respectively.[†] u_e is the exhaust velocity relative to the vehicle. The term on the right hand side is commonly identified as the *thrust* of the vehicle,

$$T \equiv \dot{m}u_e \quad (2.2)$$

and the *total impulse* I_t can be defined as the integral of thrust over the operating time.

$$I_t \equiv \int_{t_0}^{t_f} T dt \quad (2.3)$$

For constant thrust this reduces to

$$I_t = T\Delta t \quad (2.4)$$

[†]Actually, the difference between the exhaust pressure and the ambient fluid pressure has an influence on the thrust and is called *pressure thrust*. This contribution is, however negligibly small compared to the right hand side of Eq. (2.1), *momentum thrust*, as far as the electric propulsion is concerned and thus omitted here.

where $\Delta t = t_f - t_0$. By assuming that the thruster operates at constant u_e for a specified mission, the time integrals of Eq. (2.1) leads to

$$\Delta u = u_e \ln \frac{m_0}{m_f} \quad (2.5)$$

In Eq. (2.5), Δu is interpreted as a maximum velocity increment by the ejection of the propellant by Δm from the initial mass m_0 . Thus $m_f = m_0 - \Delta m$ includes the mass of the engine, power supply system, tankage, etc., plus useful payload. The ratio of m_f to m_0 is sometimes referred to as *mass ratio*, and its explicit expression can be derived by solving Eq. (2.5) for m_f/m_0 .

$$\frac{m_f}{m_0} = \exp \left(-\frac{\Delta u}{u_e} \right) \quad (2.6)$$

Eq. (2.6) implies that, since Δu is automatically determined by the mission requirement, a larger u_e can decrease the propellant mass, which inversely increases the payload mass brought to the final velocity.

In turn, the *specific impulse* I_{sp} is defined as the total impulse per unit weight of propellant

$$I_{sp} \equiv \frac{\int_{t_0}^{t_f} T dt}{g_0 \int_{t_0}^{t_f} \dot{m} dt} \quad (2.7)$$

where $g_0 = 9.8066 \text{ m/sec}^2$ is the standard acceleration of gravity at sea level. By combining with Eq. (2.3) for a constant thrust and mass flow rate, Eq. (2.7) reduces to

$$I_{sp} = \frac{T}{\dot{m}g_0} = \frac{u_e}{g_0} \quad (2.8)$$

Thus the exhaust velocity is directly related to the specific impulse by a factor of approximately 10 in mks units. Since long-range and/or long-time missions such as interplanetary flights or maintenance of satellite position and orientation are characterized by correspondingly large Δu , it is now apparent that the higher specific impulse is the most responsible factor for the choice of propulsion devices.

Thruster efficiency η is defined conventionally as the ratio of the kinetic energy rate contributes to the thrust (axial component) to the total electrical power supplied plus kinetic energy rate of incoming propellant.

$$\eta \equiv \frac{\frac{1}{2} \dot{m} u_e^2}{P + \frac{1}{2} \dot{m} u_{in}^2} = \frac{(I_{sp})_e^2}{\frac{2P}{\dot{m}g_0^2} + (I_{sp})_{in}^2} \quad (2.9)$$

where $P = IV$ is the electric power input to the thruster and the subscript "in" denote the inlet. Thruster efficiency accounts for all the energy losses, including anode/cathode heat conduction loss, viscous dissipation, thermal/chemical frozen loss, and losses due to radiation.

2.2 Simple Performance Analysis

As noted previously, more than two-dimensional analysis is inevitably required for the accurate prediction of the thruster performance. However, focussing on essential flow features, we can roughly estimate the thrust and specific impulse in the following way [12]. Although the accuracy might not be enough to be useful for practical applications, this can at least give us fundamental guidelines for the construction of more complicated models.

We model the flow within the constrictor as composed of two regions, namely arc core and the cold gas surrounding it (Fig. 2.1). From the viewpoint of fluid dynamics, it is apparent that pressure in the radial direction is almost constant. On the other hand, the temperature inside the arc can be more than 10,000 K, whereas of the order of 1,000 K at most for the cold gas. This implies that very little mass is carried inside the arc; the high temperature corresponds to low density at the same pressure. Hence the flow is essentially carried in the cold gas region, the area of which can be expressed as $A - A_a$ (A and A_a are the cross section of the constrictor and the arc column, respectively). Since the flow chokes at (or near) the constrictor exit, the mass flow rate can be expressed as

$$\begin{aligned} \dot{m} &= \rho_{\text{out}} u_{\text{out}} (A - A_a) \\ &= \frac{p_{\text{out}} c_{\text{out}} (A - A_a)}{RT_{\text{out}}} \\ &= \frac{\gamma p_{\text{out}} (A - A_a)}{c_{\text{out}}} \end{aligned} \quad (2.10)$$

where the subscript "out" denotes the outer flow property with $c = \sqrt{\gamma RT}$ being the speed of sound. In turn, the familiar mechanical interpretation of a rocket's thrust states that this thrust arises from the lack of a reaction surface for p_{out} in the area of the throat.

$$T = c_F p_{\text{out}} A \quad (2.11)$$

c_F is a nozzle coefficient of order 1-2, accounting principally for the pressure forces on the diverging nozzle bell. Accordingly, the specific impulse is given by

$$I_{\text{sp}} = \frac{T}{\dot{m} g_0} = \frac{c_F c_{\text{out}}}{\gamma g_0 (1 - A_a/A)} \quad (2.12)$$

Equation (2.12) contains crucial implications in developing more than two-dimensional models which is required for the accurate prediction of thruster performance:

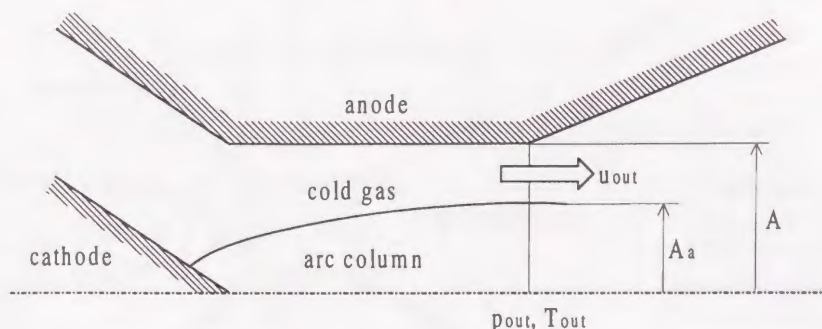


Figure 2.1: Modeling of arcjet flow in the constrictor region

1. The temperature distribution in the cold gas region must be predicted well. This also implies that, although much emphasis is placed on the reproduction of discharge phenomena inside the arc core, its complicated physics plays only a secondary role on the performance prediction.
2. The area ratio of the arc column to the constrictor (A_a/A in Eq. (2.12)) affects directly on the specific impulse, raising a requirement that the size of the arc at the constrictor exit must be predicted accurately. Since a series of transport phenomena including diffusion and thermal conduction are mainly responsible for radial arc growth, these properties must be precisely modeled.

Keeping the above mentioned in mind, we try to construct the two-dimensional models that can reproduce the arcjet physics including the arc column without relying on simplifications as introduced in the present section.

2.3 Key Issues on Arcjet Physics

We next concern some important physics that must be taken into account in the model. It is true that, despite its relatively simple configuration, the flow field inside arcjets involves so much of different physical mechanisms. They range from the well-known fluid dynamical effects to more complicated one associated with high-temperature gas dynamics, some of which are crucial and others may be neglected. The key issues are then illustrated in Fig. 2.2. The following discusses these phenomena for the purpose of the physical explanation as well as the examination of their relative importance on arcjet computations. Several excellent texts consider various aspects of these topics in detail (e.g. [33]); here we select only a few critical points.

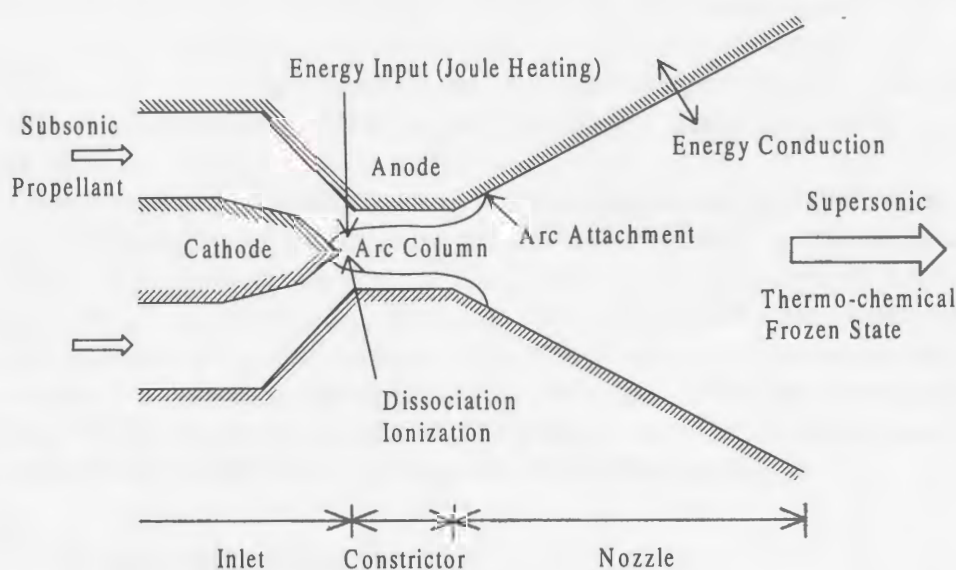
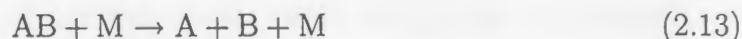


Figure 2.2: Key features of arcjet physics

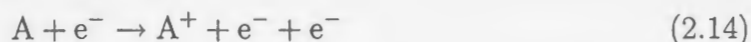
2.3.1 Dissociation/ionization processes

For a gas composed of molecular species, dissociation may take place at a given circumstance. As an example, for nitrogen gas at 1-atm pressure, the dissociation of N_2 begins when the temperature reaches 4,000 K and almost completes at 9,000 K. This reaction is mainly triggered by the collision of generic particles to the molecule considered.



The reverse reaction can also occur and is referred to as *three-body recombination*.

In turn, at sufficiently high temperatures an atom or molecule may lose one or more electrons and becomes ionized. This becomes important at a temperature more than 10,000 K for 1-atm nitrogen. Various ionization processes can be considered, but the most responsible one is the *electron impact ionization* for atomic species as far as arcjets are concerned.[†]



This reaction is categorized as a special case of *inelastic collision*. From the knowledge of elementary mechanics, it is verified that the kinetic energy of a colliding particle is transmitted to the other particle sufficiently only if the masses of the two particles are nearly equal [34]. Thus the orbits of the electrons in an atom are readily

[†]Other processes include the photoionization, field ionization, and charge-exchange ionization.

transferred by a collision of free electron with sufficient energy, which may result in ionization at some extents. In the exchange, the collision causes the free electron to slow down to an extent equivalent to the ionization energy. This indicates that the most of the ionization energy for the electron-impact ionization is subtracted from the free electron.

The dissociation and ionization can have an impact on the evaluation of thermochemical properties of gas mixture such as specific heats or gas constant. It is well known that these properties for ideal gas can be described by two of three state properties, namely density, pressure, and temperature. For chemically reacting gases, however, they also become a function of each species density considered. This results in a change of the equation of state, and ultimately, a change of flow properties. It should also be noted that these reactions occur endothermically, hence the reaction energy must be supplied from other energy sources.

2.3.2 Transport phenomena

The essence of transport phenomena lies in the random motion of gas-constituent particles. When the gas is out of equilibrium by virtue of a nonuniform spatial distribution of some macroscopic quantity, the particle moves irreversibly from one location to another, carrying with it a certain momentum, energy, and mass associated with the particle itself. The transport of these properties due to the random particle motion gives rise to a series of transport phenomena; viscosity, thermal conduction, and diffusion, correspondingly.

It is known empirically that for a large class of irreversible phenomena and under a wide range of experimental conditions, the irreversible flows can be expressed phenomenologically as linear functions of the thermodynamic forces [35]. Thus, for example, *Fourier's law* for heat conduction expresses that the components of the heat flow are linear functions of the components of the temperature gradient.

$$q = -k \frac{\partial T}{\partial x} \quad (2.15)$$

Similarly the expression of viscosity becomes

$$\tau = \mu \frac{\partial u}{\partial x} \quad (2.16)$$

Fick's law establishes a linear relation between the mass diffusion flow for species A and its concentration gradient as

$$J_A = -D_{AB} \frac{\partial n_A}{\partial x} \quad (2.17)$$

where binary diffusion is assumed for simplicity. A difficulty comes from that we need to evaluate the coefficients k , μ , and D for multi-component gas mixture assuming thermal nonequilibrium. This will be further discussed in the next chapter.

As discussed in the previous section, success of arcjet computations depends on how we can accurately predict the energy distribution outside the arc column. Regarding this, transport phenomena play a crucial role since the convection has basically nothing to do with the arc growth: there is essentially no radial velocity components in the constrictor with the pressure remaining almost constant vertically. Hence accuracy of the transport coefficient is directly related to accuracy of the performance prediction.

2.3.3 Ohmic heating

In arcjets, energy input occurs in the arc column as a volumetric heating, which is termed *Ohmic heating*.[†] If the electric current passes thorough the area S by the distance Δx and consequently the electric potential decreases to ΔV , the energy contained in the volume $S\Delta x$ must equal to the corresponding potential energy, $jS\Delta V$, where j is the current density. Hence the input energy per unit volume becomes $j\Delta V/\Delta x$. Considering that $\Delta V/\Delta x$ represents the electric field, the Ohmic heating rate S_{Joule} is finally expressed as an inner product of the current density vector j and the electric field vector E .

$$S_{\text{Joule}} = j \cdot E \quad (2.18)$$

The Ohmic heating can also be interpreted as a result of collision between electrically accelerated electron and other particles. Hence the Ohmic heating excite the electron/electric energy first, and the excited energy is transferred to heavy particles via elastic/inelastic collisions. This implies that we need to add the Ohmic heating terms to both the electron energy equation and the total energy equation constructing the equation system.

2.3.4 Chemical nonequilibrium

In general, the local speed of chemical reactions is directly related to *number* density of the gas considered (rather than *mass* density since a series of reaction takes place as a result of collision between particles, and mass of particles plays only a secondary role itself). The rate of chemical reaction, in fact, increases very rapidly with increasing the number density at a given temperature. Therefore we may encounter circumstances where the characteristic time of chemical reactions is the same order of that of the flow field due to low density, which is called *chemical nonequilibrium*. To discuss further, we define *Damköhler number* D_a as the ratio between the flow residence time and the time required for completion of chemical reactions [34].

$$D_a = \frac{\text{Flow residence time}}{\text{Time required for equilibration}} = \frac{\tau_f}{\tau_r} \quad (2.19)$$

[†]Sometimes called *Joule heating* as well.

Using this parameter, we can classify the flow state regarding chemical reaction into three types:

1. *Equilibrium flow*: wherein $\tau_f \gg \tau_r$. In this case, chemical reactions complete instantaneously so that local chemical composition of gas can be determined only by thermodynamic properties at that location, namely temperature and density (or pressure).
2. *Nonequilibrium flow*: wherein $\tau_f \sim \tau_r$. In this case, chemical composition of gas can become a function of location as well as thermodynamic properties.
3. *Frozen flow*: wherein $\tau_f \ll \tau_r$. In this case, the fluid element zips through the flow field before any chemical changes can take place and therefore chemical composition remains almost constant throughout the flow field.

For arcjets, the flow may be in chemical nonequilibrium inside the nozzle where the density is relatively low due to expansion. The atomic recombination processes occurring in the nozzle are three-body recombination, as discussed previously, and their rates are roughly proportional to the square of gas density ρ , whereas flow residence time in a nozzle is proportional to the length of the nozzle L [36]. Therefore, the Damköhler number in the nozzle is proportional to $\rho^2 L$. This becomes a criterion of the choice of chemical models.

2.3.5 Thermal nonequilibrium

Here we concentrate on the microscopic nature of a gas. For ionized gases, a molecule has several modes of internal energy, as follows (see Fig. 2.3):

1. *Translational energy*: the energy associated with the spatial motion of particle.
2. *Rotational energy*: the energy associated with the molecule's rotational velocity and its moment of inertia.
3. *Vibrational energy*: the energy associated with the molecule's linear motion in bonding direction and the potential energy due to intermolecular force (symbolized by the spring).
4. *Electron energy*: the energy associated with the spatial motion of free electron.
5. *Electronic excitation energy*: the kinetic/potential energy of the electron in orbit.

The property "temperature" can be defined for each energy mode if their energy distributions follow *Maxwellian* [33], and commonly termed as *translational temperature* T_{tr} , *rotational temperature* T_{rot} , *vibrational temperature* T_{vib} , *electron temperature* T_e , and *electronic excitation temperature* T_{ex} , correspondingly. The results of quantum

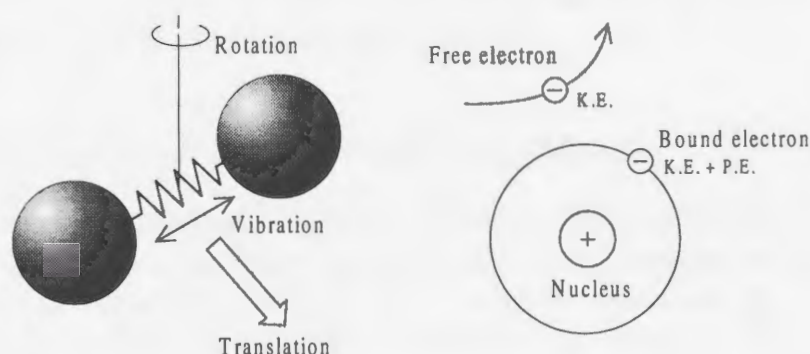


Figure 2.3: Modes of molecular energy

mechanics have shown that each of the above energies is *quantitized*, i.e., they can exist only at certain discrete values. This leads to breakdown of classical treatment of mechanics, such as the application of the energy equipartition principle [33], and can make the analysis extremely complicated.

The term *thermal nonequilibrium* is defined such that these energy modes can not be described by an unique temperature. In this case, additional equations for the conservation of each energy are required, and subsequently, corresponding energy relaxation mechanisms must be modeled and incorporated in the equations. Thermal nonequilibrium can have an impact on the evaluation of chemical reaction rates and transport properties and becomes important for low density and/or high temperature flows as is the case of chemical nonequilibrium.

2.3.6 Frozen losses

For arcjets, the degree of thermochemical nonequilibrium influences directly on the thruster performance. This is based on the fact that chemical reactions absorb or release much energy than other flow mechanisms. The dissociated or ionized particles are expected to recombine in the nozzle due to rapid decrease of temperature, hence the energy used to dissociate/ionize the gas in the arc column is recovered to kinetic energy which contributes to the thrust at some extent. However, if the density in the nozzle is low and thus chemically frozen, the gas does not substantially recombine before it leaves the nozzle and an amount of chemical energy is left in the flow, which results in the degradation of thruster performance. This kind of loss mechanism is referred to as *chemical frozen loss*.

As well, if the internal energy discussed in the previous subsection is not sufficiently equilibrated with translational energy in the nozzle, the subtracting energy does not contribute to the thrust and become a mechanism of thruster deterioration, which is termed *thermal frozen loss*.

Previous studies have shown that these frozen losses are the most responsible for thruster degradation and need to be predicted well.

2.4 Numerical Problems Expected

As will be discussed in the next chapter, the flow field inside DC arcjet thrusters can be described by the Navier-Stokes equations that have been extended to thermal and/or chemical nonequilibrium gases plus Maxwell's equations that describe the electric field. To solve these equations, time-marching algorithms have been widely used since they can apply to both inviscid and viscous flows and can be used in conjunction with virtually any spatial discretization. Although it has been becoming feasible to solve the equation set numerically owing to the advance of numerical methods, we still encounter a number of computational burden that is hard to overcome. These problems are associated with physics inherent in arcjet flows and then arise inevitably. Key issues of them are discussed in detail by the following.

2.4.1 Low-Mach number effects

The flow speed inside the thruster can vary from subsonic at the inlet to supersonic in the nozzle, so that the compressible equations must be used throughout. When the magnitude of the flow velocity is small in comparison with the acoustic speed, the convection terms of the equations become stiff and time-marching methods converge very slowly.

It is well known that a time-marching method works best when eigenvalues of the Jacobian matrix for the equation system λ are clustered. If we employ the so-called density based method (DBM), λ becomes $u, u + c$, or $u - c$ for one-dimensional inviscid flows, where u and c are the local flow speed and the speed of sound, respectively. Therefore for cases $u \ll c$, the eigenvalues can differ severely and the rate of convergence becomes considerably small.

Adding this, in the arc core, the flow is subsonic but is notably compressible because of density changes induced by volumetric heat addition, namely Ohmic heating. In this region, the temperature is of the order of 10,000 K and consequently the speed of sound becomes high, which lowers the local Mach number even when the flow speed is relatively high. Since the pressure term is of order $1/M^2$ while the advective term is of order unity in the nondimensional momentum equations, low Mach number sometimes causes the singularity for the pressure gradient terms and may smear the pressure field.

2.4.2 High-temperature effects

High-temperature effects involve many computational problems as well. Although we assume thermal and/or chemical nonequilibrium, the characteristic time of chem-

ical reactions tends to be much smaller than that of fluid motion. This influences in the way that terms associated with high-temperature effects (i.e. mass production terms and thermal relaxation terms) may become much larger than convective terms or diffusive terms at the initial stage of computation. Furthermore, since these terms are in general strongly nonlinear for the species density and temperature, a bit of numerical fluctuation can change these terms significantly and sometimes leads to breakdown of the computation.

These problems become serious especially in the prediction of electron properties. As far as arcjets are concerned, the behavior of electron determines the basic flow structure such as the arc column and needs to be predicted accurately. However, the mass of electron is by many orders of magnitude smaller than that of other particles and hence computation of the electron density/energy distribution is much liable to be suffered from numerical error.

Due to these trends, allowable time increment to integrate the flow field equations is forced to be prohibitively small and enormous amount of iterations are required to obtain steady state solutions.

2.4.3 Diffusive nature of the flow field

Typically, the scale of the arcjet thruster is of the order of millimeter, which is in contrast to many kinds of computations for hypersonic chemically reacting flows (typically order of centimeter or meter). In this case a series of transport phenomena become dominant as well as convective fluid motions and the flow field tends to be considerably diffusive. This implies the flow field becomes parabolic/elliptic rather than hyperbolic in nature and this can be a problem from the computational point of view. For time-marching algorithms associated with the compressible flow, allowable time increment Δt is basically determined by the so-called CFL condition. Unfortunately, Δt determined by this criterion is too small to perform the computation efficiently for the region where diffusive phenomenon is dominant, and consequently the scheme converges very slowly.

On the other hand, it is well known that the restriction of Δt becomes extremely severe if the parabolic terms are treated explicitly for more than two-dimensional problems [37]. Thus these terms should be discretized and solved in an implicit way. However, for solving large equation systems, direct formulation of the implicit scheme on diffusive terms involves accurate estimation of the Jacobian matrix, which requires considerable numerical operation and additional efforts to couple with the convective term. Actually it is expected to be quite expensive to solve the equations implicitly for both convective and diffusive terms within a category of time-marching algorithm, although not impossible to implement. An efficient solver which replaces the rigorous implicit formulation is thus required.

2.5 Summary

In this chapter, fundamental theories on electric propulsion, key features of arcjet physics, and expected numerical problems are discussed. Also, from the simple performance analysis, it has been shown that accurate reproduction of the arc column and consequently accurate evaluation of radial energy distribution are crucial for the performance estimation using the computational fluid dynamics technique. Computations of the arcjet flow tend to be difficult in the sense that detailed physics such as chemical reactions can have a serious effect on the basic flow structure and the thruster performance. Actually as discussed, the flow field in arcjets contains many independent phenomena which are difficult to model but indispensable to take into account. In the next chapter, basic governing equations that describe the thermochemical nonequilibrium plasma flow in the arcjet thruster are formulated and the basic physics discussed in this chapter is consistently modeled in detail.

Chapter 3

Modeling

3.1 Problem Setting

Actual arcjet thrusters can be operated in a broad range of input power, typically from several hundreds to more than 100 kW classes. Relatively high-power arcjet thrusters, such as HIPARC-R in IRS, Germany, have been developed recently to obtain both high specific impulse and high thrust levels for the application of manned interplanetary missions, to Mars for example. As opposed to these high-power thrusters, in the present study, we consider a low-power DC arcjet thruster which is expected to be utilized for north-south stationkeeping (NSSK) of satellites.

As for the propellant, hydrazine (N_2H_4) or ammonia (NH_3) is expected to be used for the practical thruster application because of their advantages in terms of specific heat and thermal conductivity, attainable exhaust speed, and storability. In this study, however, nitrogen (N_2) is selected as a preliminary step for more complicated models. The main motivations are as follows:

1. Many numerical works employ hydrogen as propellant, but few employ nitrogen.
2. Accounting of hydrazine or ammonia can make the model extremely complicated: e.g., for hydrazine, we need to assume the gas consists of at least 11 chemical species and 48 elementary reactions to take into account the decomposition only [38], and much are required for the inclusion of ionization. Furthermore, there are few available data for collision cross sections that are required to evaluate the transport properties with respect to these gas constituents.
3. For nitrogen, quite reliable experimental data and chemical models are available for wide range of conditions, most of which are derived from studies associated with hypersonic flows. Note that nitrogen is a constituent of air.

Table 3.1: Operating conditions of a typical low-power arcjet thruster

Propellant	Mass flow rate (kg/s)	Current (A)	Power (kW)	Specific power* (kJ/kg)
N ₂	10 ⁻⁴	10	0.5	5,000

* Defined by a ratio of input power to mass flow rate

Typical operating conditions of a low-power DC arcjet thruster are set and shown in Table 3.1.

Within the range of these conditions, the temperature is expected to be of the order of 20,000-30,000 K inside the arc column, and the pressure of 100 kPa at the inlet. These assumptions have been in fact verified from many experimental works.

3.2 Basic Assumptions

In order to construct the equation system, physical phenomena discussed in the preceding chapter must be modeled in detail. Needless to say, it is impossible to take into account all the physics that can be considered, and the model must be developed by balancing its accuracy with the practical limitation of computational resources. Now we examine how the model can be simplified without losing essential features regarding the state of the flow in the thruster and the physical processes involved.

3.2.1 Flow model

First and foremost, the flow is assumed to be steady and axisymmetric. It is conceivable that the arc column might constrict in three-dimensional fashion and attaches to the anode via spokes with being rotating periodically in the azimuthal direction [12]. This must change a series of energy exchange mechanisms between the fluid and the electrode wall, and then influence the prediction of thruster performance. To simulate this, we need to construct a three-dimensional equation system and to solve it by a time-accurate algorithm, which is of course prohibitively expensive. The steady and axisymmetric assumption is valid as long as we are interested in the fundamental flow structure and the effect of three-dimensional arc constriction is expected to be relatively minor.

On the other hand, the flow in the azimuthal direction, called swirl flow, must be taken into account in some cases. This flow component has an effect that the arc column is constricted well in the constrictor and consequently stabilized. In this case, unlike three-dimensional computations, we only need to add the momentum conservation equation for azimuthal direction to the equation system with omitting all azimuthal derivatives. This kind of formulation is sometimes referred to as "two

and half-dimensional" model and the computational time becomes the same order with that for purely two-dimensional cases. In fact many previous numerical works employed this model (e.g. [21], [24]), but difficulty may arise that how we set the azimuthal velocity component at the inlet, which can not be determined from the operating conditions and forced to be somewhat intuitive. In the present study, the swirl flow is assumed to have little influence on performance prediction and therefore neglected.

Next we discuss the continuity of the flow field. Specifically, the Navier-Stokes equations of continuum gas dynamics fail when gradients of the macroscopic variables become so steep that their scale length is of the same order as the average distance traveled by the molecules between collisions, or *mean free path* [39]. The ratio of the mean free path λ to the characteristic length L defines the *Knudsen number* Kn i.e.,

$$Kn = \frac{\lambda}{L} \quad (3.1)$$

The necessary condition for the validity of the continuum approach is that the Knudsen number be small compared with unity. Therefore, a question arises as to whether the Knudsen number is sufficiently small at the nozzle exit. To examine this, we conventionally evaluate the Knudsen number for perfect gas flow in the following way.

From the classical kinetic theory, the mean free path for an arbitrary gas is expressed as

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n} \quad (3.2)$$

where d is the diameter of a gas particle, particularly $d = 3.75 \text{ \AA}$ for the nitrogen molecule. We now need to evaluate the number density n at the nozzle exit. This can be done by applying the well-known quasi-one-dimensional isentropic relation between the throat and an arbitrary nozzle section.

$$\frac{A}{A^*} = \frac{1}{M} \left[\frac{1 + \frac{\gamma-1}{2} M^2}{\frac{\gamma+1}{2}} \right]^{\frac{\gamma+1}{2(\gamma-1)}} \quad (3.3)$$

$$\frac{p}{p^*} = \left[\frac{\frac{\gamma+1}{2}}{1 + \frac{\gamma-1}{2} M^2} \right]^{\frac{\gamma}{\gamma-1}} \quad (3.4)$$

$$\frac{T}{T^*} = \left[\frac{\frac{\gamma+1}{2}}{1 + \frac{\gamma-1}{2} M^2} \right] \quad (3.5)$$

where the superscript $*$ denotes the value at the throat. For typical arcjet thruster configurations, the nozzle area ratio A/A^* becomes order of 100. Further assuming

that $T^* = 300$ K and $p^* = 1$ atm, we can solve Eqs. (3.3) to (3.5) and obtain the exit number density of $n = p/kT \approx 1.2 \times 10^{23} \text{ m}^{-3}$. Substituting this into Eq. (3.2), λ becomes $1.3 \times 10^{-5} \text{ m}$. Since the characteristic length for a typical arcjet thruster is of the order of mm, corresponding Knudsen number becomes $O(10^{-2})$, which is the critical order above which the continuum assumption breaks down. Hence it may be preferable to solve the nozzle flow by the molecular approach, whereas the continuum approach can be available upstream the constrictor wherein the local density is considerably high. This implies that we need to solve the flow field by using the NS-DSMC hybrid scheme, and its implementation belongs to the state-of-art works at the present (e.g. [40]). Therefore, to simplify the analysis, we roughly assume that the continuum approach is valid through the entire flow field. Because of the parabolic nature of the flow field inside the nozzle, free molecular effects are expected to be relatively minor.

Finally, the flow field is regarded as laminar. This is a reasonable assumption since the local Reynolds number at the constrictor exit becomes order of 10^4 at most, and further decreases in the nozzle due to expansion.

3.2.2 Chemical nonequilibrium

Suppose that we employ the chemical equilibrium model for the present. In this case, chemical composition of the gas is determined locally by applying the law of mass action, and there is no need to solve additional equations which represent the mass conservation for each gas species considered. In fact, many codes that compute the equilibrium composition of various gases are available (e.g. [41]) and, by using them, the number of equation becomes the same as the perfect gas computations, so that the CPU time required is expected to be almost the same order as well. This is, of course, preferable from the computational viewpoint.[†] Nevertheless, in the present study, the assumption of chemical equilibrium is abandoned and the entire flow field is assumed to be in chemical nonequilibrium. There are two main reasons regarding this.

First, needless to say, we must simulate the discharge phenomena as well as the flow field itself. Assuming chemical equilibrium, however, we tend to predict extremely few electrons outside the arc column where the temperature is of the order of 1,000 K and hence the ionization does hardly take place. Since the electron

[†]This is not equivalent to that the scheme accordingly becomes robust. From the author's personal experience, it has been found that a numerical scheme employing a chemical equilibrium model tends to be rather fragile compared to nonequilibrium cases. This is because chemical reactions are assumed to be completed instantaneously: a bit of fluctuation of flow properties can change the chemical composition of the gas drastically, which affects the energy distribution through the flow field and sometimes leads to breakdown of the computation. On the other hand, the stiffness can be somewhat relieved for nonequilibrium computations by treating the associated source terms implicitly. It should be noted that reduction of the computational time does not always correspond to simplicity of the computation.

density and electrical conductivity are essentially zero outside the arc in this case, no mechanism exists for current to reach the anode. Previous computations remedied this problem by setting an artificial minimum value to the electrical conductivity (referred to as conductivity floor) [16], but it should be determined recursively so that the total voltage computed are equal to experimental data. In other words, it is impossible to specify the reasonable value before the computation. Therefore the chemical equilibrium computations may involve additional difficulties in spite of its simplicity.

Second, as discussed in the preceding chapter, evaluation of the frozen losses (or flow chemistry in the nozzle) is critical to predict the thruster performance. Since it is apparent that the flow inside the nozzle is in chemical nonequilibrium due to low density, there is little hope that the chemical equilibrium model can predict the nozzle chemistry accurately.

For these reasons, the assumption of chemical nonequilibrium is essential for arcjet computations.

3.2.3 Thermal nonequilibrium

The temperature can be defined only if the energy distribution for each energy mode is in accord with the Maxwell-Boltzmann distribution (or simply Maxwellian). Strictly speaking, the distributions of charged particles considerably deviate from the Maxwellian due to the externally applied electric field [42]. In this case, the energy distribution must be described by the multienergy models rather than multitemperature models, indicating that we must discard the approach based on the classical mechanics and solve the *master equation* in the state-to-state fashion with taking into account the quantum effects [43]. These approaches are, of course, far from the practical flow computations and hence we are forced to assume that the Maxwell-Boltzmann distribution is valid for all energy modes without verification.

Under this assumption, the most detailed and complicated model treats each temperature discussed in the previous chapter separately, consists of translational, rotational, vibrational, electron, and electronic excitation temperatures. Consequently we need to solve additional energy conservation equations associated with these temperatures. Such a model is referred to as multi-temperature model, and practically implemented and performed in the field of hypersonic problems by Candler and MacCormack [44], [45]. Since the chemical reactions depend on the thermal nonequilibrium state strongly, accuracy of the computations is expected to be enhanced by assuming thermal nonequilibrium. However, a question arises as to whether it is truly worthwhile to increase the number of the internal energy modes. As an example, in Ref. [45], the vibrational temperatures of each molecular species are calculated independently as well as electron temperature, resulting in a five-temperature model. In order to do so, the vibration-vibration energy exchanges among the molecules are required to be accounted for, as well as the coupling

among the electron translational mode, electronic excitation mode, and the translational/rotational modes. Since these energy transfer rates are not known accurately a fair amount of conjecture must be inevitably used. Generally speaking, this implies that not only does the model require more computing time but also it may introduce unnecessary uncertain factors associated with the energy transfer rates. Therefore a thermal model must be constructed so that the additional computational efforts are compensated by the enhancement of accuracy in terms of the simulation of detailed physics.

In the present study, the rotational temperatures for each molecular species are assumed to be equal to the translational temperature. This is because there is no simple and reliable relaxation model associated with this energy mode and also the rotational mode is considered to be equilibrated with the translational mode rapidly.[†] Further, electronic excitation energy mode are not taken into account because this is negligibly small in general.

On the other hand, the electron temperature must be separated from other temperatures. This is because, as discussed before, the mechanisms of arc attachment to the anode are involved so much with the electron temperature distribution outside the arc. The ionization processes and ambipolar diffusion become a strong function of the electron temperature and play a crucial role for the discharge phenomena.

The effect of vibrational energy nonequilibrium must have an impact for the fundamental physics of arcjets. This is because the dissociation rate is expected to be a function of both the vibrational excitation of the diatomic molecule and the translational temperature of the impacting heavy particle. However, the previous computational work has found that the energy exchange models regarding the vibrational nonequilibrium are insufficient to simulate the discharge phenomena for arcjet computations [48], although they can reproduce the energy state behind the strong shock fairly well. Thus we abandoned the inclusion of vibrational nonequilibrium models for the time being and the vibrational temperatures for each diatomic species are assumed to be equilibrated with the translational-rotational temperature (to what follows, we simply call this temperature as *heavy particle temperature* in contrast to the electron temperature). The possibility of applying the three-temperature model is discussed in the subsequent chapter.

We finally summarize that the thermal state of the flow field concerned is assumed to be expressed basically with only two temperatures, namely the heavy particle temperature and the electron temperature.

[†]The behavior of rotational temperature is of importance concerning the backflow of plume. It has been argued that the degree of backflow are essentially dictated by the internal energy of the plume constituent, which consists mostly of the rotational mode [46]. Note that the DSMC computation can readily include the rotational nonequilibrium by applying the Borgnakke-Larsen statistical model [47] and in fact the computations in Ref. [28] and [29] concern this.

3.2.4 Magnetic field

The existence of magnetic field may change the equation system and the accompanying physical properties in the following way:

1. The magnetic body force to the gas $\mathbf{j} \times \mathbf{B}$, commonly known as Lorentz force, appears in the momentum conservation equation.
2. Terms representing induced electric field, Hall effect, and ion slip appear in the Ohm's law.
3. The applied field drastically curves the trajectory of charged species, so that it affects the bulk property of the gas such as the electrical conductivity, sometimes shifts the nature from scalar to tensor.

Although effects of the magnetic field must be consistently incorporated for MPD computations since the magnetic effects are expected to be dominant through the flow field, they appear to be of little importance for arcjets due to relatively small currents. This is examined as follows.

Conventionally, the intensity of the magnetic acceleration process is scaled by the *magnetic interaction parameter* β defined as

$$\beta \equiv \frac{\sigma B^2 L}{\rho u} \quad (3.6)$$

It can be verified that β becomes of the order of unity in the range of practical interest for ideal MPD thrusters [1]. To construct a numerical estimate for arcjets, we presume the velocity u , gas density ρ , electrical conductivity σ , and characteristic length L to be 10^3 m/s, 10^{-2} kg/m³, 10^2 mhos/m, and 10^{-3} m, respectively. The arc current I under consideration is typically 10 A, from which the magnetic flux density B becomes approximately $B \approx \mu_0 I / 2\pi L = 2 \times 10^{-3}$ Wb/m². Finally we estimate the magnetic interaction parameter $\beta = 4 \times 10^{-8}$, indicating that the magnetic body force is negligibly small for low-power arcjets.

In turn, collision-free charged particles moving in the electromagnetic field show a spiral drift motion with *gyro frequency*,

$$\omega_B = \frac{eB}{m_e} \quad (3.7)$$

For dense plasma, collisions change the orbit of charged particles as well, and in this case the ratio of the gyro frequency ω_B to the collision frequency ν_c distinguishes the response of the particle swarm to the applied electromagnetic fields. If $\omega_B/\nu_c \gg 1$, the particles execute many cycles of their cycloidal drift motion before they are disturbed by collision, whereas if $\omega_B/\nu_c \ll 1$, they seldom complete one cycle of the drift motion before collision, and develop little cross-field motion. Thus the primary component of the charged particle swarm is parallel to the electric field, with only

a small deflection caused by the magnetic field. The ratio ω_B/ν_c is popularly called the *Hall parameter*, and we can generally neglect the effect of Hall current, ion slip and other factors associated with the drift motion when $\omega_B/\nu_c \ll 1$. In most cases where the density are sufficiently high, one is tempted to neglect ion currents entirely because of the large inertia of these particles compared to electron. Hence $\omega_B/\nu_c \ll 1$ with respect to electron is the necessary condition for neglecting these cross-field effects. In a similar fashion to the estimation of the magnetic interaction parameter, we evaluate Eq. (3.7) for electron and obtain $\omega_B = 3.5 \times 10^8$, whereas we roughly estimate $\nu_c = O(10^{11})$ 1/s at most. Thus the Hall parameter becomes order of 10^{-3} and it is found reasonable to neglect the effects of the magnetic field on the mobility of charged particles.

3.2.5 Others

Other assumptions required to simplify the computation are briefly discussed here. The plasma is assumed to be macroscopically neutral, so that the electron number density must be equal to the sum of the each charged heavy particle. All energy loss mechanisms associated with radiation are neglected because the escape coefficients are considerably small as far as arcjets are concerned. The mean velocities of each species are assumed to be identical, although the thermal velocities are different for heavy particles and the electron. The individual species are assumed to obey the ideal gas law, so that the equation of motion for the multi-component gas mixture can be described as a summation of partial pressure expression of each species via Dalton's law of partial pressures.

3.2.6 Summary of assumptions

It is confirmed again that the aforementioned assumptions are valid as far as we concern the low-power DC arcjet thruster with nitrogen as propellant under operating conditions of Table 3.1. Finally main issues are briefly summarized as follows.

1. The flow field is steady, axisymmetric, continuum, and laminar.
2. Swirl flow can be neglected.
3. The flow is in chemical nonequilibrium.
4. Thermal state of the flow field can be described by the heavy particle temperature and the electron temperature.
5. All magnetic effects can be neglected.
6. The plasma is macroscopically neutral.
7. Radiation losses can be neglected.

3.3 Flow Field Equations

In order to carry out numerical computation, one must first derive a set of equations that correctly account for the physics discussed so far, based on the assumptions introduced in the previous section. Within the continuum approach, the flow field in arcjet thrusters can be described by coupled time-dependent partial differential equations for the conservation of mass, momentum, and energy. These become the Navier-Stokes equations that have been augmented to include an equation for each gas species and internal energies considered. The purpose of this section is to construct the equation set with relevant arcjet physics taking into account. It must be pointed out that the present formulation owes substantially to the work of Lee [49] and we would like to obey his derivations unless any alternation is obliged to.

3.3.1 Mass conservation equation

The conservation law for a flowing gas states that the various average quantities $\langle \phi_s \rangle$ per unit particle are conserved for a volume element as

$$\begin{aligned} [\text{Time variation of } \langle \phi_s \rangle] &= [\text{Difference of inflow and outflow of } \langle \phi_s \rangle] \\ &+ [\text{Production rate of } \langle \phi_s \rangle] \end{aligned} \quad (3.8)$$

The limit of Eq. (3.8) reduces to the differential expression of the conservation equation as

$$\frac{\partial}{\partial t}(n_s \langle \phi_s \rangle) + \frac{\partial}{\partial x^j}(n_s \langle \phi_s v_s^j \rangle) = S(\langle \phi_s \rangle) \quad (3.9)$$

where n_s is the number density of species s , $\langle v_s^j \rangle$ is the average value of the j th component of particle velocity v_s^j , and $S(\langle \phi_s \rangle)$ represents the rate of change in $\langle \phi_s \rangle$ due to interactions among various species. Thus the mass conservation equation for species s is obtained by identifying $\langle \phi_s \rangle$ with the species mass m_s . The source term in this case is the mass production rate of species s due to chemical reactions and denoted by $\dot{w}_s$.

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x^j} [\rho_s (u_0^j + V_s^j)] = \dot{w}_s \quad (3.10)$$

where $\rho_s = m_s n_s$ is the mass density of species s and the summation $\sum_s \rho_s$ equals to the total density ρ . u_0 is the mass-averaged velocity component given by

$$u_0^j = \frac{\sum_s \rho_s v_s^j}{\sum_s \rho_s} = \sum_s C_s u_s^j \quad (3.11)$$

where $u_s^j = \langle v_s^j \rangle$ is the mean velocity of the species, $C_s = \rho_s/\rho$ the mass concentration of species s , and $V_s^j = u_s^j - u_0^j$ is the diffusion velocity of the species.

The summation of Eq. (3.10) over all species yields

$$\frac{\partial}{\partial t} \sum_s \rho_s + \frac{\partial}{\partial x^j} \left[\sum_s \rho_s u_0^j + \sum_s \rho_s V_s^j \right] = \sum_s \dot{w}_s \quad (3.12)$$

Since $\sum_s \dot{w}_s$ and $\sum_s \rho_s V_s^j$ must be zero by definition, we obtain the expression of total mass conservation as

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_0^j)}{\partial x^j} = 0 \quad (3.13)$$

3.3.2 Momentum conservation equation

The momentum conservation equation for each species is obtained by denoting $\langle \phi_s \rangle$ as $m_s u_s^i$. In this case, $S(m_s u_s^i)$ consists of the interaction force due to collisions $F_{\text{int},s}^j$, the electric field force $F_{E,s}^j$, and the magnetic force $F_{B,s}^j$. Note that $F_{E,s}^j$ and $F_{B,s}^j$ act on the charged particle only. Consequently, the i th momentum equation for species s becomes

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_s u_s^i) + \frac{\partial}{\partial x^j} (\rho_s u_0^i u_0^j) + \frac{\partial}{\partial x^j} (\rho_s u_0^i V_s^j + \rho_s u_0^j V_s^i) \\ + \frac{\partial p_s}{\partial x^i} - \frac{\partial \tau_s^{ij}}{\partial x^j} = F_{\text{int},s}^i + F_{E,s}^i + F_{B,s}^i \end{aligned} \quad (3.14)$$

where $p_s = \rho_s \langle c_s^2 \rangle / 3$ is defined as the average pressure over the normal components of the thermal momentum flux, and c_s^j is the random thermal velocity component with respect to u_0^j . The viscous stress $\tau_s^{ij} = -[\rho_s \langle c_s^i c_s^j \rangle - \delta^{ij} p_s]$ is defined as the negative of the thermal momentum with the pressure p_s subtracted from the normal components, and δ^{ij} is the Kronecker delta. The total momentum equation is thus obtained by summation Eq. 3.14 over all species. Since $\sum_s \rho_s V_s^j = 0$ and $\sum_s F_{\text{int},s} = 0$, this results in

$$\frac{\partial}{\partial t} (\rho u_0^i) + \frac{\partial}{\partial x^j} (\rho u_0^i u_0^j) + \frac{\partial p}{\partial x^i} = \frac{\partial \tau^{ij}}{\partial x^j} + \sum_s F_{E,s}^i + \sum_s F_{B,s}^i \quad (3.15)$$

where $p = \sum_s p_s$ is the total static pressure. Under the hypothesis of Stokes, the overall viscous shear stress $\tau^{ij} = \sum_s \tau_s^{ij}$ can be expressed as

$$\tau^{ij} = \mu \left(\frac{\partial u_0^i}{\partial x^j} + \frac{\partial u_0^j}{\partial x^i} \right) - \frac{2}{3} \mu \frac{\partial u_0^l}{\partial x^l} \delta_{ij} \quad (3.16)$$

where μ is the viscosity of mixture.

3.3.3 Energy conservation equation

The energy conservation equation for species s is obtained by identifying $\langle \phi_s \rangle$ with the total energy of the species s , that is, $m_s u_s^2/2 + \langle \epsilon_{\text{int},s} \rangle$, where $m_s u_s^2/2$ is the average kinetic energy, and $\langle \epsilon_{\text{int},s} \rangle$ is the average internal energy associated with translational, rotational, vibrational, electron-electronic, and chemical energy mode. The source term $S(\langle \phi_s \rangle)$ consists of the rate of work done by the electric/magnetic field on charged particles $(F_{E,s}^i + F_{B,s}^i)u_s^i$, the rate of energy supplied in elastic/inelastic collisions S_{int} , and the volumetric heating rate by the electric field on electron, (i.e. Ohmic heating) S_{Joule} . Thus

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho_s \left(\frac{1}{2} u_0^2 + u_0^i V_s^i + e_s \right) \right] + \frac{\partial}{\partial x^j} \left[\rho_s u_0^j \left(\frac{1}{2} u_0^2 + e_s \right) \right] + \frac{\partial q_s^j}{\partial x^j} \\ + \frac{\partial}{\partial x^j} \left[\frac{1}{2} \rho_s (u_0^2 V_s^j + u_0^j u_0^i V_s^i) \right] + \frac{\partial}{\partial x^i} (u_0^i p_s) - \frac{\partial}{\partial x^j} (u_0^i \tau_s^{ij}) \\ = (F_{E,s}^i + F_{B,s}^i) u_s^i + S_{\text{int},s} + S_{\text{Joule}} \end{aligned} \quad (3.17)$$

where e_s is the total thermodynamic energy per unit mass of species, $q_s^j = n_s \langle c_s^j \rangle [(1/2) m_s \langle c_s^2 \rangle + \langle \epsilon_{\text{int},s} \rangle]$ is the heat flux component due to random motion. The explicit expression of $S_{\text{int},s}$ is not shown here. Note that the Ohmic heating rate S_{Joule} must be added only for the case $s = e$. The overall energy conservation equation is now obtained by summation over all species, that is,

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho \left(\frac{1}{2} u_0^2 + e \right) \right] + \frac{\partial}{\partial x^j} \left[\rho u_0^j \left(\frac{1}{2} u_0^2 + e \right) \right] + \frac{\partial q^j}{\partial x^j} \\ + \frac{\partial}{\partial x^i} (u_0^i p) - \frac{\partial}{\partial x^j} (u_0^i \tau^{ij}) = \sum_s (F_{E,s}^i + F_{B,s}^i) u_s^i + S_{\text{Joule}} \end{aligned} \quad (3.18)$$

where e is the overall thermodynamic energy per unit mass defined by $e = \sum_s C_s e_s$, and $q^j = \sum_s q_s^j$ is the overall heat flux component. The summation of $S_{\text{int},s}$ vanishes by definition, whereas S_{Joule} still remains because of the above mentioned.

The flux of energy through a multicomponent gas is a result of temperature gradient and diffusion. In the present flow, there are three temperature gradients, namely translational-rotational, vibrational, and electron temperature gradients. By considering these contributions to energy transport, the j th component of the overall heat flux vector q^j can be expressed as the sum of four terms as follows

$$q^j = -(\lambda + \lambda_{\text{vib}}) \frac{\partial T}{\partial x^j} - \lambda_e \frac{\partial T_e}{\partial x^j} + \sum_s \rho_s h_s V_s^j \quad (3.19)$$

where h_s is the enthalpy of species s and $\lambda = \lambda_{\text{tr}} + \lambda_{\text{rot}}$, λ_{vib} , and λ_e are the frozen thermal conductivities of heavy particles, vibrational energy, and electrons, respectively.

3.3.4 Simplification to the equation system

The species momentum equation Eq. (3.14) is rewritten in terms of electron as

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_e u_e^i) + \frac{\partial}{\partial x^j} (\rho_e u_0^i u_0^j) + \frac{\partial}{\partial x^j} (\rho_e u_0^i V_e^j + \rho_e u_0^j V_e^i) \\ + \frac{\partial p_e}{\partial x^i} - \frac{\partial \tau_e^{ij}}{\partial x^j} = F_{\text{int},e}^i + F_{E,e}^i + F_{B,e}^i \end{aligned} \quad (3.20)$$

Although not necessary to be solved, this equation is used to simplify the other equations. Since the mass of the electron is very small compared to that of a heavy particle, Eq. (3.20) can be significantly simplified.

If we take the ratio of the dynamic pressure of the electron gas to the electron pressure and assume that the electron speed and temperature are about the same as the bulk gas, we have

$$\frac{\rho_e u_e^2}{p_e} = \frac{M_e u_e^2}{\Re T_e} \approx \frac{M_e u_e^2}{\Re T} \approx \gamma M_e M^2 \quad (3.21)$$

where γM_e is of the order of 10^{-6} and for conditions of interest, the square of the Mach number will be of the order of 10^2 at most. Therefore we can neglect the electron dynamic pressure relative to the electron pressure. In this case, we may neglect the inertial terms, i.e. the first, second, and third terms of the left hand side of Eq. (3.20). Since the viscous stress owing to electron is generally negligible, the fifth term is also neglected, as it was by Sutton and Sherman [32]. Further we assume that there is no conduction current and magnetic effect in the present flow field and this leads to $F_{\text{int},e} = F_{B,e} = 0$. Thus, Eq. (3.20) becomes

$$\frac{\partial p_e}{\partial x^i} = F_{E,e}^i \quad (3.22)$$

For electron, the electric field force per unit volume is given by

$$F_{E,e}^i = -n_e e E^i \quad (3.23)$$

where e is the electronic charge and E^i is a component of the electric field. Now Eq. (3.22) is rewritten for E^i as

$$E^i = -\frac{1}{n_e e} \frac{\partial p_e}{\partial x^i} \quad (3.24)$$

Physically, Eq. (3.24) implies that the electric field E^i can be induced by the electron pressure gradient even if the charge separation does not occur. Now the overall momentum conservation equation (3.15) can be rearranged by means of the electron momentum equation (3.24) as

$$\frac{\partial}{\partial t} (\rho u_0^i) + \frac{\partial}{\partial x^j} (\rho u_0^i u_0^j) + \frac{\partial p}{\partial x^i} - \frac{\partial \tau^{ij}}{\partial x^j} = \left(1 - \frac{n_I}{n_e}\right) \frac{\partial p_e}{\partial x^i} \quad (3.25)$$

where n_I is the number density of ionized particles and must be equal to n_e when the plasma is assumed to be macroscopically neutral. In this case, Eq. (3.25) becomes equivalent to the standard momentum conservation equation for perfect gases.

In turn, the electron energy equation takes a form

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho_e \left(\frac{1}{2} u_0^2 + u_0^i V_e^i + e_e \right) \right] + \frac{\partial}{\partial x^j} \left[\rho_e u_0^j \left(\frac{1}{2} u_0^2 + e_e \right) \right] + \frac{\partial q_e^j}{\partial x^j} \\ + \frac{\partial}{\partial x^j} \left[\frac{1}{2} \rho_e (u_0^2 V_e^j + u_0^j u_0^i V_e^i) \right] + \frac{\partial}{\partial x^i} (u_0^i p_e) - \frac{\partial}{\partial x^j} (u_0^i \tau_e^{ij}) \\ = F_{E,e} u_e^i + S_{\text{int},e} + S_{\text{Joule}} \end{aligned} \quad (3.26)$$

This must be solved if we need to obtain the electron energy distribution independent of the heavy particle energy distribution. Substituting Eqs. (3.23) and (3.24) into Eq. (3.26) with neglecting the terms associated with kinetic energy of electron, we obtain a simple form of the electron energy equation as

$$\frac{\partial(\rho_e e_e)}{\partial t} + \frac{\partial(\rho_e e_e u_0^j)}{\partial x^j} + \frac{\partial q_e^j}{\partial x^j} + p_e \frac{\partial u_0^j}{\partial x^j} = S_{\text{int},e} + S_{\text{Joule}} \quad (3.27)$$

As well, the overall energy conservation equation (3.18) can be rearranged by means of the electron momentum equation (3.24). By letting $u_s^i = u_0^i$ for all particles and neglecting the term associated with the magnetic effect, Eq. (3.18) can be written as

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho \left(\frac{1}{2} u_0^2 + e \right) \right] + \frac{\partial}{\partial x^j} \left[\rho u_0^j \left(\frac{1}{2} u_0^2 + e \right) \right] + \frac{\partial q^j}{\partial x^j} \\ + \frac{\partial}{\partial x^i} (u_0^i p) - \frac{\partial}{\partial x^j} (u_0^i \tau^{ij}) = \left(1 - \frac{n_I}{n_e} \right) u_0^i \frac{\partial p_e}{\partial x^i} + S_{\text{Joule}} \end{aligned} \quad (3.28)$$

Again, the first term of the right hand side vanishes if we assume the plasma to be neutral.

3.4 Electric Field Equations

In the magnetohydrodynamics, we need to construct the equation system by relating the flow field with the electromagnetic field. Generally the electromagnetic field is induced as a result of interaction between the electric field and magnetic field, and its reciprocal relation can be described by the *Maxwell's equations*. These equations are derived theoretically from the empirical law of Faraday, Ampere, and Gauss.

We would like to quote them as an axiom and thus without derivation here.

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad (3.29)$$

$$\nabla \times \mathbf{H} = \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t} \quad (3.30)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (3.31)$$

$$\nabla \cdot \mathbf{D} = \rho_e \quad (3.32)$$

It should be noted that the last two statements are directly derivable from the first two. The electric displacement field vector $\mathbf{D}$ and the magnetic induction field vector $\mathbf{B}$ are correspondingly related with the electric field vector $\mathbf{E}$ and the magnetic field vector $\mathbf{H}$ as follows.

$$\mathbf{D} = \epsilon_0 \mathbf{E} \quad (3.33)$$

$$\mathbf{B} = \mu_0 \mathbf{H} \quad (3.34)$$

where ϵ_0 and μ_0 are the electric permittivity and the magnetic permeability of free space, respectively.

Comparing the curl of Eq. (3.29) with the partial derivative of Eq. (3.30) yields an equation for $\mathbf{E}$:

$$\nabla^2 \mathbf{E} = \epsilon_0 \mu_0 \ddot{\mathbf{E}} \quad (3.35)$$

Equation (3.35) is a well-known wave equation and implies that free space can support propagation of plane electromagnetic waves with a phase velocity

$$c_0 = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \quad (3.36)$$

This is equivalent to the speed of light by definition. Thus time variation of the electric field is scaled as the speed of light. Considering that the time scale of the flow field is many order of magnitude longer, it is not practical to solve the electromagnetic equation in a time-marching fashion. Fortunately, since we are only interested in the steady state of the flow field, we can omit the time-derivative terms of Eqs. (3.29) to (3.32) and solve them as an elliptic system of equations.

Assuming that the magnetic field is negligibly weak, we don't need to solve Eq. (3.30). Omitting time-derivative terms of Eqs. (3.29) and (3.30), we obtain

$$\nabla \times \mathbf{E} = 0 \quad (3.37)$$

$$\nabla \times \mathbf{B} = \mathbf{j} \quad (3.38)$$

Equation (3.37) implies there exists a scalar function such that

$$\nabla \times (\nabla \phi) = 0 \quad (3.39)$$

Hence we define the electric potential ϕ as

$$\mathbf{E} = -\nabla\phi \quad (3.40)$$

The divergence of Eq. (3.38) yields the conservation of current density $\mathbf{j}$

$$\nabla \cdot \mathbf{j} = 0 \quad (3.41)$$

In turn, the current density is directly related to the electric field by an *Ohm's law*.

$$\mathbf{j} = \sigma \mathbf{E} \quad (3.42)$$

If the gaseous medium is in motion relative to the frame of reference in which the fields are specified, Maxwell's equations remain valid, but certain modifications are required in Eq. (3.42). These may be rigorously derived from considerations of relativistic invariance, or rationalized by empirical argument, in the form

$$\mathbf{j} = \sigma \left(\mathbf{E} + \mathbf{u} \times \mathbf{B} + \frac{1}{en_e} \nabla p_e \right) + \mathbf{j}_H + \mathbf{j}_I \quad (3.43)$$

where $\mathbf{j}_H$ and $\mathbf{j}_I$ are possible contributions from Hall current and ion slip that are discussed in the previous section in this chapter. The electron pressure gradient term denotes the electric field derived from the electron momentum equation (see the previous section). Equation (3.43) is referred to as *generalized Ohm's law*. Under the assumption of negligibly weak magnetic field, this reduces to

$$\mathbf{j} = \sigma \left(\mathbf{E} + \frac{1}{en_e} \nabla p_e \right) \quad (3.44)$$

Substituting Eq. (3.44) with (3.40) into Eq. (3.41), we finally obtain the basic governing equation for the electric field as

$$\nabla \cdot (\sigma \nabla \phi) = \nabla \cdot \left(\frac{\sigma}{en_e} \nabla p_e \right) \quad (3.45)$$

The above equation is an elliptic equation with respect to ϕ . Note that Eq. (3.32) is not used explicitly in the derivation of Eq. (3.45).

The electric field and the fluid field are related each other via the Ohmic heating S_{Joule} , which can be expressed as

$$S_{\text{Joule}} = \mathbf{j} \cdot \mathbf{E} = \frac{j^2}{\sigma} \quad (3.46)$$

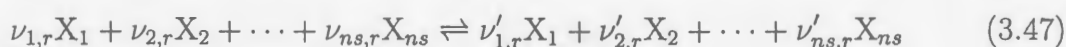
3.5 Chemical Reaction Model

3.5.1 Chemical species

With nitrogen as a working gas, we consider the gas mixture to be made up of four components: neutral molecules, neutral atoms, singly ionized positive ions, and electrons with 5 species (N_2 , N , N_2^+ , N^+ , e^-). We also specify s as an index of each species by denoting that $s = 1$: N_2 , 2: N , 3: N_2^+ , 4: N^+ , and 5: e^- .

3.5.2 Reaction rates

As stated previously, it is assumed that the chemical reactions proceed at a finite rate, hence the production rates of each species must be evaluated. Here we consider nr elemental reactions in the chemical system involving ns species ($X_1, X_2, \dots, X_{ns}$) of the general form



where $\nu_{s,r}$ and $\nu'_{s,r}$ are the stoichiometric coefficients of the reactants and products of species s in the reaction r , respectively. Note that the above formulation involves all chemical species, and therefore if a given chemical species X_s does not occur on one side or the other of the equation, then the corresponding value of ν_s or ν'_s must be zero.

The evaluation of the rates of chemical reactions, commonly called *chemical kinetics*, is a complex and difficult science, both experimentally and theoretically. Although a number of knowledge has been accumulated, the field is still an incomplete state of development, and no general theory exists. It is in fact doubtful whether we can estimate the rates correctly at any cases with only using macroscopic parameters such as temperature or density. However, it has been verified that the phenomenon can be simulated quite satisfactorily by taking up the simplest of the several theories, namely the so-called *collision theory* and we employ this with taking into account the effects of thermal nonequilibrium.

In the framework of this theory, the rate of formation of any one of the *products* in the reaction r can be expressed by an equation of the form

$$\left(\frac{d[X_s]}{dt} \right)_{f,r} = \nu'_{s,r} k_{f,r} [X_{1,r}]^{\nu_{1,r}} [X_{2,r}]^{\nu_{2,r}} \dots [X_{ns,r}]^{\nu_{ns,r}} \quad (3.48)$$

where $[X_s] \equiv \rho_s/M_s$ is the mole density of species s . The stoichiometric coefficient ν'_s is included explicitly, since the change in the number of moles of a given species as a result of the reaction must be in proportional to its stoichiometric coefficient. The so-called *rate coefficient* for a forward reaction r , $k_{f,r}$, is assumed to be a function of

the temperature only. Similarly, the rate of disappearance of any one of the *reactants* is given by

$$\left(\frac{d[X_s]}{dt}\right)_{b,r} = \nu_{s,r} k_{b,r} [X_{1,r}]^{\nu'_{1,r}} [X_{2,r}]^{\nu'_{2,r}} \cdots [X_{ns,r}]^{\nu'_{ns,r}} \quad (3.49)$$

where a negative sign is included since the coefficient $\nu_{s,r}$ is positive by definition. Thus the net mass production rates of species s , $\dot{w}_s$ in Eq. (3.10), can be evaluated by combining Eq. (3.48) and (3.49) and summing over all reactions r , which results in

$$\dot{w}_s = M_s \sum_{r=1}^{nr} (\nu'_{s,r} - \nu_{s,r}) (L_{f,r} - L_{b,r}) \quad (3.50)$$

where

$$L_{f,r} = k_{f,r} \prod_{j=1}^{ns} \left(\frac{\rho_j}{M_j}\right)^{\nu_{j,r}} \quad (3.51)$$

$$L_{b,r} = k_{b,r} \prod_{j=1}^{ns} \left(\frac{\rho_j}{M_j}\right)^{\nu'_{j,r}} \quad (3.52)$$

A question then arises how we estimate the forward/backward rate coefficient k with respect to temperature. Regarding this, before any theory was constructed, it was recognized on experimental grounds that for many reactions a plot of $\ln k$ versus $1/T$ gives an essentially straight line of negative slope, which leads to a relation of the form

$$k = CT^\epsilon \exp(-\theta_r/T) \quad (3.53)$$

where the constant C , η , and ϵ are independent of T . The factor T^η is multiplied to take into account the slight deviation of the $\ln k$ versus $1/T$ from the straight line. This equation is commonly called *Arrhenius equation*, and θ_r has a dimension of temperature and then called the characteristic temperature of reaction r .

In turn, by applying Eq. (3.50) at equilibrium condition and invoking the law of mass action, we can rewrite Eq. (3.50) as

$$\frac{k_{f,r}}{k_{b,r}} = K_r^{\text{eq}} \quad (3.54)$$

Here K_r^{eq} is the equilibrium constant in the law of mass action applied to the reaction (3.47), namely

$$K_r^{\text{eq}} = \frac{\prod_{j=1}^{ns} \left(\frac{\rho_j^*}{M_j}\right)^{\nu'_{j,r}}}{\prod_{j=1}^{ns} \left(\frac{\rho_j^*}{M_j}\right)^{\nu_{j,r}}} \quad (3.55)$$

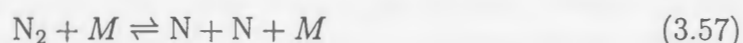
where the superscript * denotes the equilibrium state. Note that K_r^{eq} is a function of temperature only. With Eq. (3.54), the backward rate coefficient can be rewritten as

$$k_{b,r} = k_{f,r} / K_r^{\text{eq}} \quad (3.56)$$

3.5.3 Reaction model for nitrogen

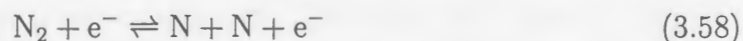
In nitrogen at sufficiently high temperature, the molecular species can dissociate through the collision between other heavy particles or free electrons. In turn, electrons are produced first by the associative ionization process and the ion so produced then transfers its charge to other neutral particles through the charge exchange reaction. When the resulting density of the electrons reaches a certain threshold value, the collision of electrons with neutral atoms begins to contribute significantly to the ion production. To describe these phenomena correctly, one must know the rate coefficients for the 5 types of reactions, total of 8 elemental reactions as [52]

- 1) Heavy particle impact dissociation/recombination:

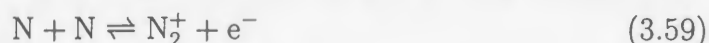


where M is an unspecified heavy particle, i.e. $M = \text{N}_2, \text{N}, \text{N}_2^+, \text{N}^+$.

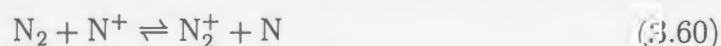
- 2) Electron impact dissociation/recombination:



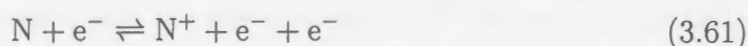
- 3) Associative ionization:



- 4) Charge exchange:



- 5) Electron impact ionization:



Since the 1950's, a great deal of experimental data associated with these reactions has been gathered in the field of hypersonic reentry problems and the rate coefficients have been determined subsequently. These coefficients so derived are, unfortunately,

reliable typically up to 15,000 K and hence we are obliged to extrapolate them at higher temperatures. Recently, in Refs. [34] and [54], Park determined the rate coefficients for the aforementioned reactions from analysis of an up-to-date experimental data base. His model reproduced the experimental data of the radiation behind a strong shock wave at least quantitatively for nitrogen [52], and appears to be quite reliable at higher temperatures.

According to this, the expression of forward/backward rate coefficients Eq. (3.53) are extended to more generalized form as

$$k_{f,r}(T_{f,r}) = C_r T_{f,r}^{s_r} \exp(-\theta_r/T_{f,r}) \quad (3.62)$$

$$k_{b,r}(T_{b,r}) = k_{f,r}(T_{b,r})/K_r^{\text{eq}}(T_{b,r}) \quad (3.63)$$

where $T_{f,r}$ and $T_{b,r}$ are the *effective temperature* for the reaction r . Both the forward and reverse rates of the reactions (3.58) and (3.61) are determined only by T_e , whereas those of reaction (3.60) are probably determined only by T . For reaction (3.59), the forward rate is determined by the T , whereas the reverse rate is determined by T_e . The values of the constants C_r , s_r , and θ_r are obtained from Ref. [54][†] and tabulated in Table 3.2 for each reaction with the effective temperature.

For the dissociation reaction (3.57), which is most important in terms of the energy involved, the reverse rate is dictated by T . But the expression for the forward rate coefficient is presently indeterminable because it is likely to be affected by both T and T_{vib} . It is well known that the dissociation rate of thermally nonequilibrium flows becomes substantially smaller than that under thermal equilibrium. This is because the dissociation occurs mostly from high vibrational levels close to the dissociation limits. Under the present assumption discussed in Section 2, there is no room to take into account these effect and hence we inevitably assume that this reaction is simply expressed by T .

The equilibrium constants K_r^{eq} are, as discussed previously, functions of temperature only and curve-fit formula of [53] are employed in the present computation as

$$\ln(K_r^{\text{eq}}) = A_{1,r}Z^5 + A_{2,r}Z^4 + A_{3,r}Z^3 + A_{4,r}Z^2 + A_{5,r}Z + A_{6,r} \quad (3.64)$$

where $Z = \ln(10^4/T)$. The coefficients $A_{1,r}, \dots, A_{6,r}$ are taken from [53] and tabulated in the appendix.

[†]It should be mentioned that there is a typographical error for the nitrogen ionization rates ($r = 8$ in Table 3.2) in the famous textbook of Park, Ref. [34]. If we use the tabulated value of [34] without modification, the reaction rate is underpredicted one order of magnitude [54]. Unfortunately, since this textbook is widely accepted without being recognized this fact, a number of previous computations employed his model must involve numerical error associated with this. Regarding arcjet computations, the computation of Ref. [26] used this wrong expression and thus must have underpredicted the electron production rate considerably.

Table 3.2: Properties of reaction model for nitrogen

r	Reactants		Products	C_r	s_r	θ_r	$T_{f,r}$	$T_{b,r}$
1	$N_2 + N_2$	$\rightleftharpoons$	$N + N + N_2$	7.0×10^{21}	-1.60	113,200	T	T
2	$N_2 + N$	$\rightleftharpoons$	$N + N + N$	3.0×10^{22}	-1.60	113,200	T	T
3	$N_2 + N_2^+$	$\rightleftharpoons$	$N + N + N_2^+$	7.0×10^{21}	-1.60	113,200	T	T
4	$N_2 + N^+$	$\rightleftharpoons$	$N + N + N^+$	3.0×10^{22}	-1.60	113,200	T	T
5	$N_2 + e^-$	$\rightleftharpoons$	$N + N + e^-$	1.2×10^{25}	-1.60	113,200	T_e	T_e
6	$N + N$	$\rightleftharpoons$	$N_2^+ + e^-$	4.4×10^7	1.50	67,500	T	T_e
7	$N_2 + N^+$	$\rightleftharpoons$	$N_2^+ + N$	1.0×10^{12}	0.50	12,200	T	T
8	$N + e^-$	$\rightleftharpoons$	$N^+ + e^- + e^-$	2.5×10^{34}	-3.82	168,600	T_e	T_e

3.6 Thermodynamic Relations

3.6.1 Thermodynamic properties

For a gas, if the partitioning of energy for all modes can be described by the Maxwell-Boltzmann distribution at each temperature, then the energy per unit mass of species s in the gas can be expressed as

$$e_s = \int_{T_{\text{ref}}}^T C_{v,s} dT + \Delta e_s^0 \quad (3.65)$$

where $C_{v,s}$ is the specific heat at constant volume for species s and Δe_s^0 is the energy of formation of species s at temperature T_{ref} . T_{ref} is a reference temperature and taken to absolute zero in the present study. Similarly, the enthalpy per unit mass of species s is expressed as

$$h_s = \int_{T_{\text{ref}}}^T C_{p,s} dT + \Delta h_s^0 \quad (3.66)$$

where $C_{p,s} = C_{v,s} + R_s$ is the specific heat at constant pressure and Δh_s^0 is the enthalpy of formation of species s at temperature T_{ref} , which becomes $\Delta h_s^0 = \Delta e_s^0$ here.

Although tabulated values and polynomial curve fits for $C_{p,s}$ and h_s are readily available (e.g. [51]), we explicitly express them in terms of each energy mode. This is required in order to take into account the effect of thermal nonequilibrium and high temperature effects such as the vibrational excitation.

For diatomic species, each energy mode of species s can be expressed as follows

$$e_s = e_{tr,s} + e_{rot,s} + e_{vib,s} + \Delta h_s^0 \quad (3.67)$$

$$h_s = e_s + R_s T \quad (3.68)$$

$$e_{tr,s} = \frac{3}{2} R_s T \quad (3.69)$$

$$e_{rot,s} = R_s T \quad (3.70)$$

$$e_{vib,s} = \frac{R_s \Theta_{vib,s}}{\exp(\Theta_{vib,s}/T_{vib}) - 1} \quad (3.71)$$

So that the specific heats for each energy mode of species s become

$$C_{v,s} = C_{v,tr,s} + C_{v,rot,s} + C_{v,vib,s} \quad (3.72)$$

$$C_{p,s} = C_{v,s} + R_s \quad (3.73)$$

$$C_{v,tr,s} = \frac{\partial e_{tr,s}}{\partial T} = \frac{3}{2} R_s \quad (3.74)$$

$$C_{v,rot,s} = \frac{\partial e_{rot,s}}{\partial T} = R_s \quad (3.75)$$

$$C_{v,vib,s} = \frac{\partial e_{vib,s}}{\partial T_{vib}} = R_s \left[\frac{(\Theta_{vib,s}/2T_{vib})}{\sinh(\Theta_{vib,s}/2T_{vib})} \right]^2 \quad (3.76)$$

Similarly for atomic species,

$$e_s = e_{tr,s} = \frac{3}{2} R_s T + \Delta h_s^0 \quad (3.77)$$

$$h_s = e_s + R_s T = \frac{5}{2} R_s T + \Delta h_s^0 \quad (3.78)$$

$$C_{v,s} = C_{v,tr,s} = \frac{3}{2} R_s \quad (3.79)$$

$$C_{p,s} = C_{v,s} + R_s = \frac{5}{2} R_s \quad (3.80)$$

For electron,

$$e_e = e_{tr,e} = \frac{3}{2} R_e T_e \quad (3.81)$$

$$h_e = e_e + R_e T_e = \frac{5}{2} R_e T_e \quad (3.82)$$

$$C_{v,e} = C_{v,tr,e} = \frac{3}{2} R_e \quad (3.83)$$

$$C_{p,e} = C_{v,e} + R_e = \frac{5}{2} R_e \quad (3.84)$$

Values for Δh_s^0 , M_s , and other physical constants for the 5 species considered herein are presented in Table 3.3.

Table 3.3: Species data

Species	M_s , kg/mole	$\Theta_{\text{vib},s}$, K	Δh_s^0 , J/kg	$E_{D,s}$, J/kg	$E_{I,s}$, J/kg
N ₂	28×10^{-3}	3,353	0	3.365×10^7	—
N	14×10^{-3}	—	3.364×10^7	—	1.002×10^8
N ₂ ⁺	28×10^{-3}	3,129	5.372×10^7	—	—
N ⁺	14×10^{-3}	—	1.339×10^8	—	—
e ⁻	5.486×10^{-7}	—	0	—	—

3.6.2 Equation of state

For a gas under the assumption of thermochemical nonequilibrium, the partial pressure of species s is defined by

$$p_s = \rho_s R_s T \quad (3.85)$$

where s represents a species of heavy particle. Similarly for free electron,

$$p_e = \rho_e R_e T_e \quad (3.86)$$

Therefore the total static pressure p is derived from the application of Dalton's law of partial pressure as

$$p = \sum_s p_s = \sum_{s \neq e} \rho_s R_s T + \rho_e R_e T_e = \rho \hat{R} T + p_e \quad (3.87)$$

where the gas constant of gas mixture except for the electron energy mode $\hat{R}$ is defined by

$$\hat{R} = \sum_{s \neq e} \frac{\rho_s}{\rho} R_s \quad (3.88)$$

Here we consider the specific heat of species s except for the contribution of vibrational/electron energy mode as

$$C'_{v,s} = C_{v,\text{tr},s} + C_{v,\text{rot},s} \quad (3.89)$$

$$C'_{p,s} = C_{p,\text{tr},s} + C_{p,\text{rot},s} \quad (3.90)$$

It should be noted that $C'_{v,s}$ and $C'_{p,s}$ are related with R_s as $C'_{p,s} - C'_{v,s} = R_s$. Similar to $\hat{R}$, the specific heat of mixture gas are defined by

$$\hat{C}'_v = \sum_{s \neq e} \frac{\rho_s}{\rho} C'_{v,s} \quad (3.91)$$

$$\hat{C}'_p = \sum_{s \neq e} \frac{\rho_s}{\rho} C'_{p,s} \quad (3.92)$$

Hence we obtain $\widehat{C}'_p - \widehat{C}'_v = \widehat{R}$. Further defining the ratio of specific heat of mixture by $\widehat{\gamma} = \widehat{C}'_p / \widehat{C}'_v$, we have

$$p = (\widehat{\gamma} - 1)\rho\widehat{C}'_v T + p_e \quad (3.93)$$

On the other hand, the total energy of the gas flow per unit volume E is a summation of the internal energy and the kinetic energy of the flow, so that

$$\begin{aligned} E &= \sum_s \rho_s e_s + \frac{1}{2} \rho q^2 \\ &= \rho\widehat{C}'_v T + \sum_{s=M} \rho_s e_{\text{vib},s} + \rho_e e_e + \sum_s \rho_s \Delta h_s^0 + \frac{1}{2} \rho q^2 \end{aligned} \quad (3.94)$$

where $q^2 = u_j u_j$. Combining Eq. (3.94) with Eq. (3.93), we obtain

$$p = (\widehat{\gamma} - 1) \left[E - E_{\text{vib}} - E_e - \sum_s \rho_s \Delta h_s^0 - \frac{1}{2} \rho q^2 \right] + p_e \quad (3.95)$$

where $E_{\text{vib}} = \sum \rho_s e_{\text{vib},s}$ and $E_e = \rho_e e_e$. Conversely, E can be expressed for p as

$$E = \frac{p - p_e}{\widehat{\gamma} - 1} + E_{\text{vib}} + E_e + \sum_s \rho_s \Delta h_s^0 + \frac{1}{2} \rho q^2 \quad (3.96)$$

These relations are used in demand.

3.7 Transport Properties

3.7.1 Chapman-Enskog procedure

As stated in Chapter 2, Sec. 3, the basic mechanism of the transport phenomena is dominated by the random motion of the particles, so that they must be treated from the microscopic point of view. Necessarily, we need to describe the phenomena starting from the Boltzmann equation

$$\frac{\partial(nf)}{\partial t} + c \frac{\partial(nf)}{\partial x} = n^2 \iint [f(c')f(\xi') - f(c)f(\xi)] g \sigma d\Omega d\xi \quad (3.97)$$

and solve it independently from the flow field equation itself. This is, of course, practically impossible and an approximate method that enables us to evaluate the phenomena using only macroscopic properties is required. This can be realized by assuming that all the transport phenomena arise by slight deviation from the equilibrium velocity distribution. In this case, the velocity distribution function f may be expressed in the form of the power series as

$$f = f_0(1 + \Phi_1 + \Phi_2 + \cdots) \quad (3.98)$$

where f_0 is an equilibrium function known as the Maxwell distribution, and Φ_i is the perturbation term assumed small. Analytical solutions of the Boltzmann equation with taking only the first perturbation term (i.e. for $f = f_0(1 + \Phi_1)$) were found independently by Chapman and by Enskog, and commonly referred to as *the first Chapman-Enskog approximation*. Their methods differed widely but gave identical results (In Ref. [55], we can find an interesting historical summary of the development of the theory).

The Chapman-Enskog method is characterized by extreme mathematical complexity and then only an outline of the procedure is described below. Substituting Eq. (3.98) into Eq. (3.97) and keeping the perturbation terms up to first-order, the nonlinear Boltzmann equation can be transformed to a linearized equation for Φ_1 . To solve this equation, it is *assumed* that the perturbation is proportional to the various gradients of composition, pressure, temperature, etc. with the coefficients of proportionality (i.e. transport coefficients) being unknown functions of molecular velocities. Then we need to find these functions, each one of which satisfies a linear integrodifferential equation obtained from the linearized Boltzmann equation. To do this, the functions are expanded as power series in the component of the molecular velocities by using Sonine polynomials. When these expansions are substituted back into the integral expressions for the transport coefficients, it turns out that each transport coefficient is exactly equal to just one of the expansion coefficients. The detail of the procedure can be found in [55] and [56].

When the Chapman-Enskog theory is applied to a mixture of monoatomic gases, we obtain the expression of the viscous stress τ^{ij} , heat flux q^j , and diffusion velocity V_s^j for species s as

$$\tau^{ij} = \mu \left(\frac{\partial u_0^i}{\partial x^j} + \frac{\partial u_0^j}{\partial x^i} \right) - \frac{2}{3} \mu \frac{\partial u_0^l}{\partial x^l} \delta_{ij} \quad (3.99)$$

$$q^j = -\lambda \frac{\partial T}{\partial x^j} + \frac{5}{2} kT \sum_s n_s V_s^j - nkT \sum_s \frac{D_s^T}{\rho_s} d_s^j \quad (3.100)$$

$$V_s^j = \frac{n^2}{n_s \rho} \sum_r m_r D_{sr} d_r^j - \frac{D_s^T}{\rho} \frac{\partial \ln T}{\partial x^j} \quad (3.101)$$

where

$$d_s^j \equiv \frac{\partial}{\partial x^j} \left(\frac{n_s}{n} \right) + \left(\frac{n_s}{n} - \frac{\rho_s}{\rho} \right) \frac{\partial \ln p}{\partial x^j} - \frac{\rho_s}{p} \left(F_s^j - \sum_r \frac{\rho_r}{\rho} F_r^j \right) \quad (3.102)$$

D_{sr} and D_s^T are referred to as the *multicomponent diffusion coefficients* and *multicomponent thermal diffusion coefficients*, respectively. The expression of the viscous stress and the heat flux are identical to Eqs. (3.16) and Eqs. (3.19) respectively, except for inclusion of the third term in the right-hand side of Eq. (3.100), representing the thermal diffusion. The expression of d_s^j is discussed in the subsequent

subsection. It can now be verified that the substitution of these relationship into the Maxwell's transport equations gives rise to the familiar Navier-Stokes equations [39], indicating that the flow field equations can be derived from the rigorous kinetic theory as well.

It should be mentioned that the form of the phenomenological transport equations, (i.e. Eq. (2.15) to (2.17) in Chapter 2, Sec. 3) does not follow automatically from a mathematical solution of the Boltzmann equation. In our derivations, we take for granted that the phenomenological equations are correct, and seeks "normal" solutions of the Boltzmann equations that lead to these equations, ignoring the many other possible types of solutions. The solutions are, in other words, forced into the desired form [57].

The Chapman-Enskog procedure is also available for obtaining the transport properties of a gas mixture from the molecular constituent species. In this case, for example, formulas for both the viscosity μ and translational component of thermal conductivity λ_{tr} of a gas mixture are of the general form

$$\mu^{(1)} \text{ or } \lambda_{tr}^{(1)} = - \left| \begin{array}{cccc} A_{11} & \cdots & A_{1\nu} & X_1 \\ \vdots & & \vdots & \vdots \\ A_{\nu 1} & \cdots & A_{\nu\nu} & X_\nu \\ X_1 & \cdots & X_\nu & 0 \end{array} \right| / |A_{ij}| \quad (3.103)$$

where X_i is the mole fraction of the i th species, $\nu = ns$ is the total number of species present in the mixture, and the matrix elements A_{ij} are different for viscosity and thermal conductivity. Other transport properties including diffusion coefficient and electrical conductivity can be derived in the similar fashion. Although these rigorous equations describe the transport properties of gas mixtures very well, the expressions are cumbersome and practical calculation is extremely expensive. To alleviate this, various approximate formulas that replace Eq. (3.103) have been proposed. Among them, if the approximations of Ref. [58] to [60] are employed, relatively simple formula that reproduce the results of Eq. (3.103) to within a fraction of a few percent in most cases can be obtained [61]. These approximations are further extended for thermal nonequilibrium cases in Ref. [49], [62], and [53] and employed in the present study.

3.7.2 Expression of transport coefficients

By following Ref. [53], the viscosity, thermal conductivity, and the binary diffusion coefficient for gas mixture in thermal nonequilibrium can be described as follows.

Mixture viscosity:

$$\mu = \sum_{i \neq e^-} \left[\frac{m_i X_i}{\sum_{j \neq e^-} X_j \Delta_{i,j}^{(2)}(T) + X_e \Delta_{i,e}^{(2)}(T_e)} \right] + \frac{m_e X_e}{\sum_j X_j \Delta_{e,j}^{(2)}(T_e)} \quad (3.104)$$

Thermal conductivity:

Translational component of thermal conductivity in a mixture except for electrons:

$$\lambda_{tr} = \frac{15}{4} k \sum_{i \neq e} \left[\frac{X_i}{\sum_{j \neq e} \alpha_{ij} X_j \Delta_{i,j}^{(2)}(T) + 3.54 X_e \Delta_{i,e}^{(2)}(T_e)} \right] \quad (3.105)$$

Rotational component of thermal conductivity in a mixture:

$$\lambda_{rot} = k \sum_{i=M} \left[\frac{X_i}{\sum_{j \neq e} X_j \Delta_{i,j}^{(1)}(T) + X_e \Delta_{i,e}^{(1)}(T_e)} \right] \quad (3.106)$$

Vibrational component of thermal conductivity in a mixture:

$$\lambda_{vib} = k \sum_{i=M} \left[\frac{\left(\frac{C_{vib i}}{R_i} \right) X_i}{\sum_{j \neq e} X_j \Delta_{i,j}^{(1)}(T) + X_e \Delta_{i,e}^{(1)}(T_e)} \right] \quad (3.107)$$

Thermal conductivity of electrons:

$$\lambda_e = \frac{15}{4} k \frac{X_e}{\sum_{j \neq e} 1.45 X_j \Delta_{e,j}^{(2)}(T_e) + X_e \Delta_{e,e}^{(2)}(T_e)} \quad (3.108)$$

Electrical conductivity:

$$\sigma = \frac{e^2}{k T_e} \frac{X_e}{\sum_{j \neq e} X_j \Delta_{e,j}^{(1)}(T_e)} \quad (3.109)$$

Binary diffusion coefficient: * †

$$\mathcal{D}_{ij} = \frac{kT}{p\Delta_{i,j}^{(1)}(T)}, \quad \text{for } i \neq e \text{ and } j \neq e \quad (3.110)$$

$$\mathcal{D}_{ij} = \frac{kT_e}{p\Delta_{i,j}^{(1)}(T_e)}, \quad \text{for } i = e \text{ or } j = e \quad (3.111)$$

where

$$X_i = \frac{\rho_i}{M_i} \quad (3.112)$$

$$\Delta_{i,j}^{(1)}(T) = \frac{8}{3} \left[\frac{2m_i m_j}{\pi kT(m_i + m_j)} \right]^{1/2} \pi \bar{\Omega}_{i,j}^{(1,1)} \quad (3.113)$$

$$\Delta_{i,j}^{(2)}(T) = \frac{16}{5} \left[\frac{2m_i m_j}{\pi kT(m_i + m_j)} \right]^{1/2} \pi \bar{\Omega}_{i,j}^{(2,2)} \quad (3.114)$$

$$\alpha_{ij} = 1 + \frac{[1 - (m_i/m_j)][0.45 - 2.54(m_i/m_j)]}{[1 + (m_i/m_j)]^2} \quad (3.115)$$

Collision cross section:

The collision cross sections $\pi \bar{\Omega}_{i,j}^{(1,1)}$ and $\pi \bar{\Omega}_{i,j}^{(2,2)}$ are the weighted averages of the cross sections for collisions between species i and j , which are defined as

$$\pi \bar{\Omega}_{i,j}^{(l,s)} = \frac{\int_0^\infty \int_0^\pi \exp(-\gamma^2) \gamma^{2s+3} (1 - \cos^l \chi) 4\pi \sigma_{i,j} \sin \chi d\chi d\gamma}{\int_0^\infty \int_0^\pi \exp(-\gamma^2) \gamma^{2s+3} (1 - \cos^l \chi) \sin \chi d\chi d\gamma} \quad (3.116)$$

where $\sigma_{i,j} = \sigma_{i,j}(\chi, \gamma)$ is the differential scattering cross section for the collision pair i - j , χ the scattering angle in the center-of-mass system, $\gamma = [m_i m_j / (2(m_i + m_j)kT)]^{1/2} g$ the reduced velocity, g the relative velocity of the colliding particles.

If the symmetrical equality is postulated, there are 15 possible binary interactions for nitrogen with 5 species, and corresponding cross section data are required. These values have been curve-fit in Ref. [53] using the following relations

$$\pi \bar{\Omega}_{i,j}^{(1,1)} = \left[\exp \left(D_{\pi \bar{\Omega}_{i,j}^{(1,1)}} \right) \right] T^{[A_{\pi \bar{\Omega}_{i,j}^{(1,1)}} (\ln T)^2 + B_{\pi \bar{\Omega}_{i,j}^{(1,1)}} \ln T + C_{\pi \bar{\Omega}_{i,j}^{(1,1)}}]} \quad (3.117)$$

$$\pi \bar{\Omega}_{i,j}^{(2,2)} = \left[\exp \left(D_{\pi \bar{\Omega}_{i,j}^{(2,2)}} \right) \right] T^{[A_{\pi \bar{\Omega}_{i,j}^{(2,2)}} (\ln T)^2 + B_{\pi \bar{\Omega}_{i,j}^{(2,2)}} \ln T + C_{\pi \bar{\Omega}_{i,j}^{(2,2)}}]} \quad (3.118)$$

They are given by the following function of temperatures in the unit of Å². The coefficients $A_{\pi \bar{\Omega}_{i,j}^{(l,s)}}$, $B_{\pi \bar{\Omega}_{i,j}^{(l,s)}}$, $C_{\pi \bar{\Omega}_{i,j}^{(l,s)}}$, and $D_{\pi \bar{\Omega}_{i,j}^{(l,s)}}$ are tabulated in the appendix.

*Note that the binary diffusion coefficient is obtained from the *complete* first Chapman-Enskog approximation [56].

†There is a mismatch for the evaluation of $\mathcal{D}_{ij}$ in Ref. [53]. The unit of the pressure p must be in [dyn/cm²] rather than atmospheres.

For the pair of species for which both are ions, the above collision cross sections must be corrected for the given electron pressure p_e by multiplying the following factor:

$$\ln \Lambda(p_e) = \frac{1}{2} \ln \left[2.09 \times 10^{-2} \left(\frac{T}{1000 p_e^{1/4}} \right)^4 + 1.52 \left(\frac{T}{1000 p_e^{1/4}} \right)^{8/3} \right] \quad (3.119)$$

where p_e is the electron pressure in atmospheres. Similarly, for the pair of species for which both are electrons or a combination of electron and ion, the above collision cross sections must be corrected by multiplying the following factor:

$$\ln \Lambda(p_e) = \frac{1}{2} \ln \left[2.09 \times 10^{-2} \left(\frac{T_e}{1000 p_e^{1/4}} \right)^4 + 1.52 \left(\frac{T_e}{1000 p_e^{1/4}} \right)^{8/3} \right] \quad (3.120)$$

3.7.3 Diffusion velocity

Effective diffusion coefficient:

The evaluation of diffusion velocity for a multi-component gas mixture involves a peculiar operation compared to that of other transport properties. For arguments, Eqs. (3.101) and (3.102) are written again here.

$$V_s^j = \frac{n^2}{n_s \rho} \sum_r m_r D_{sr} d_r^j - \frac{D_s^T}{\rho} \frac{\partial \ln T}{\partial x^j} \quad (3.121)$$

$$d_s^j \equiv \frac{\partial}{\partial x^j} \left(\frac{n_s}{n} \right) + \left(\frac{n_s}{n} - \frac{\rho_s}{\rho} \right) \frac{\partial \ln p}{\partial x^j} - \frac{\rho_s}{p} \left(F_s^j - \sum_r \frac{\rho_r}{\rho} F_r^j \right) \quad (3.122)$$

Equation (3.121) indicates that there are four driving factors that induce the microscopic transport of mass: (i) the gradient in concentration (referred to as *ordinary diffusion*), (ii) the gradient in temperature (*thermal diffusion*), (iii) the gradient in pressure (*pressure diffusion*), and (iv) the gradient in external forces F_s^j (*forced diffusion*). Of the four, thermal and pressure diffusion are second-order effects that are only important when there are large differences between the atomic masses of the constituent species (also note that these effects are proportional to the gradient in the logarithm of p and T rather than the gradient of themselves). Hence we can neglect these effects for the condition of interest and accordingly the third term of Eq. (3.100) vanishes. Furthermore, the effect of external forces such as those due to existence of the electric field are neglected for the time being. In this case, Eqs. (3.121) and (3.122) can be rewritten as

$$V_s^j = \frac{n^2}{n_s \rho} \sum_r m_r D_{sr} d_r^j \quad (3.123)$$

$$d_s^j = \frac{\partial}{\partial x^j} \left(\frac{n_s}{n} \right) \quad (3.124)$$

For certain hydrodynamics applications it is sometimes convenient to replace the relations given in Eqs. (3.123) and (3.124) by [56]

$$\sum_{k=1}^{ns} \frac{n_s n_k}{n^2 \mathcal{D}_{sk}} (V_k^j - V_s^j) = \frac{\partial}{\partial x^j} \left(\frac{n_s}{n} \right) \quad (3.125)$$

Hence the multicomponent diffusion coefficients D_{sk} are related to the binary diffusion coefficients $\mathcal{D}_{sk}$. Also it must be noted that there is a relation for each species diffusion velocities as

$$\sum_{s=1}^{ns} \rho_s V_s^j = 0 \quad (3.126)$$

Since the diffusion velocities are defined relative to the net momentum of the mixture, they are constrained to carry no momentum. Calculating V_s^j requires solving Eq. (3.125) subject to the constraint in Eq. (3.126). This requires the inversion of $(ns \times ns)$ matrix, so that the operation count scales as $(ns)^3$, facing with the problem of the high computational cost.

To alleviate this, in Ref. [63], Jones and Boris proposed an efficient algorithm which requires no matrix inversion to solve Eq. (3.125). The idea is that we rewrite the diffusion velocity in a perturbation expansion form as [†]

$$V_s^j = -\frac{\rho - \rho_s}{\rho} \frac{n^2 \bar{D}_s}{(n - n_s)n_s} [\delta_{sk} + A_{sk} + A_{sl}A_{lk} + \dots] d_k^j \quad (3.127)$$

where

$$\bar{D}_s \equiv \frac{n - n_s}{\sum_{k=1}^{ns} (n_k / \mathcal{D}_{sk})} \quad (3.128)$$

$$A_{sk} \equiv \frac{\rho_s}{\rho} \delta_{sk} + \frac{n_s}{\mathcal{D}_{sk}} \frac{\rho - \rho_s}{\rho} \frac{\bar{D}_s}{n - n_k} (1 - \delta_{sk}) \quad (3.129)$$

Hence rewriting Eq. (3.127) as

$$V_s^j = V_{s0}^j + \delta V_s^j + \delta^2 V_s^j + \dots \quad (3.130)$$

we obtain the zeroth order velocity

$$V_{s0}^j = -\frac{\rho - \rho_s}{\rho} \frac{n^2 \bar{D}_s}{(n - n_s)n_s} d_s^j \quad (3.131)$$

[†]The convergence of this expansion is verified in [63].

subsequently for the first and second order

$$\delta V_s^j = \left(\sum_{k=1}^{ns} A_{sk} d_k^j \right) V_{s0}^j \quad (3.132)$$

$$\delta^2 V_s^j = \left(\sum_k^{ns} \sum_l^{ns} A_{sk} A_{kl} d_l^j \right) V_{s0}^j \quad (3.133)$$

etc. In the numerical evaluation of Eq. (3.127), none of the indicated multiplication has to be performed and the computational cost reduces to order of $(ns)^2$. Obviously the accuracy of the algorithm depends on how to truncate the expansion term. In the present study, only the zeroth order expression is employed and other higher-order terms are discarded. Although it is argued in [65] that Eq. (3.127) may not even give correct sign for the diffusive flux unless the terms are kept up to at least first order (i.e. remain the A_{sk} term), the truth is still doubtful and no example is reported in [65]. Above all, it should be noted that the zeroth order expression Eq. (3.131) is totally identical to the famous formula of Curtiss and Hirschfelder [64], that is,

$$V_s^j = - \frac{1 - C_s}{\sum_{k \neq s} X_k / \mathcal{D}_{sk}} \frac{1}{X_s} \frac{\partial X_s}{\partial x^j} \quad (3.134)$$

Since it has been confirmed that the formula of Curtiss and Hirschfelder can explain the diffusive phenomena quite well, we employ this without any modification and examination of the higher-order correction should be addressed in the future. Hence if one defines the effective diffusion coefficient D_s as

$$D_s \equiv \frac{1 - C_s}{\sum_{k \neq s} X_k / \mathcal{D}_{sk}} \frac{C_s}{X_s} \quad (3.135)$$

finally the diffusion velocity of species s is given by

$$\rho_s V_s^j = -\rho D_s \frac{\partial X_s}{\partial x^j} \quad (3.136)$$

Diffusion coefficient of ion:

Electrons have higher thermal velocities and tend to diffuse faster than ions. A positive charge is then left behind, and an electric field is set up as to decelerate electrons and to accelerate ions. Thus, the diffusions of ions and electrons are linked by the electric field. In the present work, this effect is approximately considered by assuming *ambipolar diffusion*. In this case, the diffusion coefficients for ions can be

approximated by

$$D_s^a = \left(1 + \frac{T_e}{T}\right) D_s \quad (3.137)$$

where D_s is the effective diffusion coefficient of ionic species in the absence of electric field.

Diffusion coefficient of electron:

The effective diffusion coefficient of electron can be obtained by equating the mass averaged diffusion velocity of ions and that of electron as follows:

$$D_e = \frac{m_e \sum_{s=1} D_s^a X_s}{\sum_{s=1} m_s X_s} \quad (3.138)$$

3.8 Elastic/Inelastic Losses

The effect of the energy loss due to elastic and inelastic collisions appears in the electron energy conservation equation Eq. (3.27) as $S_{\text{int},e}$ and must be modeled. As is the case for the evaluation of the transport properties, rigorous treatment of these effects is extremely complex, sometimes we may be obliged to start from the quantum mechanical approaches and naturally both theoretical and computational tasks become tedious. As long as we formulate $S_{\text{int},e}$ in conjunction with the flow field equations, a simple model that describes the phenomenon from the macroscopic viewpoint is necessary.

In Ref. [66], Appleton and Bray constructed an electron energy equation that includes elastic/inelastic interaction terms by assuming Maxwellian velocity distribution for the electron energy mode. In the present model, we extend their formulation to include some relevant mechanisms that are important for diatomic species such as nitrogen.

Aside from the elastic collisions between electron and heavy particles, the electron loses its energy by the electron-impact dissociation/ionization reactions. This is a main inelastic loss mechanism for atomic gases, but additional effects must be taken into account for a plasma composed of molecular species. It is well known that molecular gases, particularly N_2 , can readily absorb collisional energy from the free electrons into their vibrational modes, so that the energy source term representing this effect must be modeled. The energy exchange rate between the electron and the rotational modes may become important in some occasions as well. In turn, a series of radiative effects can be neglected for arcjet computations as discussed in Section 2.

Consistently incorporating these mechanisms, now we can show the explicit expression of $S_{\text{int},e}$ as

$$S_{\text{int},e} = Q_{\text{T-e}} + Q_{\text{R-e}} - Q_{\text{e-v}} + Q_{\text{D}}^e + Q_{\text{I}}^e \quad (3.139)$$

where Q is the electron energy transfer rate per unit volume due to:

$$\begin{aligned} Q_{\text{T-e}} &= \text{elastic collisions with heavy particles} \\ Q_{\text{R-e}} &= \text{collisions with diatomic species} \\ Q_{\text{e-v}} &= \text{vibrational excitations by the electron impact} \\ Q_{\text{D}}^e &= \text{electron-impact dissociation/recombination} \\ Q_{\text{I}}^e &= \text{electron-impact ionization/recombination} \end{aligned}$$

These terms are modeled independently and described below.

3.8.1 Translation-electron energy exchange

The rate of the translational energy transfer between heavy particles and electrons $Q_{\text{T-e}}$ is given by

$$Q_{\text{T-e}} = \sum_{s \neq e} n_e \frac{2m_e}{m_s} \nu_{e,s} \frac{3}{2} k (T - T_e) \quad (3.140)$$

where $\nu_{e,s}$ the collision frequency between electrons and other particles [66]. For an ionic particle s , the interaction is described by the well-known Coulomb potential, and then the effective collision frequency is expressed in SI units as

$$\nu_{e,s} = 3.64 \times 10^{-6} n_s \ln(\Lambda/T_e^{3/2}) \quad (3.141)$$

$$\Lambda = 1.24 \times 10^7 (T_e/n_e)^{1/2} \quad (3.142)$$

For neutral species, the following expression is used.

$$\nu_{e,s} = n_s \sigma_{e,s} \left(\frac{8kT_e}{\pi m_e} \right)^{1/2} \quad (3.143)$$

where the effective electron-neutral energy exchange cross section is defined by a curve fit of the form [52]

$$\sigma_{e,s} = \tilde{a}_s + \tilde{b}_s T_e + \tilde{c}_s T_e^2 \quad (3.144)$$

and the constants $\tilde{a}_s$, $\tilde{b}_s$, and $\tilde{c}_s$ are presented in Table 3.4.

Table 3.4: Constants for curve fits of $\sigma_{e,s}$

s	$\tilde{a}_s$	$\tilde{b}_s$	$\tilde{c}_s$
N ₂	7.5×10^{-20}	5.5×10^{-24}	-1.0×10^{-28}
N	5.0×10^{-20}	0	0

3.8.2 Rotation-electron energy exchange

The energy transfer between the rotational energy mode and electron energy mode should be also considered. This is because electrons interact with the molecular multipoles produced by deformation of electron cloud in the formation of molecular bonds [67]. Using an energy loss factor, $g_{\text{rot},s}$, the energy transfer rate is written as

$$Q_{\text{R-e}} = \sum_{s=\text{M}} n_e \frac{2m_e}{m_i} g_{\text{rot},s} \nu_{e,s} \frac{3}{2} k(T - T_e) \quad (3.145)$$

The factor $g_{\text{rot},s}$ is the ratio of $Q_{\text{R-e}}$ to $Q_{\text{T-e}}$ for molecular species s . In the present work, we assume $g_{\text{rot},\text{N}_2} = 10$ [68]. The rotational excitation for molecular positive ions is governed by the long-range Coulomb interaction, so that the large excitation cross section is expected. Two theoretical results are cited in Ref. [69], but it is uncertain whether the calculated values are quantitatively valid in the present conditions. In this analysis, it is assumed that $g_{\text{rot},\text{N}_2^+}$ is equal to those for the corresponding neutral molecules.

3.8.3 Electron-vibration energy exchange

It is well known that the nitrogen-electron coupling is much stronger than the coupling between the electron and other molecules [70] and thus should be taken into account. In Refs [71] and [72], Lee calculated the cross section and relaxation time for the vibrational excitation of the nitrogen molecules by electron-impact applying a quantum mechanical treatment, which is based on the concept that the vibrational excitation occurs through the formation of an intermediate negative ion state (compound resonant state). The calculated cross sections are in very good agreement with the experimental data, hence the relaxation time is fairly reliable. Using the relaxation time $\tau_{\text{N}_2-\text{e}}$, the e-V energy transfer rate is given by the following conventional form:

$$Q_{\text{e-V}} = \rho_{\text{N}_2} \frac{e_{\text{vib},\text{N}_2}^{\text{eq}}(T_e) - e_{\text{vib},\text{N}_2}(T_{\text{vib}})}{\tau_{\text{N}_2-\text{e}}} \quad (3.146)$$

The relaxation time is evaluated using the following curve fit equation:[§]

$$\log_{10}(p_e \tau_e) = \begin{cases} 3.91Z^2 - 30.36Z + 48.90, & 1,000 \leq T_e \leq 7,000\text{K} \\ 1.30Z^2 - 9.09Z + 5.70, & 7,000 \leq T_e \leq 50,000\text{K} \end{cases} \quad (3.147)$$

where

$$Z = \log_{10}(T_e) \quad (3.148)$$

and p_e is the electron pressure in atmospheres.

3.8.4 Electron energy loss due to chemical reactions

In both electron-impact dissociation and ionization, dissociation/ionization energy is mainly extracted from the electron energy [34], so that the loss of the electron energy due to these reactions may be written as

$$Q_D^e = E_{D,N_2} \dot{w}_{N_2}^e \quad (3.149)$$

$$Q_I^e = E_{I,N} \dot{w}_N^e \quad (3.150)$$

where $w_{N_2}^e$ and w_N^e are mass production rate of N_2 and N due to electron impact dissociation and ionization, respectively.

3.9 Summary of Governing Equations

Finally, the basic governing equations for both the flow field and the electric field are summarized in conjunction with the expressions of transport phenomena and elastic/inelastic source terms developed so far as follows.

Total mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (3.151)$$

Momentum conservation equation:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j + \delta_{ij} p)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] \quad (3.152)$$

[§]There is a deficiency in the original expression of Eq. (3.143): if the coefficients in [72] are used without modification, a discontinuity arises at $T_e = 7,000$ K. To prevent this, we shifted the original value of 5.58 to 5.70 in Eq. (3.147).

Total energy conservation equation:

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} [(E + p)u_j] &= \frac{\partial}{\partial x_j} \left[(\lambda + \lambda_{\text{vib}}) \frac{\partial T}{\partial x_j} + \lambda_e \frac{\partial T_e}{\partial x_j} \right] \\ &+ \frac{\partial}{\partial x_j} \left(\rho \sum_{s=1}^{ns} h_s D_s \frac{\partial X_s}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left[u_i \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} u_i \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] + j_j E_j \end{aligned} \quad (3.153)$$

Species mass conservation equation:

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial (\rho_s u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_s \frac{\partial X_s}{\partial x_j} \right) + \dot{w}_s \quad (3.154)$$

Electron energy conservation equation:

$$\begin{aligned} \frac{\partial E_e}{\partial t} + \frac{\partial (E_e u_j)}{\partial x_j} &= \frac{\partial}{\partial x_j} \left(\lambda_e \frac{\partial T_e}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho h_e D_e \frac{\partial X_e}{\partial x_j} \right) \\ &- p_e \frac{\partial u_j}{\partial x_j} + Q_{T-e} + Q_{R-e} - Q_{e-v} + Q_D^e + Q_I^e + j_j E_j \end{aligned} \quad (3.155)$$

Equation of state:

$$p = \sum_{s \neq e} \rho_s R_s T + \rho_e R_e T_e \quad (3.156)$$

Electric field equation:

$$\nabla \cdot (\sigma \nabla \phi) = \nabla \cdot \left(\frac{\sigma}{en_e} \nabla p_e \right) \quad (3.157)$$

where

$$E = E_{\text{tr}} + E_{\text{rot}} + E_{\text{vib}} + E_e + \sum_{s=1}^{ns} \rho_s \Delta h_s^0 + \frac{1}{2} \rho u_j u_j \quad (3.158)$$

$$E_{\text{tr}} = \sum_{s \neq e} \frac{3}{2} \rho_s R_s T \quad (3.159)$$

$$E_{\text{rot}} = \sum_{s=M} \rho_s R_s T \quad (3.160)$$

$$E_{\text{vib}} = \sum_{s=M} \frac{\rho_s R_s \Theta_{\text{vib},s}}{\exp(\Theta_{\text{vib},s}/T) - 1} \quad (3.161)$$

$$E_e = \frac{3}{2} \rho_e R_e T_e \quad (3.162)$$

Here we make a comment on the above equations. Since $\sum_{s=1}^{ns} \rho_s = \rho$ holds, we can consider two approaches regarding the construction of the equation system. One is to solve the total mass conservation equation and omit the one of ns species mass conservation equations. In this case, if the n th species equation is excluded, the species density ρ_n can be computed as $\rho_n = \rho - \sum_{s \neq n} \rho_s$. Assuming charge neutral, we can further omit one additional equation for ionized species or electron conservation. Another is to omit the total mass conservation equation and evaluate the global density as $\rho = \sum_{s=1}^{ns} \rho_s$. These approaches reduce the number of the governing equation and thus seems to be computationally efficient.

However, in the present study, *all* species mass conservation equations are simultaneously solved as well as the total mass conservation equation. This formulation makes the equation system redundant and also makes the Jacobian matrix indeterminate. In spite of them, this approach is employed because of the following:

1. If one of the species variables is expressed as a combination of others, the numerical errors acquired in each computing step, is accumulated in that species, and
2. Conservation of the total mass is of particularly importance for internal flow computations: if the global density is calculated as the sum of all the species, we may be suffered from numerical errors associated with the treatment of the source terms or diffusive terms in the species mass conservation equations [73].

In addition, although the redundancy may result in a discrepancy in which the sum of all species concentrations does not satisfy the overall mass conservation due to numerical errors, this was remedied by multiplying each species concentration values by the same factor, that is,

$$\rho_s \rightarrow f \rho_s, \quad f = \rho / \sum_{s=1}^{ns} \rho_s \quad (3.163)$$

thereby satisfying the total mass conservation that is free from numerical errors included in the solution of species conservation equations [74].

Although a question remains that the Jacobian matrix can become singular in this formulation and hence the characteristic theory may break down, there is no mathematical contradiction only if we do not explicitly use the *physical* constrain of $\sum_{s=1}^{ns} \rho_s = \rho$ in constructing the Jacobian matrix. This is further discussed in the appendix.

Chapter 4

Implementation

4.1 Introductory Remarks

Needless to say, we can not analytically solve the equation system developed in the previous chapter, and hence need to find the approximate solutions in a numerical way. Since both the flow field and the electric field are described by partial differential equations, they must be discretized in space and suitable methods must be applied to each term considering their mathematical natures. In solving the equations in a time-marching manner, the inviscid terms of the fluid field equations must be discretized by taking into account the hyperbolic nature, so that one needs to construct the numerical flux in an upwind fashion. On the other hand, all terms associated with the transport phenomena have parabolic properties and thus they must be solved in a different manner from the inviscid terms. This is also true for the electric field equation which has an elliptic nature. The source terms representing the thermochemical nonequilibrium effects and the heat addition due to the Ohmic heating are, furthermore, tend to be extremely nonlinear with respect to flow properties, requiring some strategies to enhance stability of computations.

Since the late 1980's, many attempts have been made to solve the flow field that is in thermal and/or chemical nonequilibrium. These efforts have been directed mostly to resolve the strong nonlinear phenomena such as shock wave without imposing excessive numerical dissipation, which might degrade the accuracy of the computation for viscous flow fields. A number of time-evolution algorithms that enable us to obtain converged solutions within satisfied computational cost have been proposed with great success.

These numerical methods can also be applied to the arcjet computations, but additional efforts may be required to get rid of numerical difficulties associated with the physics inherent to arcjet thrusters as discussed in Chapter 2, Sec. 4. It should be kept in mind that a numerical scheme does not always reflect the physical model as expected. In other words, no matter how we construct a physical model completely, it will lose its completeness if accuracy of the employed numerical

scheme is insufficient. Commonly, numerical method involves intrinsic error which is accompanied in return for stabilization of the code, and numerical algorithms must be constructed in order to enhance the stability with imposing less numerical dissipation.

The purpose of the present chapter is, therefore, to describe how we should implement the physical model developed in the previous chapter with efforts being directed to enhance both accuracy and computational efficiency. Key topics discussed are as follows:

1. Finite volume discretization of the equation system
2. Construction of the numerical flux for convective terms
3. Construction of the numerical flux for diffusive terms
4. Implementation of the time-integration algorithm
5. Solution method for the electron energy equation
6. Solution method for the electric field equation

Care is taken so that the numerical algorithms are described in a way that the reader can construct the program directly from the expressions presented. The motivation is based on the author's personal opinion that the description of the numerical algorithm must be practical even at the expense of simplicity. Hence it is mentioned in advance that the expressions in the present chapter can be somewhat complicated although it might not always be necessary.

4.2 Finite Volume Formulation

Application of the computational fluid dynamics (CFD) to practical flow field owes much to introduction of the generalized curvilinear coordinates, originally proposed by Steger [75]. In this case, we transform the equation system from the physical domain (x, y, z) to computational domain (ξ, η, ζ) where the partial derivative terms $\partial/\partial\xi$, $\partial/\partial\eta$, and $\partial/\partial\zeta$ can be discretized as a finite difference method in the same manner as Cartesian mesh. This enables us to compute the flow field for a complicated geometry where it is difficult to impose boundary conditions if we use the conventional orthogonal meshes. However, although the idea of generalized coordinate system is very useful for most cases, recent numerical methods have been becoming very close to finite volume methods in nature. This is apparent if we employ the cell-centered scheme as indicated in Fig. 4.1. The physical properties $P_{i,j}$ are all defined at the center of the each computational mesh. On the other hand, in the recent sophisticated numerical schemes, fluxes are defined at the cell interface denoted by the subscript $1/2$. Hence even though the space derivative are

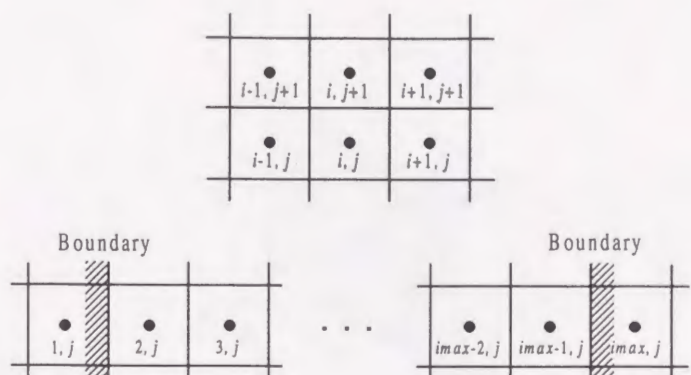


Figure 4.1: Finite volume mesh

evaluated in a finite difference fashion (e.g. $(\partial P / \partial \xi)_{i+1/2} = P_{i+1} - P_i$), the scheme is very similar to finite volume methods in the sense that we evaluate the difference of inflow and outflow of the physical properties by the flux defined at the cell interface. For these reasons, we term the discretization algorithm described subsequently as *finite volume formulation*.

To begin with, it is convenient to rewrite the flow field governing equation system Eqs. (3.151) to (3.155) in conservative form as

$$\frac{d}{dt} \iiint Q dV + \iint \mathbf{F}_j dA_j = \iiint \mathbf{W} dV \quad (4.1)$$

where $\mathbf{Q} = [\rho, \rho u_i, E, \rho s, E_e]^t$ is the vector of conservative variables to be solved and $\mathbf{F}$ is the inviscid/viscous fluxes. The source vector $\mathbf{W}$ may include the Ohmic heating term, the mass production terms, and the thermal relaxation terms. Further A_k denotes the k -component of the area vector $\mathbf{A}$ and V is the volume of the control volume. Now we apply the finite volume formulation taking into account the axisymmetric condition. For a conventional numerical scheme, one transfers the equation system from Cartesian coordinates (x, y, z) to cylindrical coordinates (r, θ, z) and set the azimuthal derivatives $\partial / \partial \theta$ to zero. This results in an equation set composed of two-dimensional equations and additional source terms which represent the axisymmetric effect. In the present computation, instead of using above approach, we discretized the governing equations in a three-dimensional fashion for an infinitely thin control volume under the axisymmetric assumption [76]. The advantage of this discretization is that the scheme becomes rigorously conservative (i.e. the free stream can be captured without the error associated with the treatment of metrics terms). This is desirable for internal flow computations, especially for cases where the energy conversion processes are of interest.

Generally, in a finite volume method, the governing equation Eq. (4.1) is dis-

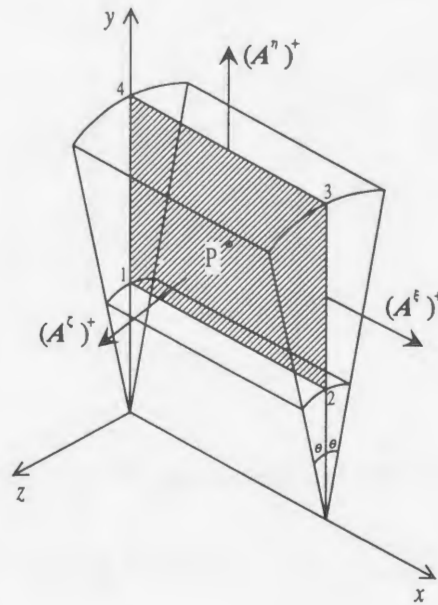


Figure 4.2: Quasi three-dimensional control volume

cretized for an arbitrary control volume by the following formula:

$$\frac{V}{\Delta t} \Delta Q + \sum_j (\mathbf{F}_j A_j) = V \cdot \mathbf{W} \quad (4.2)$$

where the subscript j denotes the index of the adjacent control volume and $\mathbf{F}_j$ is the numerical flux defined at the cell interface. We consider here a control volume P , so that the cell 1-2-3-4 on $x-y$ plane is rotated by 2θ around x axis as shown in Fig. 4.2. The physical properties are all defined at the center of the control volume. The area vector $(\mathbf{A}^\xi)^\pm$, $(\mathbf{A}^\eta)^\pm$, and $(\mathbf{A}^\zeta)^\pm$ can be expressed as

$$\begin{aligned} (\mathbf{A}^\xi)^+ &= (y_3 + y_2)\theta[(y_3 - y_2), -(x_3 - x_2), 0] \\ (\mathbf{A}^\xi)^- &= (y_4 + y_1)\theta[(y_4 - y_1), -(x_4 - x_1), 0] \\ (\mathbf{A}^\eta)^+ &= (y_3 + y_4)\theta[-(y_3 - y_4), (x_3 - x_4), 0] \\ (\mathbf{A}^\eta)^- &= (y_2 + y_1)\theta[-(y_2 - y_1), (x_2 - x_1), 0] \\ (\mathbf{A}^\zeta)^\pm &= S[0, \mp\theta, 1] \end{aligned} \quad (4.3)$$

where S denotes the cross section of the control volume and can be evaluated as

$$S = |(x_3 - x_1)(y_4 - y_2) - (y_3 - y_1)(x_4 - x_2)|/2 \quad (4.4)$$

Applying Pappus-Guldinus theorem, we can evaluate the volume of P as

$$\begin{aligned} V &= \theta[(y_1 + y_2 + y_3)|(x_1 - x_2)(y_1 - y_3) - (y_1 - y_2)(x_1 - x_3)| \\ &\quad + (y_1 + y_3 + y_4)|(x_1 - x_3)(y_1 - y_4) - (y_1 - y_3)(x_1 - x_4)|]/3 \end{aligned} \quad (4.5)$$

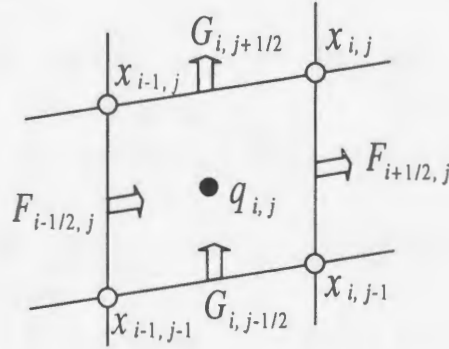


Figure 4.3: Finite volume cell system

Substituting Eq. (4.3) into Eq. (4.2) yields

$$\frac{V}{\Delta t} \Delta Q + (F_k A_k^\xi)^+ - (F_k A_k^\xi)^- + (F_k A_k^\eta)^+ - (F_k A_k^\eta)^- + H = V \cdot W \quad (4.6)$$

where

$$H = 2\theta S \begin{bmatrix} 0 \\ 0 \\ -p + \tau_{yy} - \tau_{zy} \\ (\tau_{yy} - \tau_{zy})v \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (4.7)$$

We have assumed here $\theta \ll 1$. Since all the terms of Eq. (4.6) are multiplied by θ , θ can be set to 1 without losing generality. The expression of the axisymmetric source terms H is much simpler than that for the cylindrical coordinate system, hence the present formulation is also efficient from the computational standpoint (note that $\tilde{F}_v$ and $\tilde{G}_v$ are defined at the cell interface, whereas H should be evaluated at the center point).

Now we evaluate the actual expression of Eq. (4.6). To do this, the finite volume cell is rewritten in terms of grid index as shown Fig. 4.3. The index (i, j) is defined at the center of the control volume for physical properties, whereas at the node in the right top of the cell for grid points and hence the cell $P_{i,j}$ is constructed by the four nodes, i.e. (i, j) , $(i, j-1)$, $(i-1, j)$, and $(i-1, j-1)$. In this cell system, Eq. (4.3)

can be rewritten as follows:

$$\begin{aligned} (A^\xi)^+ &= (y_{i,j} + y_{i,j-1})[(y_{i,j} - y_{i,j-1}), -(x_{i,j} - x_{i,j-1}), 0] \\ &= [2\bar{y}(y_\eta, -x_\eta, 0)]_{i+1/2,j} \end{aligned} \quad (4.8)$$

$$\begin{aligned} (A^\xi)^- &= (y_{i-1,j} + y_{i-1,j-1})[(y_{i-1,j} - y_{i-1,j-1}), -(x_{i-1,j} - x_{i-1,j-1}), 0] \\ &= [2\bar{y}(y_\eta, -x_\eta, 0)]_{i-1/2,j} \end{aligned} \quad (4.9)$$

$$\begin{aligned} (A^\eta)^+ &= (y_{i,j} + y_{i-1,j})[-(y_{i,j} - y_{i-1,j}), (x_{i,j} - x_{i-1,j}), 0] \\ &= [2\bar{y}(-y_\xi, x_\xi, 0)]_{i,j+1/2} \end{aligned} \quad (4.10)$$

$$\begin{aligned} (A^\eta)^- &= (y_{i,j-1} + y_{i-1,j-1})[-(y_{i,j-1} - y_{i-1,j-1}), (x_{i,j-1} - x_{i-1,j-1}), 0] \\ &= [2\bar{y}(-y_\xi, x_\xi, 0)]_{i,j-1/2} \end{aligned} \quad (4.11)$$

where, for example, $\bar{y}_{i+1/2,j} = (y_{i,j} + y_{i,j-1})/2$. Substituting Eqs. (4.8) to (4.11) into Eq. (4.6), we obtain

$$\begin{aligned} \frac{V_{i,j}}{\Delta t} \Delta Q_{i,j} &+ [2\bar{y}(\tilde{F} - \tilde{F}_v)]_{i+1/2,j} - [2\bar{y}(\tilde{F} - \tilde{F}_v)]_{i-1/2,j} \\ &+ [2\bar{y}(\tilde{G} - \tilde{G}_v)]_{i,j+1/2} - [2\bar{y}(\tilde{G} - \tilde{G}_v)]_{i,j-1/2} + H_{i,j} = (V \cdot W)_{i,j} \end{aligned} \quad (4.12)$$

where

$$\tilde{F} = y_\eta F - x_\eta G, \quad \tilde{F}_v = y_\eta F_v - x_\eta G_v \quad (4.13)$$

$$\tilde{G} = -y_\xi F + x_\xi G, \quad \tilde{G}_v = -y_\xi F_v + x_\xi G_v \quad (4.14)$$

F , G , F_v , and G_v , are the inviscid/viscous fluxes in Cartesian coordinate. The actual expressions of $\tilde{F}$, $\tilde{F}_v$, $\tilde{G}$, and $\tilde{G}_v$ are

$$\tilde{F} = \begin{bmatrix} \rho U \\ \rho u U + y_\eta p \\ \rho v U - x_\eta p \\ (E + p)U \\ \rho_1 U \\ \vdots \\ \rho_{ns} U \\ E_e U \end{bmatrix}, \quad \tilde{F}_v = \begin{bmatrix} 0 \\ y_\eta \tau_{xx} - x_\eta \tau_{xy} \\ y_\eta \tau_{yx} - x_\eta \tau_{yy} \\ y_\eta \beta_x - x_\eta \beta_y \\ -y_\eta J_{1,x} + x_\eta J_{1,y} \\ \vdots \\ -y_\eta J_{ns,x} + x_\eta J_{ns,y} \\ -y_\eta q_{e,x} + x_\eta q_{e,y} \end{bmatrix} \quad (4.15)$$

$$\tilde{G} = \begin{bmatrix} \rho V \\ \rho u V - y_\xi p \\ \rho v V + x_\xi p \\ (E + p)V \\ \rho_1 V \\ \vdots \\ \rho_{ns} V \\ E_e V \end{bmatrix}, \quad \tilde{G}_v = \begin{bmatrix} 0 \\ -y_\xi \tau_{xx} + x_\xi \tau_{xy} \\ -y_\xi \tau_{yx} + x_\xi \tau_{yy} \\ -y_\xi \beta_x + x_\xi \beta_y \\ y_\xi J_{1,x} - x_\xi J_{1,y} \\ \vdots \\ y_\xi J_{ns,x} - x_\xi J_{ns,y} \\ y_\xi q_{e,x} - x_\xi q_{e,y} \end{bmatrix} \quad (4.16)$$

U and V are the contravariant velocity defined as

$$U = y_\eta u - x_\eta v, \quad V = -y_\xi u + x_\xi v \quad (4.17)$$

and in this case each term associated with transport phenomena can be defined as follows:

$$\tau_{xx} = \frac{2}{3}\mu \left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{v}{y} \right) \quad (4.18)$$

$$\tau_{yy} = \frac{2}{3}\mu \left(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} - \frac{v}{y} \right) \quad (4.19)$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right) \quad (4.20)$$

$$\tau_{yz} = \tau_{zy} = \mu \left(2\frac{\partial v}{\partial y} - \frac{v}{y} \right) \quad (4.21)$$

Further,

$$\beta_x = u\tau_{xx} + v\tau_{xy} + (\lambda + \lambda_{\text{vib}})\frac{\partial T}{\partial x} + \lambda_e \frac{\partial T_e}{\partial x} + \rho \sum_{s=1}^{ns} h_s D_s \frac{\partial X_s}{\partial x} \quad (4.22)$$

$$\beta_y = u\tau_{xy} + v\tau_{yy} + (\lambda + \lambda_{\text{vib}})\frac{\partial T}{\partial y} + \lambda_e \frac{\partial T_e}{\partial y} + \rho \sum_{s=1}^{ns} h_s D_s \frac{\partial X_s}{\partial y} \quad (4.23)$$

$$J_{s,x} = -\rho D_s \frac{\partial X_s}{\partial x} \quad (4.24)$$

$$J_{s,y} = -\rho D_s \frac{\partial X_s}{\partial y} \quad (4.25)$$

$$q_{e,x} = -\lambda_e \frac{\partial T_e}{\partial x} - \rho h_e D_e \frac{\partial X_e}{\partial x} \quad (4.26)$$

$$q_{e,y} = -\lambda_e \frac{\partial T_e}{\partial y} - \rho h_e D_e \frac{\partial X_e}{\partial y} \quad (4.27)$$

Finally all metrics are defined at each cell interface as

$$(x_\xi)_{j+1/2} = x_{i,j} - x_{i-1,j} \quad (4.28)$$

$$(y_\xi)_{j+1/2} = y_{i,j} - y_{i-1,j} \quad (4.29)$$

$$(x_\eta)_{i+1/2} = x_{i,j} - x_{i,j-1} \quad (4.30)$$

$$(y_\eta)_{i+1/2} = y_{i,j} - y_{i,j-1} \quad (4.31)$$

From the above definitions, for example, x_η at the cell interface $j + 1/2$ can be evaluated as $(x_\eta)_{j+1/2} = [(x_\eta)_{i+1/2,j} + (x_\eta)_{i-1/2,j} + (x_\eta)_{i+1/2,j+1} + (x_\eta)_{i-1/2,j+1}]/4$.

4.3 Inviscid Flux

4.3.1 Recent progress on inviscid numerical flux for compressible flows

As widely recognized, the existence of strong shock wave with large density gradients is one of the distinctive characteristics of the hypersonic flow environment and numerical computation of weak solutions to flow problems with such a strong discontinuity necessitates special consideration. To date, many computational methods associated with hypersonic chemically reacting flows have been proposed and the development is still one of the state-of-art works. They are briefly overviewed below.

To reproduce shock waves both accurately and stable, one needs to discretize the convective terms by taking into account their hyperbolic nature. This implies that the solution of hyperbolic conservation laws must be based on exploiting the information obtained by considering a sequence of so-called Riemann problems in which we need to solve the locally one-dimensional Euler equations for discontinuous neighboring states, that is,

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0, \quad Q(t=0) = \begin{cases} Q_L & \text{if } x < 0 \\ Q_R & \text{if } x > 0 \end{cases} \quad (4.32)$$

where Q and F denote conservative vectors and flux, respectively. The group of schemes known as flux difference splitting (FDS) methods evaluate the inviscid numerical flux by solving the Riemann problem exactly or approximately. Among them, the Roe scheme [77] solves Eq. (4.1) approximately by linearizing the problem and evaluates the numerical flux in a simple form. This can be applied for various compressible flow computations with great success, but accuracy of the scheme is the first order and there is no room to extend to higher accuracy. Hence another approach to obtain more than second order accuracy was required.

In Ref. [78] Harten advocated the idea of total variation diminishing (TVD), whereby a scheme is constructed under the condition that the variation of the numerical solution does not produce any new extremum. This concept, when applied

to central schemes, leads to particular forms of artificial viscosity without empirical constants and prevents the generation of numerical oscillations if the scheme is extended to higher-order accuracy. The group of schemes based on the idea of Harten is generally referred to as *TVD scheme*, and have widely applied in broad range of high-speed compressible flow computations. Essential contributions in these directions are summarized in [79].

Although the higher-accuracy FDS methods such as the TVD scheme can resolve shock waves clearly, sometimes they are liable to capture a series of unphysical solutions including the carbuncle phenomenon for blunt-body flows, oscillations behind slow-moving shocks, and the expansion shock at sonic points [80]. This is mostly due to the fact that the Riemann problems are solved approximately in one-dimensional manner. Since these trends become notable with increasing Mach number, their application to hypersonic problems have been cumbersome.

On the other hand, the group of schemes called flux vector splitting (FVS) methods divide the flux vector $\mathbf{F}$ into positive and negative parts as

$$\mathbf{F}(\mathbf{Q}) = \mathbf{F}(\mathbf{Q})^- + \mathbf{F}(\mathbf{Q})^+ \quad (4.33)$$

which gives the numerical flux at cell interface between the states $\mathbf{Q}_L$ and $\mathbf{Q}_R$

$$\mathbf{F}_{1/2}(\mathbf{Q}_L, \mathbf{Q}_R) = \mathbf{F}(\mathbf{Q}_L)^+ + \mathbf{F}(\mathbf{Q}_R)^- \quad (4.34)$$

This can be possible since the inviscid flux vector has a homogeneous nature, $\mathbf{F} = A\mathbf{Q}$, where A denotes the Jacobian matrix with respect to the conservative variable $\mathbf{Q}$. In the FVS scheme, the interaction of neighboring states is accomplished through mixing of *pseudo-particles* that move in and out of each cell according to a given velocity distribution. Hence we can interpret the FVS scheme as we solve the Boltzmann equation omitting the collision term. The scheme of Steger and Warming [81], van Leer [82], and Hänel [83] belong to this splitting method. Although these schemes are first-order accuracy for themselves, we can readily extend to higher accuracy by applying the MUSCL (Monotone Upstream-centered Scheme for Conservation Laws) methods proposed by van Leer [84], [85]. The FVS schemes are very robust and less liable to cause unphysical phenomena for higher Mach number flow computations compared to FDS schemes. However, in return for robustness, we are much suffered from the excessive numerical dissipation and they are not suitable to viscous computations.

Recently, there have been another approach to develop less-dissipative upwind schemes in which the surplus dissipation of the FVS is reduced by introducing the flavor of FDS into FVS schemes. In [86], Liou and Steffen proposed a promising scheme named Advection Upstream Splitting Method (AUSM), in which the cell-face advection Mach number is appropriately defined to determine the upwind extrapolation for the convective quantities. The AUSM can capture a stationary discontinuity with no numerical dissipation and is robust enough to calculate the higher Mach number flows. Owing to success of the AUSM, many efforts have been

moved towards the construction of the FDS/FVS hybrid scheme and the AUSM-class schemes are becoming a mainstream of the compressible flow computations replacing FDS or FVS. In the present study, we employ a kind of FDS/FVS hybrid scheme, AUSM-DV, proposed by Wada [87], to evaluate the numerical flux for inviscid terms and they are subsequently discussed in detail. While maintaining the same level of accuracy, AUSM+MUSCL approach is much robust and efficient than FDS and less suffered from numerical dissipation than FVS. These characteristics are preferable even when there exists no strong nonlinear phenomena such as shock waves in the flow field.

4.3.2 MUSCL

The purpose of the present section is to derive the high-accuracy numerical flux denoted as $\tilde{F}_{i+1/2,j}$ and $\tilde{G}_{i,j+1/2}$ in Eq. (4.12). Based on the finite volume formulation discussed in the previous section, accuracy of the numerical flux becomes first order at most if the distribution of the physical properties inside the cell shown in Fig. 4.2 are assumed to be piecewisely constant, and additional methods are required in order to obtain more than second order accuracy. This can be achieved by applying the Monotone Upwind Scheme for Conservation Law (MUSCL) of van Leer [84], [85]. The essence of the method is a one-dimensional Lagrangean scheme that may be regarded as a second-order sequel to Godunov's method, and the basic idea is summarized as follows:

1. The second-order accuracy is achieved by reconstructing the distributions of the state quantities inside the cell to be linear, rather than uniform as in Godunov's original method [88] that is first order.
2. Several monotonicity algorithms are applied to ensure positivity, monotonicity and nonlinear stability.
3. The Riemann flux is applied to obtain the numerical flux at the cell interface where there may exist a discontinuity.

In the present MUSCL approach, physical properties at a cell interface can be evaluated by reconstructing the distributions of the physical properties inside the cell adjacent to the interface, which is equivalent to extrapolating the cell-center values toward the cell interface. Care must be taken to maintain the monotonicity of the distribution and to prevent numerical oscillations by introducing the limiter. These efforts yield the expression of newly defined physical properties at the cell interface

for the present finite volume formulation as [89]

$$q_{i+1/2}^- = q_i + \frac{l_i}{2} \minmod(\Delta_i^-, \Delta_i^+) \quad (4.35)$$

$$q_{i+1/2}^+ = q_{i+1} - \frac{l_{i+1}}{2} \minmod(\Delta_{i+1}^+, \Delta_{i+1}^-) \quad (4.36)$$

$$q_{j+1/2}^- = q_j + \frac{l_j}{2} \minmod(\Delta_j^-, \Delta_j^+) \quad (4.37)$$

$$q_{j+1/2}^+ = q_{j+1} - \frac{l_{j+1}}{2} \minmod(\Delta_{j+1}^+, \Delta_{j+1}^-) \quad (4.38)$$

where

$$\minmod(a, b) = \max[0, \min\{a \cdot \text{sgn}(b), b \cdot \text{sgn}(a)\}] \text{sgn}(a) \quad (4.39)$$

$$\Delta_i^+ = \frac{2(q_{i+1} - q_i)}{(l_i + l_{i+1})} \quad (4.40)$$

$$\Delta_i^- = \frac{2(q_i - q_{i-1})}{(l_{i-1} + l_i)} \quad (4.41)$$

$$\Delta_j^+ = \frac{2(q_{j+1} - q_j)}{(l_j + l_{j+1})} \quad (4.42)$$

$$\Delta_j^- = \frac{2(q_j - q_{j-1})}{(l_{j-1} + l_j)} \quad (4.43)$$

$$l_i = \left[(\sqrt{x_\xi^2 + y_\xi^2})_{i,j+1/2} + (\sqrt{x_\xi^2 + y_\xi^2})_{i,j-1/2} \right] / 2 \quad (4.44)$$

$$l_j = \left[(\sqrt{x_\eta^2 + y_\eta^2})_{i+1/2,j} + (\sqrt{x_\eta^2 + y_\eta^2})_{i-1/2,j} \right] / 2 \quad (4.45)$$

Note that l implies the length of the cell.

A question remains how we select the property q to be reconstructed. There are at least two choices regarding this, namely conservative variables $[\rho, \rho u, \rho v, E, \rho_s]^t$ and primitive variables $[\rho, u, v, p, \rho_s]^t$. As pointed out by Yee [79], the choice of the dependent variables on which limiters are applied plays an important role in the stability and convergence rate. In fact, many previous studies have pointed out that selecting primitive variables are marginally better than selecting conservative variables, and we determine to follow them. Since the stability problem is mostly associated with the numerical oscillations around the shock wave, this choice of the dependent variables is expected to be relatively minor for shock-free problems.

4.3.3 AUSM-DV scheme

To what follows, we try to construct the two-dimensional inviscid numerical flux $\mathbf{F}$ for perfect gases in Cartesian coordinates at the cell interface $i + 1/2$, i.e.

$$\mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \end{bmatrix} \quad (4.46)$$

and we simply express it as $\mathbf{F}_{1/2}$. The physical properties defined at the control volume (i, j) and $(i + 1, j)$ are denoted as L and R , respectively. Extension to thermochemical nonequilibrium flow cases in the present finite volume formulation is straightforward and discussed later.

The essence of the AUSM is to split $\mathbf{F}_{1/2}$ into advection contribution $\mathbf{F}_{1/2}^a$ and pressure contribution $\mathbf{F}_{1/2}^p$ as $\mathbf{F}_{1/2} = \mathbf{F}_{1/2}^a + \mathbf{F}_{1/2}^p$. The two contributions are treated separately. The numerical flux for the advection term is constructed in an upwind manner as is the case for FDS methods, so that

$$\begin{aligned} \mathbf{F}_{1/2}^a &= \frac{1}{2} [(\rho u)_{1/2}(\Psi_L + \Psi_R) - |(\rho u)_{1/2}|(\Psi_R - \Psi_L)] \\ &= \begin{bmatrix} (\rho u)_{1/2} \\ (\rho u)_{1/2}(u_L + u_R) - |(\rho u)_{1/2}|(u_R - u_L) \\ (\rho u)_{1/2}(v_L + v_R) - |(\rho u)_{1/2}|(v_R - v_L) \\ (\rho u)_{1/2}(H_L + H_R) - |(\rho u)_{1/2}|(H_R - H_L) \end{bmatrix} \end{aligned} \quad (4.47)$$

where $\Psi = [1, u, v, H]^t$. On the other hand, the pressure flux is split in the same manner as FVS methods, hence

$$\mathbf{F}_{1/2}^p = \begin{bmatrix} 0 \\ p_{1/2} \\ 0 \\ 0 \end{bmatrix} \quad (4.48)$$

The interface mass flux $(\rho u)_{1/2}$ and the interface pressure $p_{1/2}$ are expressed in terms of sets of polynomials in Mach number, defined as

$$M_{L/R} \equiv \frac{u_{L/R}}{c_{1/2}} \quad (4.49)$$

It is important to note that M_L and M_R are defined by a common speed of sound $c_{1/2}$. In this case, $c_{1/2}$ is simply defined by

$$c_{1/2} = \max(c_L, c_R) \quad (4.50)$$

To evaluate the interface values, we use the following three sets of Mach number polynomials

$$\Gamma_{(1)}^{\pm} = \frac{M \pm |M|}{2} \quad (4.51)$$

$$\Gamma_{(2)}^{\pm} = \begin{cases} \pm \frac{(M \pm 1)^2}{4}, & |M| < 1 \\ \Gamma_{(1)}^{\pm}, & \text{otherwise} \end{cases} \quad (4.52)$$

$$\Gamma_{(3)}^{\pm} = \begin{cases} \frac{(M \pm 1)^2(2 \mp M)}{(1/M)\Gamma_{(1)}^{\pm}}, & |M| < 1 \\ \Gamma_{(1)}^{\pm}, & \text{otherwise} \end{cases} \quad (4.53)$$

The numerals in the subscripts of Eqs. (4.51) to (4.53) indicate the degree of the polynomials. With these, $(\rho u)_{1/2}$ and $p_{1/2}$ are defined as

$$(\rho u)_{1/2} = \rho_L u_L^+ + \rho_R u_R^- = c_{1/2} (\rho_L m_{1/2}^+ + \rho_R m_{1/2}^-) \quad (4.54)$$

$$p_{1/2} = \Gamma_{(3)}^+(M_L) \cdot p_L + \Gamma_{(3)}^-(M_R) \cdot p_R \quad (4.55)$$

where

$$u_L^+ = c_{1/2} m_{1/2}^+ \quad (4.56)$$

$$u_R^- = c_{1/2} m_{1/2}^- \quad (4.57)$$

$$m_{1/2}^+ = \Gamma_{(1)}^+(M_L) + \alpha_L [\Gamma_{(2)}^+(M_L) - \Gamma_{(1)}^+(M_L)] \quad (4.58)$$

$$m_{1/2}^- = \Gamma_{(1)}^-(M_R) + \alpha_R [\Gamma_{(2)}^-(M_R) - \Gamma_{(1)}^-(M_R)] \quad (4.59)$$

and

$$\alpha_L = \frac{2(p/\rho)_L}{(p/\rho)_L + (p/\rho)_R} \quad (4.60)$$

$$\alpha_R = \frac{2(p/\rho)_R}{(p/\rho)_L + (p/\rho)_R} \quad (4.61)$$

Since the above scheme discretize all the advection terms by the upwind differencing, this is classified as a group of "AUSM-D" methods [87], where "D" denotes the flux Difference splitting biased scheme.

Owing to the second terms of Eqs. (4.58) and (4.59), the AUSM-D scheme is less suffered from numerical dissipation compared to conventional FVS schemes. To examine this, we consider a stationary contact discontinuity where $u_L = u_R = 0$; $p_L = p_R$. By substituting Eqs. (4.56) to (4.59) into Eq. (4.54), we can readily confirm that the mass flux $(\rho u)_{1/2}$ becomes zero as it should be. Normally this condition is not satisfied for any FVS schemes and this is a main cause of producing the excessive numerical dissipation.

Although the AUSM-D scheme can be used as an independent scheme, as is the case for other FDS schemes, we sometimes encounter numerical instabilities if there exist strong shock waves or rapid expansions. The idea of the AUSM-DV method is, therefore, to combine the above AUSM-D scheme with a kind of flux vector splitting method which is much more robust than FDS. We conventionally term this FVS-class scheme as "AUSM-V", where "V" implies the FVS.

For the AUSM-V, the term $(\rho u^2)_{1/2}$ in the x -momentum flux can be expressed as

$$(\rho u^2)_{1/2}^V = u_L^+(\rho u)_L + u_R^-(\rho u)_R \quad (4.62)$$

where u_L^+ and u_R^- are the same as Eqs. (4.56) to (4.57). Whereas for the AUSM-D,

$$(\rho u^2)_{1/2}^D = \frac{1}{2} [(\rho u)_{1/2}(u_L + u_R) - |(\rho u)_{1/2}|(u_R - u_L)] \quad (4.63)$$

The $(\rho u^2)_{1/2}$ of the AUSM-DV method is thus expressed as a combination of $(\rho u^2)_{1/2}^D$ and $(\rho u^2)_{1/2}^V$,

$$(\rho u^2)_{1/2}^{DV} = \left(\frac{1}{2} - s\right) (\rho u^2)_{1/2}^D + \left(\frac{1}{2} + s\right) (\rho u^2)_{1/2}^V \quad (4.64)$$

In Ref. [87], Wada determined the blending parameter s in a numerically experimental way, which results in

$$s = \frac{1}{2} \min \left(1, 10 \frac{|p_R - p_L|}{\min(p_L, p_R)} \right) \quad (4.65)$$

Now we summarize the AUSM-DV scheme as follows.

$$\mathbf{F}_{1/2} = \begin{bmatrix} (\rho u)_{1/2} \\ (\rho u^2)_{1/2}^{DV} + p_{1/2} \\ (\rho u)_{1/2}(v_L + v_R) - |(\rho u)_{1/2}|(v_R - v_L) \\ (\rho u)_{1/2}(H_L + H_R) - |(\rho u)_{1/2}|(H_R - H_L) \end{bmatrix} \quad (4.66)$$

It should also be noted that the energy flux of Eq. (4.66) $F_{\text{energy}}^\pm$ can be expressed in terms of the mass flux $F_{\text{mass}}^\pm$ as

$$F_{\text{energy}}^\pm = F_{\text{mass}}^\pm H \quad (4.67)$$

The above relation implies that the AUSM-DV scheme can rigorously conserve the total enthalpy, which should always be satisfied from the physical viewpoint but sometimes fails for a certain numerical scheme. This property is favorable for computations where the energy transfer phenomena should be simulated accurately, such as the case for arcjet flows.

Finally we apply the AUSM-DV numerical flux to the present finite volume formulation with the MUSCL procedure. For $\tilde{\mathbf{F}}$ in Eq. (4.12),

$$\tilde{\mathbf{F}}_{1/2} = \begin{bmatrix} (\rho U)_{1/2} \\ (\rho u U)_{1/2}^{DV} + (y_\eta p)_{1/2} \\ (\rho)_{1/2}(v_L + v_R) - |(\rho U)_{1/2}|(v_R - v_L) - (x_\eta p)_{1/2} \\ (\rho U)_{1/2}(H_L + H_R) - |(\rho U)_{1/2}|(H_R - H_L) \\ (\rho)_{1/2}(C_{1,L} + C_{1,R}) - |(\rho U)_{1/2}|(C_{1,L} - C_{1,R}) \\ \vdots \\ (\rho U)_{1/2}(C_{ns,L} + C_{ns,R}) - |(\rho U)_{1/2}|(C_{ns,R} - C_{ns,L}) \\ (\rho U)_{1/2}((C_e e_e)_L + (C_e e_e)_R) - |(\rho U)_{1/2}|((C_e e_e)_R - (C_e e_e)_L) \end{bmatrix} \quad (4.68)$$

where, for example, $v_L = v_{i+1/2}^+$ and $v_R = v_{i+1/2}^-$, whose values are obtained from Eqs. (4.39) and (4.41). Further,

$$(\rho U)_{1/2} = \rho_L U_L^+ + \rho_R U_R^- \quad (4.69)$$

$$(\rho u U)_{1/2}^D = \frac{1}{2} [(\rho U)_{1/2}(u_L + u_R) - |(\rho U)_{1/2}|(u_R - u_L)] \quad (4.70)$$

$$(\rho u U)_{1/2}^V = U_L^+(\rho u)_L + U_R^-(\rho u)_R \quad (4.71)$$

Similarly for $\tilde{\mathbf{G}}$,

$$\tilde{\mathbf{G}}_{1/2} = \begin{bmatrix} (\rho V)_{1/2} \\ (\rho v V)_{1/2}^{DV} + (x_\xi p)_{1/2} \\ (\rho V)_{1/2}(u_L + u_R) - |(\rho V)_{1/2}|(u_R - u_L) - (y_\xi p)_{1/2} \\ (\rho V)_{1/2}(H_L + H_R) - |(\rho V)_{1/2}|(H_R - H_L) \\ (\rho V)_{1/2}(C_{1,L} + C_{1,R}) - |(\rho V)_{1/2}|(C_{1,R} - C_{1,L}) \\ \vdots \\ (\rho V)_{1/2}(C_{ns,L} + C_{ns,R}) - |(\rho V)_{1/2}|(C_{ns,R} - C_{ns,L}) \\ (\rho V)_{1/2}((C_e e_e)_L + (C_e e_e)_R) - |(\rho V)_{1/2}|((C_e e_e)_R - (C_e e_e)_L) \end{bmatrix} \quad (4.72)$$

where, for example, $u_L = v_{j+1/2}^+$ and $u_R = v_{j+1/2}^-$, whose values are obtained from Eqs. (4.42) and (4.43). And,

$$(\rho V)_{1/2} = \rho_L V_L^+ + \rho_R V_R^- \quad (4.73)$$

$$(\rho v V)_{1/2}^D = \frac{1}{2} [(\rho V)_{1/2}(v_L + v_R) - |(\rho V)_{1/2}|(v_R - v_L)] \quad (4.74)$$

$$(\rho v V)_{1/2}^V = V_L^+(\rho v)_L + V_R^-(\rho v)_R \quad (4.75)$$

$M_{L/R}$ in Eq. (4.49) is evaluated by U or V . The velocity components u and v should not be confused with the contravariant velocities U and V .

4.3.4 Entropy-fix procedure

Although the AUSM-DV method appears to be robust and accurate for most problems, it sometimes permits the formation of stable *expansion shocks* near sonic points

and converges to aphysical solutions. This becomes serious if a strong expansion is present in the flow field. From a physical perspective, the formation of expansion shocks can be interpreted as being related to the linearized representation of expansion waves by the approximate Riemann solver [80]. The propagation of a rarefaction wave is characterized by the leading and trailing characteristics of the fan. Especially at sonic points, the leading and trailing characteristics of rarefaction waves propagate in opposite directions and thus the solution changes associated with the waves are propagated in both directions. Since the group of FDS schemes only approximately simulate its propagation in one-dimensional manner, sometimes they may fail to correctly predict the direction of the propagation, which result in the generation of unphysical phenomena such as expansion shocks.

As a remedy for these difficulties, in the present study, the entropy-fix procedure is employed [87]. There are two cases where an expansive sonic point is found across the cell interface:

$$\text{Case A: } u_L - c_L < 0 \quad \text{and} \quad u_R - c_R > 0$$

$$\text{Case B: } u_L + c_L < 0 \quad \text{and} \quad u_R + c_R > 0$$

Thus the entropy-fix is applied when a *single* expansion wave is detected. The procedure are depicted in Algorithm 4.1. When the procedure is applied to Eq.

ALGORITHM 4.1: Entropy-fix procedure

```

if ( A and B ) then
    no modification
elseif ( A ) then
     $F_{1/2} := F_{1/2} - C\Delta(u - c)\Delta(\rho\Psi)$ 
elseif ( B ) then
     $F_{1/2} := F_{1/2} - C\Delta(u + c)\Delta(\rho\Psi)$ 
else
    no modification
endif

```

where $\Delta(\cdot) \equiv (\cdot)_R - (\cdot)_L$, $C = 0.125$.

(4.68) or (4.72), the velocity u is replaced by the contravariant velocity U or V . It is apparent that the AUSM-DV scheme keeps the enthalpy conservation property even though the entropy-fix method changes the original form.

4.3.5 Preconditioning

As with most upwind methods, the cell-interface values of the inviscid numerical flux for AUSM-DV can be expressed as a combination of the central difference terms and

the artificial dissipation terms. Since the AUSM-DV method splits convective terms into the advective contribution and the pressure contribution, we can generally write them as

$$(\rho u)_{1/2} = \frac{1}{2}[(\rho u)_L + (\rho u)_R + \Phi_{1/2}] \quad (4.76)$$

$$p_{1/2} = \frac{1}{2}[p_L + p_R + \Psi_{1/2}] \quad (4.77)$$

where Φ and Ψ represent the artificial dissipation. Various upwind splitting methods can be classified as to how they evaluate the dissipation terms at the critical location such as sonic or stagnation points. It is widely recognized that the AUSM-class schemes lose their accuracy and robustness with decreasing Mach number, and this is because the dissipation term is scaled by the speed of sound. In Ref. [90], it is verified that the AUSM splitting tends to smear the velocity field solution severely when the Mach number becomes low due to the excessive dissipation for the pressure splitting. Moreover, the original AUSM-DV scheme is sometimes suffered from the even-odd decoupling phenomena as the Mach number is lowered, showing central difference discretization behavior. To remedy them, we modify the original AUSM-DV scheme by applying the preconditioning technique.[†] The basic idea is that the diffusive contributions should be scaled by the velocity magnitude rather than by the speed of sound as the local Mach number decreases [90].

In the present preconditioning, the interface speed of sound $c_{1/2}$ in Eq. (4.50) is preconditioned as

$$\tilde{c}_{1/2} = f_{1/2} c_{1/2} \quad (4.78)$$

where the quantity $f_{1/2}$ is given as

$$f_{1/2} = \frac{\sqrt{(1 - M_{\text{ref}}^2)M_{1/2}^2 + 4M_{\text{ref}}^2}}{(1 + M_{\text{ref}}^2)} \quad (4.79)$$

Then $M_{L/R}$ is replaced by

$$\tilde{M}_{L/R} = \frac{u_{L/R}}{\tilde{c}_{1/2}} \quad (4.80)$$

By using $\tilde{M}_{L/R}$, the cell interface Mach numbers $\bar{M}_{L/R}$ are defined as follows:

$$\bar{M}_L = \frac{1}{2} \left[(1 + M_{\text{ref}}^2) \tilde{M}_L + (1 - M_{\text{ref}}^2) \tilde{M}_R \right] \quad (4.81)$$

$$\bar{M}_R = \frac{1}{2} \left[(1 + M_{\text{ref}}^2) \tilde{M}_R + (1 - M_{\text{ref}}^2) \tilde{M}_L \right] \quad (4.82)$$

[†]Note that the present preconditioning is applied to the inviscid numerical flux itself, and this should be distinguished from the time-derivative preconditioning technique [91].

By this, the dissipation term Φ can be scaled with the velocity magnitude rather than the speed of sound, and hence we can alleviate the difficulty mentioned above.

In turn, to prevent even-odd decoupling, the mass flux terms $(\rho u)_{1/2}$ can be preconditioned for the split Mach numbers $m_{1/2}^\pm$ in Eqs. (4.58) and (4.59) as

$$m_{1/2}^+ = \Gamma_{(1)}^+(\bar{M}_L) + \frac{\alpha_L}{2} \left\{ \left(1 + \frac{1}{M_{\text{ref}}^2} \right) [\Gamma_{(2)}^+(\bar{M}_L) - \Gamma_{(1)}^+(\bar{M}_L)] \right. \\ \left. + \left(1 - \frac{1}{M_{\text{ref}}^2} \right) [\Gamma_{(2)}^-(\bar{M}_R) - \Gamma_{(1)}^-(\bar{M}_R)] \right\} \quad (4.83)$$

$$m_{1/2}^- = \Gamma_{(1)}^-(\bar{M}_R) + \frac{\alpha_R}{2} \left\{ \left(1 + \frac{1}{M_{\text{ref}}^2} \right) [\Gamma_{(2)}^-(\bar{M}_R) - \Gamma_{(1)}^-(\bar{M}_R)] \right. \\ \left. + \left(1 - \frac{1}{M_{\text{ref}}^2} \right) [\Gamma_{(2)}^+(\bar{M}_L) - \Gamma_{(1)}^+(\bar{M}_L)] \right\} \quad (4.84)$$

4.4 Viscous Flux

In a time-marching scheme, all diffusive terms associated with the transport properties, i.e. viscosity, heat conduction, and mass/energy diffusion indicate parabolic nature [92]. From the physical viewpoint, this implies that time-evolution of physical state depends on every direction with the same degree of influence, as opposed to hyperbolic problems where there exist limited zones of influence and thus space derivative terms should be treated in an upwind way. Therefore, in order to correctly implement this trend in the computation, all the diffusive terms should be discretized in a central-difference fashion.

We need to evaluate the viscous flux of the form

$$(\tilde{\mathbf{F}}_v)_{i+1/2,j} = \begin{bmatrix} 0 \\ y_\eta \tau_{xx} - x_\eta \tau_{xy} \\ y_\eta \tau_{yx} - x_\eta \tau_{yy} \\ y_\eta \beta_x - x_\eta \beta_y \\ -y_\eta J_{1,x} + x_\eta J_{1,y} \\ \vdots \\ -y_\eta J_{ns,x} + x_\eta J_{ns,y} \\ -y_\eta q_{e,x} + x_\eta q_{e,y} \end{bmatrix}_{i+1/2,j} \quad (\tilde{\mathbf{G}}_v)_{i,j+1/2} = \begin{bmatrix} 0 \\ -y_\xi \tau_{xx} + x_\xi \tau_{xy} \\ -y_\xi \tau_{yx} + x_\xi \tau_{yy} \\ -y_\xi \beta_x + x_\xi \beta_y \\ y_\xi J_{1,x} - x_\xi J_{1,y} \\ \vdots \\ y_\xi J_{ns,x} - x_\xi J_{ns,y} \\ y_\xi q_{e,x} - x_\xi q_{e,y} \end{bmatrix}_{i,j+1/2} \quad (4.85)$$

Obviously the space derivatives appear in the above viscous flux should be evaluated separately for $\tilde{\mathbf{F}}_{i+1/2}$ and $\tilde{\mathbf{G}}_{j+1/2}$ since they are defined in the different cell interface; namely at $i + 1/2$ and at $j + 1/2$. With this in mind, we express the discretized forms of these terms in detail below.

For simplicity, we denote $\partial u / \partial x$ as u_x , and so on. We evaluate the spatial derivatives with respect to the computational domain (ξ, η) instead of the physical domain (x, y) . In this case the spatial velocity gradients can be evaluated as

$$u_x = \xi_x u_\xi + \eta_x u_\eta \quad (4.86)$$

$$u_y = \xi_y u_\xi + \eta_y u_\eta \quad (4.87)$$

$$v_x = \xi_x v_\xi + \eta_x v_\eta \quad (4.88)$$

$$v_y = \xi_y v_\xi + \eta_y v_\eta \quad (4.89)$$

Note that the following relations hold

$$\xi_x = J \cdot y_\eta \quad (4.90)$$

$$\xi_y = -J \cdot x_\eta \quad (4.91)$$

$$\eta_y = J \cdot x_\xi \quad (4.92)$$

$$\eta_x = -J \cdot y_\xi \quad (4.93)$$

$$J = 1/(x_\xi y_\eta - x_\eta y_\xi) \quad (4.94)$$

With these, each stress tensor can be expressed as

$$\tau_{xx} = J \cdot \frac{2}{3} \mu [2(y_\eta u_\xi - y_\xi u_\eta) - (-x_\eta v_\xi + x_\xi v_\eta) - v/(y \cdot J)] \quad (4.95)$$

$$\tau_{yy} = J \cdot \frac{2}{3} \mu [2(-x_\eta v_\xi + x_\xi v_\eta) - (y_\eta u_\xi - y_\xi u_\eta) - v/(y \cdot J)] \quad (4.96)$$

$$\tau_{xy} = J \cdot \mu (-x_\eta u_\xi + x_\xi u_\eta + y_\eta v_\xi - y_\xi v_\eta) \quad (4.97)$$

Putting Eqs. (4.95) to (4.97) into Eq. (4.85), we obtain

$$\begin{aligned} (y_\eta \tau_{xx} - x_\eta \tau_{xy})_{i+1/2} = (J\mu)_{i+1/2} & \left[\left(\gamma + \frac{y_\eta^2}{3} \right) u_\xi - \left(\beta + \frac{y_\xi y_\eta}{3} \right) u_\eta \right. \\ & \left. - \frac{x_\eta y_\eta}{3} v_\xi - \left(\varepsilon - \frac{x_\xi y_\eta}{3} \right) v_\eta - \frac{2}{3} \frac{y_\eta v}{y J} \right]_{i+1/2} \end{aligned} \quad (4.98)$$

$$\begin{aligned} (-y_\xi \tau_{xx} + x_\xi \tau_{xy})_{j+1/2} = (J\mu)_{j+1/2} & \left[-\left(\beta + \frac{y_\xi y_\eta}{3} \right) u_\xi + \left(\alpha + \frac{y_\xi^2}{3} \right) u_\eta \right. \\ & \left. + \left(\varepsilon + \frac{x_\eta y_\xi}{3} \right) v_\xi - \frac{x_\xi y_\xi}{3} v_\eta + \frac{2}{3} \frac{y_\xi v}{y J} \right]_{j+1/2} \end{aligned} \quad (4.99)$$

$$\begin{aligned} (y_\eta \tau_{xy} - x_\eta \tau_{yy})_{i+1/2} = (J\mu)_{i+1/2} & \left[-\frac{x_\eta y_\eta}{3} u_\xi + \left(\varepsilon + \frac{x_\eta y_\xi}{3} \right) u_\eta \right. \\ & \left. + \left(\gamma + \frac{x_\eta^2}{3} \right) v_\xi - \left(\beta + \frac{x_\xi x_\eta}{3} \right) v_\eta + \frac{2}{3} \frac{x_\eta v}{y J} \right]_{i+1/2} \end{aligned} \quad (4.100)$$

$$\begin{aligned}
 (-y_\xi \tau_{xy} + x_\xi \tau_{yy})_{j+1/2} = (J\mu)_{j+1/2} & \left[-\left(\varepsilon - \frac{x_\xi y_\eta}{3}\right) u_\xi - \frac{x_\xi y_\xi}{3} u_\eta \right. \\
 & \left. - \left(\beta + \frac{x_\xi x_\eta}{3}\right) v_\xi + \left(\alpha + \frac{x_\xi^2}{3}\right) v_\eta - \frac{2}{3} \frac{x_\xi v}{yJ} \right]_{j+1/2}
 \end{aligned} \quad (4.101)$$

where

$$\alpha = x_\xi^2 + y_\xi^2 \quad (4.102)$$

$$\beta = x_\xi x_\eta + y_\xi y_\eta \quad (4.103)$$

$$\gamma = x_\eta^2 + y_\eta^2 \quad (4.104)$$

$$\varepsilon = x_\xi y_\eta - x_\eta y_\xi \quad (4.105)$$

On the other hand, the mass diffusion flux can be expressed as

$$J_{s,x} = -D_s \frac{\partial X_s}{\partial x} = -J \cdot D_s [y_\eta X_{s,\xi} - y_\xi X_{s,\eta}] \quad (4.106)$$

$$J_{s,y} = -D_s \frac{\partial X_s}{\partial y} = -J \cdot D_s [-x_\eta X_{s,\xi} + x_\xi X_{s,\eta}] \quad (4.107)$$

$$(4.108)$$

Thus,

$$(-y_\eta J_{s,x} + x_\eta J_{s,y})_{i+1/2} = (JD_s)_{i+1/2} [\gamma X_{s,\xi} - \beta X_{s,\eta}]_{i+1/2} \quad (4.109)$$

$$(y_\xi J_{s,x} - x_\xi J_{s,y})_{j+1/2} = (JD_s)_{j+1/2} [-\beta X_{s,\xi} + \alpha X_{s,\eta}]_{j+1/2} \quad (4.110)$$

The heat flux can be expressed in the same form. For energy flux,

$$\begin{aligned}
 (y_\eta \beta_x - x_\eta \beta_y)_{i+1/2} &= [u (y_\eta \tau_{xx} - x_\eta \tau_{xy})]_{i+1/2} + [v (y_\eta \tau_{xy} - x_\eta \tau_{yy})]_{i+1/2} \\
 &+ (J(\lambda + \lambda_{\text{vib}}))_{i+1/2} [\gamma T_\xi - \beta T_\eta]_{i+1/2} + (J\lambda_e)_{i+1/2} [\gamma T_{e,\xi} - \beta T_{e,\eta}]_{i+1/2} \\
 &+ \sum_{s=1}^{ns} (JD_s)_{i+1/2} [\gamma X_{s,\xi} - \beta X_{s,\eta}]_{i+1/2}
 \end{aligned} \quad (4.111)$$

Similarly,

$$\begin{aligned}
 (-y_\xi \beta_x + x_\xi \beta_y)_{j+1/2} &= [u (-y_\xi \tau_{xx} + x_\xi \tau_{xy})]_{j+1/2} + [v (-y_\xi \tau_{xy} + x_\xi \tau_{yy})]_{j+1/2} \\
 &+ (J(\lambda + \lambda_{\text{vib}}))_{j+1/2} [-\beta T_\xi + \alpha T_\eta]_{j+1/2} + (J\lambda_e)_{j+1/2} [-\beta T_{e,\xi} + \alpha T_{e,\eta}]_{j+1/2} \\
 &+ \sum_{s=1}^{ns} (JD_s)_{j+1/2} [-\beta X_{s,\xi} + \alpha X_{s,\eta}]_{j+1/2}
 \end{aligned} \quad (4.112)$$

The derivatives for computational domain $\partial/\partial\xi$ and $\partial/\partial\eta$ are defined separately for the cell interface $i + 1/2$ and $j + 1/2$, e.g. for u ,

$$(u_\xi)_{i+1/2} = u_{i+1,j} - u_{i,j} \quad (4.113)$$

$$(u_\eta)_{i+1/2} = \frac{1}{2} \left(\frac{u_{i,j+1} - u_{i,j-1}}{2} + \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2} \right) \quad (4.114)$$

$$(u_\xi)_{j+1/2} = \frac{1}{2} \left(\frac{u_{i+1,j} - u_{i-1,j}}{2} + \frac{u_{i+1,j+1} - u_{i-1,j+1}}{2} \right) \quad (4.115)$$

$$(u_\eta)_{j+1/2} = u_{i,j+1} - u_{i,j} \quad (4.116)$$

Finally the cell interface values of the transport coefficients for the viscosity and thermal conductivity are estimated in the following formula:

$$\frac{1}{\mu_{i+1/2}} = \frac{1}{2} \left(\frac{1}{\mu_i} + \frac{1}{\mu_{i+1}} \right), \quad \frac{1}{\lambda_{i+1/2}} = \frac{1}{2} \left(\frac{1}{\lambda_i} + \frac{1}{\lambda_{i+1}} \right) \quad (4.117)$$

$$\frac{1}{\mu_{j+1/2}} = \frac{1}{2} \left(\frac{1}{\mu_j} + \frac{1}{\mu_{j+1}} \right), \quad \frac{1}{\lambda_{j+1/2}} = \frac{1}{2} \left(\frac{1}{\lambda_j} + \frac{1}{\lambda_{j+1}} \right) \quad (4.118)$$

If the coefficient at i or $i + 1$ is zero, the averaged value at $i + 1/2$ must be zero. The above formula prevents evaluating excessive diffusion speed if there exist large gradients [93]. However, this is not recommended for diffusion coefficients. This is because, say, if $(D_s)_i \neq 0$ and $(D_s)_{i+1} = 0$, $(D_s)_{i+1/2}$ becomes zero by definition and the diffusion mechanism would never carry the mass from i to $i + 1$, which is apparently unreasonable from the physical viewpoint. Therefore the cell interface values for each diffusion coefficient are evaluated by the simple arithmetic averaging as

$$(D_s)_{i+1/2} = \frac{(D_s)_i + (D_s)_{i+1}}{2} \quad (4.119)$$

$$(D_s)_{j+1/2} = \frac{(D_s)_j + (D_s)_{j+1}}{2} \quad (4.120)$$

4.5 Time-Integration Scheme

4.5.1 Implicit method

In a time-marching method, we need to update the solution in time and obtain a steady state solution as an asymptotic solution for large time steps. Based on Eq. (4.12), a time-marching scheme can be described in generalized form as

$$\frac{V_{i,j}}{\Delta t} \Delta Q_{i,j} = R_{i,j} \quad (4.121)$$

where $\Delta Q_{i,j} = Q_{i,j}^{n+1} - Q_{i,j}^n$ and the solution is updated as $Q_{i,j}^{n+1} = Q_{i,j}^n + \Delta Q_{i,j}^n$. Further,

$$\begin{aligned} \mathbf{R}_{i,j} = & - \left[2\bar{y} (\tilde{\mathbf{F}} - \tilde{\mathbf{F}}_v) \right]_{i+1/2,j} + \left[2\bar{y} (\tilde{\mathbf{F}} - \tilde{\mathbf{F}}_v) \right]_{i-1/2,j} \\ & - \left[2\bar{y} (\tilde{\mathbf{G}} - \tilde{\mathbf{G}}_v) \right]_{i,j+1/2} + \left[2\bar{y} (\tilde{\mathbf{G}} - \tilde{\mathbf{G}}_v) \right]_{i,j-1/2} - H_{i,j} + (\mathbf{V} \cdot \mathbf{W})_{i,j} \end{aligned} \quad (4.122)$$

is a right-hand residual vector for the control volume (i, j) and should equal zero for steady state problems. Hence a time-marching method can be characterized how we treat the residual term with respect to time. If we evaluate $\mathbf{R}$ for time step n where all properties are already known, we can construct a series of *explicit* scheme. In this case, we can obtain the value of $Q_{i,j}$ at $n+1$ step as $Q_{i,j}^{n+1} = Q_{i,j}^n + \Delta t V_{i,j} \mathbf{R}_{i,j}^n$, so that we require no additional computational operation other than evaluate $\mathbf{R}_{i,j}^n$. In fact, early efforts in the development of temporal discretization methods focused on explicit schemes such as multistage Runge-Kutta schemes combined with convergence acceleration techniques as local time-stepping or implicit residual smoothing method. Every explicit methods has an average that they are easy to implement, vectorize/parallelize, and require only limited memory storage. However, the allowable time increment Δt for an explicit scheme to be performed stable is prohibitively small for more than two-dimensional problems in high-Reynolds number compressible flows, so that the rate of convergence for large-scale problems and especially for the solution of the Navier-Stokes equations is very poor. This trend is more evident for flows that include very low Mach number region but are compressible, as already discussed in Chapter 2, Sec. 3. It should be noted that, in order to obtain the time-evolution solution at a control volume, the explicit scheme uses the information only for its adjacent control volumes, being unable to represent parabolic/elliptic nature of the equation system in which the solution depends upon the entire physical domain.

An alternative approach is to evaluate $\mathbf{R}_{i,j}$ at the time step $n+1$, i.e. $\mathbf{R}_{i,j}^{n+1}$. Since the properties at $n+1$ are not known explicitly, we need to approximately evaluate the value of $\mathbf{R}_{i,j}^{n+1}$ by linearizing it in time.

$$\begin{aligned} \mathbf{R}_{i,j}^{n+1} & \approx \mathbf{R}_{i,j}^n + \Delta t \left(\frac{\partial \mathbf{R}_{i,j}}{\partial t} \right)^n \\ & = \mathbf{R}_{i,j}^n + \Delta t \left(\frac{\partial \mathbf{R}_{i,j}}{\partial Q} \right)^n \left(\frac{\partial Q}{\partial t} \right)^n \\ & = \mathbf{R}_{i,j}^n + \left(\frac{\partial \mathbf{R}_{i,j}}{\partial Q} \right)^n \Delta Q_{i,j}^n \end{aligned} \quad (4.123)$$

The term $\partial \mathbf{R}_{i,j} / \partial Q$ represents symbolically the Jacobian matrix. It involves the linearization of both inviscid and viscous flux vectors. Substituting Eq. (4.123) into

Eq. (4.121), we obtain

$$[\text{L.H.S.}] \Delta Q^n = \frac{\Delta t}{V_{i,j}} R_{i,j}^n \quad (4.124)$$

where

$$\text{L.H.S.} \equiv I - \frac{\Delta t}{V_{i,j}} \cdot \left(\frac{\partial R_{i,j}}{\partial Q} \right)^n \quad (4.125)$$

Hence ΔQ^n can be obtained by inverting the right-hand-side matrix [L.H.S.] in Eq. (4.124), which results in a group of *implicit* schemes. It is apparent that Eq. (4.124) reduces to the standard Newton's method for solving a system of nonlinear equations as Δt tends to infinity. Newton's method is known to have a quadratic convergence property, so that the scheme Eq. (4.124) is expected to converge fast if large Δt is allowed. Note that the Jacobian matrix $\partial R_{i,j} / \partial Q$ (which should be distinguished from $\partial R_{i,j} / \partial Q_{i,j}$) is a matrix of the derivatives of $R_{i,j}$ for Q at each control volume ($1 \leq i \leq imax$, $1 \leq j \leq jmax$), implying that the time-evolution of Q depends on the entire domain and hence representing the parabolic/elliptic nature correctly.

However, two additional difficulties arise for constructing the implicit scheme. First, explicit formulation of the Jacobian matrix resulting from the exact linearization of the second-order numerical flux for both inviscid and viscous terms are extremely complicated to derive and expensive to compute, if not impossible to perform. Second, direct inversion of the L.H.S. matrix is enormously expensive since the Jacobian matrix is composed of $(neqns \times imax \times jmax)^2$ elements. To alleviate these difficulties, we first consider the implication of Eq. (4.124) by rewriting in the following [94]

$$[\text{Numerics}] \Delta Q_{i,j}^n = [\text{Physics}] \quad (4.126)$$

The term on the right-hand-side, [Physics], represents a accurate approximation to the complete governing equations, i.e. the residual vectors evaluated by the second-order numerical flux as discussed in the previous sections. On the other hand, the role of the left-hand-matrix, [Numerics], is just to lead the solution to convergence. Since the left hand side vanishes to zero for steady state problems, the Jacobian matrix itself has nothing to do with accuracy of the solution finally obtained. Therefore, we can reconstruct the left hand side in more liberal way so that the Jacobian matrix is approximated to more convenient form from the computational viewpoint. To what follows, we try to approximate the left hand side for the present equation system containing thermochemical source terms.

4.5.2 Point-implicit procedure

The implicit treatment of the thermochemical source terms is particularly important since these terms introduce an additional stiffness into the equation set causing, the

algorithm to be unstable except for very small Δt . The explicit solution algorithm is widely regarded as unsuitable for the computation of thermochemical nonequilibrium flows. This comes from the fact that the time scale associated with chemistry tends to be very small compared to the time step required for an effective calculation. Hence, $\mathbf{W}_{i,j}$ in Eq. (4.122) is treated implicitly here. The point-implicit method, firstly proposed by Bussing and Murmann [95], eliminates the stiffness problems and allows the solution to be updated with a time step dictated by the CFL condition. In this method, L.H.S. in Eq. (4.125) is approximately factored as

$$\begin{aligned} [L.H.S.] &= I - \frac{\Delta t}{V} \cdot \left(\frac{\partial(\mathbf{R} - \mathbf{W})}{\partial \mathbf{Q}} + \frac{\partial \mathbf{W}}{\partial \mathbf{Q}} \right) \\ &\approx \left(I - \Delta t \widehat{\mathbf{H}} \right) \cdot \left(I - \frac{\Delta t}{V} \cdot \frac{\partial(\mathbf{R} - \mathbf{W})}{\partial \mathbf{Q}} \right) \end{aligned} \quad (4.127)$$

where $\widehat{\mathbf{H}} = \partial \mathbf{W} / \partial \mathbf{Q}$. Since the first factor of Eq. (4.127) is $(neqns \times neqns)$ matrix, it can be inverted directly. In order to relieve strong nonlinearity of $\mathbf{W}$, $\widehat{\mathbf{H}}$ should be evaluated without any approximation. Although quite complicated, this is possible for the present chemical model and described in the Appendix.

4.5.3 LU-SGS method

Modern implicit methods are characterized by how they approximate the L.H.S. and among them, in the present study, we employ the Lower-Upper Symmetric Gauss Seidel (LU-SGS) method since it is robust and efficient. We now describe the practical implementation of the method below.

To begin with, we try to derive the expression of the Jacobian matrix without explicitly differentiating Eq. (4.122) with respect to $\mathbf{Q}$. For convenience we first go back to Eq. (4.12) and rewrite it as

$$\begin{aligned} \frac{V_{i,j}}{\Delta t} \Delta \mathbf{Q}^n + \left[2\bar{y} \left(\tilde{\mathbf{F}} - \tilde{\mathbf{F}}_v \right) \right]_{i+1/2}^{n+1} - \left[2\bar{y} \left(\tilde{\mathbf{F}} - \tilde{\mathbf{F}}_v \right) \right]_{i-1/2}^{n+1} \\ + \left[2\bar{y} \left(\tilde{\mathbf{G}} - \tilde{\mathbf{G}}_v \right) \right]_{j+1/2}^{n+1} - \left[2\bar{y} \left(\tilde{\mathbf{G}} - \tilde{\mathbf{G}}_v \right) \right]_{j-1/2}^{n+1} + \mathbf{H}_{i,j}^{n+1} = (\mathbf{V} \cdot \mathbf{W})_{i,j}^{n+1} \end{aligned} \quad (4.128)$$

Linearizing this in time and taking consistency with Eq. (4.127), we obtain

$$\begin{aligned} &\left(I - \Delta t \widehat{\mathbf{H}}_{i,j} \right) \\ &\times \left[I + \frac{\Delta t}{V_{i,j}} \left(\left[2\bar{y} \left(\tilde{\mathbf{A}} - \tilde{\mathbf{A}}_v \right) \right]_{i+1/2}^n - \left[2\bar{y} \left(\tilde{\mathbf{A}} - \tilde{\mathbf{A}}_v \right) \right]_{i-1/2}^n \right. \right. \\ &\quad \left. \left. + \left[2\bar{y} \left(\tilde{\mathbf{B}} - \tilde{\mathbf{B}}_v \right) \right]_{j+1/2}^n - \left[2\bar{y} \left(\tilde{\mathbf{B}} - \tilde{\mathbf{B}}_v \right) \right]_{j-1/2}^n \right) \right] \Delta \mathbf{Q}^n = \frac{\Delta t}{V_{i,j}} \mathbf{R}_{i,j}^n \end{aligned} \quad (4.129)$$

R is given in Eq. (4.122). And,

$$\tilde{A} = \frac{\partial \tilde{F}}{\partial Q} = y_\eta A - x_\eta B \quad (4.130)$$

$$\tilde{A}_v = \frac{\partial \tilde{F}_v}{\partial Q} = y_\eta A_v - x_\eta B_v \quad (4.131)$$

$$\tilde{B} = \frac{\partial \tilde{G}}{\partial Q} = -y_\xi A + x_\xi B \quad (4.132)$$

$$\tilde{B}_v = \frac{\partial \tilde{G}_v}{\partial Q} = -y_\xi A_v + x_\xi B_v \quad (4.133)$$

$$\hat{H} = \frac{\partial W}{\partial Q} \quad (4.134)$$

where A , B , A_v , and B_v are the Jacobian matrices in Cartesian coordinates. The contribution of $H_{i,j}$ is neglected in Eq. (4.129) because this is relatively minor.

The cell-interface values of inviscid terms A and B are evaluated by applying the first-order FVS scheme as

$$(A)_{i+1/2} = (A)_i^+ + (A)_{i+1}^- \quad (4.135)$$

$$(A)_{i-1/2} = (A)_i^- + (A)_{i-1}^+ \quad (4.136)$$

$$(B)_{j+1/2} = (B)_j^+ + (B)_{j+1}^- \quad (4.137)$$

$$(B)_{j-1/2} = (B)_j^- + (B)_{j-1}^+ \quad (4.138)$$

where A and B are split into $A^\pm$ and $B^\pm$ according to the signs of their eigen values. In Ref. [96], Jameson and Yoon proposed an approximate formula of evaluating $A^\pm$ and $B^\pm$ as

$$X^\pm = \frac{1}{2}[X \pm \beta \sigma(X)I] \quad (4.139)$$

where X is A or B , $\sigma(X)$ is the spectral radius of X , which is given by

$$\sigma(X) = \max_i [|\lambda_i|] \quad (4.140)$$

λ represents eigenvalues of X , and β is a constant that is larger than unity. Stability and convergence can be controlled by adjusting β either manually or automatically. In the present study, $\beta = 1.1$ is set throughout the computation. The actual expressions of $\tilde{A}$ and $\tilde{B}$ are described in the appendix.

In turn, since the elements of the viscous flux F_v and G_v contain space derivatives $\partial/\partial x^j$ for primitive variables, evaluation of the Jacobian matrices A_v and B_v is somewhat cumbersome. For convenience, we express the viscous flux F_v and G_v in the following form

$$A_v = \left[\frac{\partial F_v}{\partial Q} - \frac{\partial}{\partial x^j} \left(\frac{\partial F_v}{\partial Q_{x^j}} \right) \right] + \frac{\partial}{\partial x^j} \left(\frac{\partial F_v}{\partial Q_{x^j}} \right) \quad (4.141)$$

$$B_v = \left[\frac{\partial G_v}{\partial Q} - \frac{\partial}{\partial x^j} \left(\frac{\partial G_v}{\partial Q_{x^j}} \right) \right] + \frac{\partial}{\partial x^j} \left(\frac{\partial G_v}{\partial Q_{x^j}} \right) \quad (4.142)$$

The subscript x^j denotes the space derivative with respect to j -components. In the above equations, the first terms of the right hand side include only the secondary terms associated with derivatives for transport properties or metrics and is thus expected to be comparatively small. On the other hand, although we can explicitly express the second terms in an analytical form, they are still complicated and then replaced by a diagonal matrix with the spectral radius of $\partial F_v / \partial Q_{x^j}$ or $\partial G_v / \partial Q_{x^j}$ [97], i.e.

$$A_v \approx \frac{\partial}{\partial x^j} \left(\frac{\partial F_v}{\partial Q_{x^j}} \right) \approx \frac{\partial P}{\partial x} \quad (4.143)$$

$$B_v \approx \frac{\partial}{\partial x^j} \left(\frac{\partial G_v}{\partial Q_{x^j}} \right) \approx \frac{\partial P}{\partial y} \quad (4.144)$$

$$P = \frac{2\mu}{\rho} I \quad (4.145)$$

Hence the viscous Jacobian matrices become

$$\tilde{A}_v \approx y_\eta P_x - x_\eta P_y \quad (4.146)$$

$$\tilde{B}_v \approx -y_\xi P_x + x_\xi P_y \quad (4.147)$$

The space derivatives P_x and P_y can be discretized in the same procedure as used in Section 4 with omitting the cross-derivative terms for simplicity, which results in,

$$(\tilde{A}_v)_{i+1/2} = (J\gamma P_\xi)_{i+1/2} = (J\gamma)_{i+1/2} (P_{i+1,j} - P_{i,j}) \quad (4.148)$$

$$(\tilde{B}_v)_{j+1/2} = (J\alpha P_\eta)_{j+1/2} = (J\alpha)_{j+1/2} (P_{i,j+1} - P_{i,j}) \quad (4.149)$$

Substituting Eqs. (4.130) to (4.139) into Eq. (4.129) and further simplifying, we finally obtain

$$(I - \Delta t \widehat{H}_{i,j}) (D + L + U) \Delta Q^n = R_{i,j}^n \quad (4.150)$$

where

$$\begin{aligned} D &= I + \frac{\Delta t}{V_{i,j}} \left[\frac{\bar{y}_{i+1/2} + \bar{y}_{i-1/2}}{2} \{ \sigma(A_{i,j}) + 2(J\gamma P)_{i,j} \} \right. \\ &\quad \left. + \frac{\bar{y}_{j+1/2} + \bar{y}_{j-1/2}}{2} \{ \sigma(B_{i,j}) + 2(J\alpha P)_{i,j} \} \right] \\ L &= -\Delta t \left[\bar{y}_{i-1/2} (\tilde{A}^+ + J\gamma P)_{i-1,j} + \bar{y}_{j-1/2} (\tilde{B}^+ + J\alpha P)_{i,j-1} \right] \\ U &= \Delta t \left[\bar{y}_{i+1/2} (\tilde{A}^- - J\gamma P)_{i+1,j} + \bar{y}_{j+1/2} (\tilde{B}^+ - J\alpha P)_{i,j+1} \right] \end{aligned} \quad (4.151)$$

ALGORITHM 4.2: Point implicit + LU-SGS procedure

Solve $(I - \Delta t \widehat{H})(D + L)D^{-1}(D + U)\Delta Q^n = R^n$.

1. Point implicit: $(I - \Delta t \widehat{H})\Delta Q^{(1)} = R$
 For $i = 2, imax - 1$, step = 1, do:
 For $j = 2, jmax - 1$, step = 1, do:

$$\Delta Q_{i,j}^{(1)} = (I - \Delta t \widehat{H}_{i,j})^{-1} R_{i,j}^n$$

 EndDo
2. Lower sweep: $(D + L)\Delta Q^{(2)} = Q^{(1)}$
 For $i = 2, imax - 1$, step = 1, do:
 For $j = 2, jmax - 1$, step = 1, do:

$$\Delta Q_{i,j}^{(2)} = D_{i,j}^{-1} (\Delta Q_{i,j}^{(1)} - L\Delta Q_{i-1,j}^{(2)} - L\Delta Q_{i,j-1}^{(2)})$$

 EndDo
3. Upper sweep: $(D + U)\Delta Q^n = DQ^{(2)}$
 For $i = imax - 1, 2$, step = -1, do:
 For $j = jmax - 1, 2$, step = -1, do:

$$\Delta Q_{i,j}^n = \Delta Q_{i,j}^{(2)} - D_{i,j}^{-1} (U\Delta Q_{i+1,j}^{(2)} + U\Delta Q_{i,j+1}^{(2)})$$

 EndDo

The matrices D , L , and U represent the diagonal, strict lower, and strict upper matrix, respectively. In the LU-SGS scheme, the second factor of Eq. (4.150) is approximately factored as

$$(D + L + U) \approx (D + L)D^{-1}(D + U) \quad (4.152)$$

Finally the resulting equation can be solved as illustrated in ALGORITHM 4.2. Note that D reduces to a scalar diagonal matrix, so that no matrix inversion is required to obtain $\Delta Q^{(2)}$ or ΔQ^n in Steps 2 and 3 of ALGORITHM 4.2, reducing a great amount of operating time. In the present algorithm, all boundary conditions are treated explicitly and hence ΔQ are set to zero for each boundary point. Although the original LU-SGS algorithm takes the sweep direction as $i + j = \text{const.}$ oblique lines, conventional sweep procedure shown in ALGORITHM 4.2 is employed. This is simple to implement and do not degrade the convergence property of the algorithm as far as vector processor is not utilized.

It is also possible to implement the LU-SGS algorithm without separating W from the inviscid/viscous Jacobian matrix [98]. This approach, however, may cause numerical instability since the inversion of $\widehat{H}$ must include the factorization error coming from the approximation of $(D + L + U)$. If one employs the point implicit

procedure, inherent numerical error associated with the matrix inversion is of the order of round-off error at most. This difference is critical for cases where chemical source terms becomes extremely stiff.

4.6 Electron Energy Equation Solver

Assuming thermal nonequilibrium flow, we must solve the electron energy equation to obtain the electron energy distribution. Unfortunately, the equation system becomes extremely stiff when the electron energy is coupled with the flow field equations. This is because of the following:

1. Electron thermal conductivity becomes very large for highly ionized plasma, sometimes scales as $T_e^{5/2}$.
2. The energy exchange rate between the electron and vibrational mode and the energy loss rate due to electron impact dissociation/ionization [48] tend to be extremely stiff.
3. Since T_e is evaluated from the electron energy defined as $E_e = 3/2\rho_e R_e T_e$, it tends to fluctuate severely: both E_e and ρ_e are normally very small compared to other flow properties, and they are liable to be suffered from numerical error.

To remedy them, we uncouple the electron energy equation from other flow field equations and solve with respect to the electron temperature. This is in spirit the same idea as [99] where they iteratively solved the electron energy equation in steady form. In the present algorithm, instead of obtaining a converged solution at each time step, we rewrite the equation in delta form. In this case, we do not need to obtain converged solutions of T_e for each time step, but need to obtain updating value ΔT_e required for global convergence of the flow field equations. The residual vector for the electron energy equation $\mathbf{R}_e$ is linearized with respect to T_e , which results in

$$\mathbf{A}\Delta T_e = \mathbf{R}_e \quad (4.153)$$

where $\mathbf{A}$ is the Jacobian matrix defined as $\mathbf{A} = \partial \mathbf{R}_e / \partial T_e$. We derive the actual expression of $\mathbf{R}_e$ and $\mathbf{A}$ for completeness.

$$\begin{aligned} (R_e)_{i,j} = & - \left[2\bar{y} (\tilde{F}_e - \tilde{F}_{e,v}) \right]_{i+1/2} + \left[2\bar{y} (\tilde{F}_e - \tilde{F}_{e,v}) \right]_{i-1/2} \\ & - \left[2\bar{y} (\tilde{G}_e - \tilde{G}_{e,v}) \right]_{j+1/2} + \left[2\bar{y} (\tilde{G}_e - \tilde{G}_{e,v}) \right]_{j-1/2} \\ & + \left[V \cdot \left(-p_e \frac{\partial u_j}{\partial x_j} + Q_{T-e} + Q_{R-e} - Q_{e-v} + Q_D^e + Q_I^e + j_l E_l \right) \right]_{i,j} \end{aligned} \quad (4.154)$$

Instead of directly differentiating Eqs. (4.68) and (4.72) with respect to T_e , we simply evaluate the convective contribution of $\mathbf{A}$ as an first-order upwind manner as

$$\begin{aligned} (A\Delta T_e)_{i,j}^{\text{conv}} = & (A_e^+ \Delta T_e)_{i,j} - (A_e^+ \Delta T_e)_{i-1,j} + (A_e^- \Delta T_e)_{i+1,j} - (A_e^- \Delta T_e)_{i,j} \\ & + (B_e^+ \Delta T_e)_{i,j} - (B_e^+ \Delta T_e)_{i,j-1} + (B_e^- \Delta T_e)_{i,j+1} - (B_e^- \Delta T_e)_{i,j} \end{aligned} \quad (4.155)$$

where

$$A_e^\pm = \frac{3}{2} \rho_e R_e V \frac{U' \pm |U'|}{2}, \quad B_e^\pm = \frac{3}{2} \rho_e R_e V \frac{V' \pm |V'|}{2} \quad (4.156)$$

$$U' = \xi_x u + \xi_y v, \quad V' = \eta_x u + \eta_y v \quad (4.157)$$

In turn, we evaluate the viscous contribution of $\mathbf{A}$ by differentiating the discretized form of the electron energy flux with omitting the cross-derivative contributions, which results in

$$\begin{aligned} (A\Delta T_e)_{i,j}^{\text{vis}} = & -\bar{A}_{i+1/2}^\xi (\Delta T_{e,i+1,j} - \Delta T_{e,i,j}) + \bar{A}_{i-1/2}^\xi (\Delta T_{e,i,j} - \Delta T_{e,i-1,j}) \\ & -\bar{A}_{j+1/2}^\eta (\Delta T_{e,i,j+1} - \Delta T_{e,i,j}) + \bar{A}_{j-1/2}^\eta (\Delta T_{e,i,j} - \Delta T_{e,i,j-1}) \end{aligned} \quad (4.158)$$

where

$$\bar{A}^\xi = 2\bar{\gamma} J \lambda_e \gamma, \quad \bar{A}^\eta = 2\bar{\gamma} J \lambda_e \alpha \quad (4.159)$$

The terms associated with the diffusion are omitted from the above equation for simplicity. The source terms are rigorously differentiated for T_e and we obtain

$$(A\Delta T_e)_{i,j}^{\text{source}} = A_{i,j}^{\text{source}} \Delta T_{e,i,j} \quad (4.160)$$

where

$$\begin{aligned} A_{i,j}^{\text{source}} = & \rho_e R_e \frac{\partial u_j}{\partial x_j} + \frac{Q_{T-e} + Q_{R-e}}{T - T_e} - 3\rho_e (T - T_e) \sum_s (1 + g_{\text{rot},s}) R_s \frac{\partial \nu_{e,s}}{\partial T_e} \\ & + \frac{1}{\tau_{N_2,e}} \left(\rho_{N_2} C_{\text{vib},N_2}^{\text{eq}} - Q_{e-v} \frac{\partial \tau_{N_2,e}}{\partial T_e} \right) - E_{D,N_2} \frac{\partial \dot{w}_{N_2}^e}{\partial T_e} - E_{I,N} \frac{\partial \dot{w}_N^e}{\partial T_e} \end{aligned} \quad (4.161)$$

The electron temperature derivatives of $\nu_{e,s}$, $\tau_{N_2,e}$, $\dot{w}_{N_2}^e$, and $\dot{w}_N^e$ can be obtained by differentiating Eqs. (3.140), (3.146), (3.149), and (3.150), respectively.

For the same reason discussed in the preceding section, we do not need to invert $\mathbf{A}$ exactly and hence Eq. (4.153) is solved approximately at each time step by using

the standard line relaxation method. Combining Eqs. (4.155) to (4.161), we rewrite Eq. (4.154) for (i, j) as

$$A\Delta T_{e,i,j-1} + B\Delta T_{e,i,j} + C\Delta T_{e,i,j+1} = R_{e,i,j} - D\Delta T_{e,i-1,j} - E\Delta T_{e,i+1,j} \quad (4.162)$$

where

$$\begin{aligned} A &= -B_{i,j-1}^+ - \bar{A}_{j-1/2}^\eta \\ B &= A_{i,j}^+ - A_{i,j}^- + B_{i,j}^+ - B_{i,j}^- + \bar{A}_{i+1/2}^\xi + \bar{A}_{i-1/2}^\xi + \bar{A}_{j+1/2}^\eta + \bar{A}_{j-1/2}^\eta + A_{i,j}^{\text{source}} \\ C &= B_{i,j+1}^+ - \bar{A}_{j+1/2}^\eta \\ D &= -A_{i-1,j}^+ - \bar{A}_{i-1/2}^\xi \\ E &= A_{i+1,j}^- - \bar{A}_{i+1/2}^\xi \end{aligned}$$

Note that the time derivative term is not included in Eq. (4.162). Equation (4.162) consists a scalar tridiagonal system of equations and hence can readily be solved implicitly in the j -direction for ΔT_e by using the Thomas algorithm [92].

The line relaxation methods can further be subdivided into Gauss-Seidel (GS) and non-Gauss-Seidel (NGS) methods [100]. For the GS methods, $\Delta T_{e,i-1,j}$ and $\Delta T_{e,i+1,j}$ in the right hand side of Eq. (4.162) are evaluated using the latest available values. This is preferable if exact solutions of Eq. (4.162) are required since changes in the solution propagates quickly, but the equation must be solved iteratively. In contrast, $\Delta T_{e,i-1,j}$ and $\Delta T_{e,i+1,j}$ in NGS methods are computed using previous time step values even if values of the current level are available for some lines. We employ this approach because only approximate solutions of Eq. (4.162) are required, and further set as $\Delta T_{e,i-1,j} = \Delta T_{e,i+1,j} = 0$. Many practical computational works have verified that this approximation does not affect the final results [101]. In this case, only one iteration is required to obtain ΔT_e for all points and thus very efficient.

Furthermore, to prevent excessive variation of T_e , ΔT_e is limited by the following:

$$\Delta T_e = \text{sgn}(\Delta T_e) \cdot \min[|\Delta T_e|, |\Delta T_e|_{\min}] \quad (4.163)$$

where $|\Delta T_e|_{\min} = 100$ K is found to work well.

As for boundary conditions, zero electron temperature gradient is imposed for all boundaries including the electrode wall, i.e.

$$\frac{\partial T_e}{\partial n} = 0 \quad (4.164)$$

This condition is simply implemented as $(T_e)_{i,1} = (T_e)_{i,2}$ at the cathode wall for example.

To initiate the calculation, we firstly solve the flow field assuming thermal equilibrium (one temperature calculation), then the converged solution is used as an initial condition for the two temperature calculation.

4.7 Electric Field Solver

4.7.1 Basic discretization

As for the electric field, we need to obtain a converged solution of Eq. (3.157) per time step of the flow field computation to evaluate the Ohmic heating term in the energy conservation equation of Eq. (3.153) or Eq. (3.155). Since this term plays a critical role to determine flow structure including the arc column, Eq. (3.157) must be solved with good accuracy. Adding this, it is not the electric potential ϕ itself but the space derivatives of ϕ (which is more sensitive to accuracy of the solution) that determines the Ohmic heating. If we evaluate this term by the electric potential distribution with poor accuracy, it tends to fluctuate severely and the flow field equation will never converge. Hence developing an efficient electric field solver for faster convergence is crucial.

Since Eq. (3.41) represents the conservation law with respect to the electrical density j , we can apply the finite volume approach described in Section 2, that is,

$$\begin{aligned} & [2\bar{y}(y_\eta j_x - x_\eta j_y)]_{i+1/2} - [2\bar{y}(y_\eta j_x - x_\eta j_y)]_{i-1/2} \\ & + [2\bar{y}(-y_\xi j_x + x_\xi j_y)]_{j+1/2} - [2\bar{y}(-y_\xi j_x + x_\xi j_y)]_{j-1/2} = 0 \end{aligned} \quad (4.165)$$

Considering that the above equation is elliptic in nature, we evaluate j_x and j_y in a central difference form as

$$\begin{aligned} j_x &= \sigma \left(-\phi_x + \frac{1}{en_e} p_{e,x} \right) \\ &= \sigma \left[-(\xi_x \phi_\xi + \eta_x \phi_\eta) + \frac{1}{en_e} (\xi_x p_{e,\xi} + \eta_x p_{e,\eta}) \right] \\ &= J\sigma \left[-(y_\eta \phi_\xi - y_\xi \phi_\eta) + \frac{1}{en_e} (y_\eta p_{e,\xi} - y_\xi p_{e,\eta}) \right] \end{aligned} \quad (4.166)$$

$$\begin{aligned} j_y &= \sigma \left(-\phi_y + \frac{1}{en_e} p_{e,y} \right) \\ &= \sigma \left[-(\xi_y \phi_\xi + \eta_y \phi_\eta) + \frac{1}{en_e} (\xi_y p_{e,\xi} + \eta_y p_{e,\eta}) \right] \\ &= J\sigma \left[-(-x_\eta \phi_\xi + x_\xi \phi_\eta) + \frac{1}{en_e} (-x_\eta p_{e,\xi} + x_\xi p_{e,\eta}) \right] \end{aligned} \quad (4.167)$$

From Eqs. (4.165) to (4.167), we have

$$\begin{aligned} & [\bar{A}(-\gamma \phi_\xi + \beta \phi_\eta)]_{i+1/2} - [\bar{A}(-\gamma \phi_\xi + \beta \phi_\eta)]_{i-1/2} \\ & + [\bar{A}(\beta \phi_\xi - \alpha \phi_\eta)]_{j+1/2} - [\bar{A}(\beta \phi_\xi - \alpha \phi_\eta)]_{j-1/2} = F_{i,j} \end{aligned} \quad (4.168)$$

where $\bar{A} = 2\bar{y}J\sigma$, and

$$(\phi_\xi)_{i+1/2} = \phi_{i+1,j} - \phi_{i,j} \quad (4.169)$$

$$(\phi_\eta)_{i+1/2} = \frac{1}{2} \left(\frac{\phi_{i,j+1} - \phi_{i,j-1}}{2} + \frac{\phi_{i+1,j+1} - \phi_{i+1,j-1}}{2} \right) \quad (4.170)$$

$$(\phi_\xi)_{j+1/2} = \frac{1}{2} \left(\frac{\phi_{i+1,j} - \phi_{i-1,j}}{2} + \frac{\phi_{i+1,j+1} - \phi_{i-1,j+1}}{2} \right) \quad (4.171)$$

$$(\phi_\eta)_{j+1/2} = \phi_{i,j+1} - \phi_{i,j} \quad (4.172)$$

The metrics terms J , α , β , γ , and the cell-interface values of σ are evaluated in the same way as the viscous terms. $F_{i,j}$ represents the term associated with the electron pressure gradient

$$\begin{aligned} F_{i,j} = & - \left[\frac{\bar{A}}{en_e} (\gamma p_{e,\xi} - \beta p_{e,\eta}) \right]_{i+1/2} + \left[\frac{\bar{A}}{en_e} (\gamma p_{e,\xi} - \beta p_{e,\eta}) \right]_{j+1/2} \\ & - \left[\frac{\bar{A}}{en_e} (-\beta p_{e,\xi} + \alpha p_{e,\eta}) \right]_{j+1/2} + \left[\frac{\bar{A}}{en_e} (-\beta p_{e,\xi} + \alpha p_{e,\eta}) \right]_{j-1/2} \end{aligned} \quad (4.173)$$

and is treated as a constant in the present solver. $p_{e,\xi}$ and $p_{e,\eta}$ are discretized in the same fashion as ϕ_ξ and ϕ_η .

Finally the total current I can be evaluated by the following formula

$$\begin{aligned} I &= \sum_{j=1}^{jmax-1} I_j / (jmax - 1) \\ I_j &= \sum_{i=2}^{imax-1} |2\pi\bar{y}(-y_\xi j_x + x_\xi j_y)|_{i,j+1/2} \\ &= \pi \sum_{i=2}^{imax-1} \left| \bar{A} \left[\beta\phi_\xi - \alpha\phi_\eta + \frac{1}{en_e} (-\beta p_{e,\xi} + \alpha p_{e,\eta}) \right] \right|_{i,j+1/2} \end{aligned} \quad (4.174)$$

4.7.2 GMRES method

Equation (4.168) results in a linear system of the equations with respect to ϕ of the form

$$\mathbf{A}\phi = \mathbf{F} \quad (4.175)$$

where $\mathbf{A}$ is the $(imax \times jmax)^2$ coefficient matrix, ϕ and $\mathbf{F}$ are the $(imax \times jmax)$ vectors whose component are $\phi_{i,j}$ and $F_{i,j}$, respectively. The (i, j) component of the product $\mathbf{A}\phi$ is equivalent to the left hand side of Eq. (4.168). As opposed to the flow field solver, we need to invert $\mathbf{A}$ *exactly* to obtain the solution of Eq. (4.165), but the direct inversion is enormously expensive. Hence one commonly uses a series

of relaxation scheme such as Gauss-Seidel, SLOR (Successive Line OverRelaxation), or ILU (Incomplete LU factorization) method. These algorithms solve Eq. (4.175) iteratively. Unfortunately, a significant number of iteration is required to obtain converged solutions, especially if severe convergence criterion is imposed. Since Eq. (4.175) must be solved at each time step of the flow field computation, an efficient algorithm is required.

In this study, $\mathbf{A}$ is inverted by the Generalized Minimal RESidual (GMRES) method of Saad and Schultz [102]. This is a generalization of the conjugate gradient method for solving a linear system where the coefficient matrix is not symmetric and/or positive definite. The use of GMRES combined with preconditioning techniques is becoming widespread in many fields. We describe the basic procedure of the algorithm below.

First, we set initial guess of the solution vector as ϕ_0 , then the first search direction becomes

$$\mathbf{v}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\| \quad (4.176)$$

where $\mathbf{r}_0 = \mathbf{F} - \mathbf{A}\phi_0$ is the initial residual. We now find an approximate solution of Eq. (4.175) as

$$\phi = \phi_0 + \sum_{k=1}^m a_k \mathbf{v}_k \quad (4.177)$$

In Eq. (4.177), vectors $\mathbf{v}_k$ constitute a basis for the m -dimensional Krylov subspace

$$K_m = \text{span}[\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^{m-1}\mathbf{r}_0] \quad (4.178)$$

and coefficients a_k are chosen so as to minimize the residual norm

$$J = \|\mathbf{F} - \mathbf{A}\phi\| = \|\mathbf{r}_0 - \mathbf{A}\mathbf{z}\| \quad (4.179)$$

where $\mathbf{z} = \sum_{k=1}^m a_k \mathbf{v}_k$. Once the first search direction is specified, m -orthonormal basis vectors $\mathbf{v}_k$ can be recursively generated through the Arnoldi process [102]. Set $h_{i,j}$ as

$$h_{i,j} = (\mathbf{A}\mathbf{v}_j, \mathbf{v}_i) \quad (4.180)$$

then the next search direction $\mathbf{v}_{j+1}$ can be obtained through the Gram-Schmidt's orthogonalization procedure as

$$\hat{\mathbf{v}}_{j+1} = \mathbf{A}\mathbf{v}_j - \sum_{i=1}^j h_{i,j} \mathbf{v}_i \quad (4.181)$$

Further setting

$$h_{j+1,j} = \|\hat{\mathbf{v}}_{j+1}\| \quad (4.182)$$

ALGORITHM 4.3: Preconditioned GMRES method

$r_0 = F - A\phi_0$	initial residual
$v_1 = r_0 / \ r_0\ $	define initial Krylov
For $j = 1, 2, \dots, m, \dots$ until satisfied do:	
$x_j = P^{-1}v_j$	preconditioning
$w_j = Ax_j$	matrix-vector product
For $i = 1, j$ do:	
$h_{i,j} = (w_j, v_i)$	set Hessenberg matrix
EndDo	
$\hat{v}_{j+1} = w_j - \sum_{i=1}^j h_{i,j}v_i$	Gram-Schmidt step
$h_{j+1,j} = \ \hat{v}_{j+1}\ $	
$v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$	define Krylov vector
$a = \min \ \beta e_1 - H_m a\ $	least squares solve
if $\ F - A\phi\ < \epsilon$ exit	convergence check
EndDo	
$z = \sum_{i=1}^m a_i v_i$	
$\Delta\phi = P^{-1}z$	preconditioning
$\phi = \phi_0 + \Delta\phi$	find solution

we obtain v_{j+1} as $v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$. Next we want to solve the least squares problem of Eq. (4.179). It is easily verified that Eq. (4.179) is equivalent to

$$J(a) = \|\beta e_1 - H_m a\| \quad (4.183)$$

Here, $\beta = \|r_0\|$ and the vector e_1 is the first column of the $(m+1) \times (m+1)$ identity matrix. H_m is the upper $(m+1) \times m$ Hessenberg matrix whose entries are $h_{i,j}$. Minimization of Eq. (4.183) with respect to a is a well known least squares problem and can be readily solved through QR algorithm.

In case the residual norm Eq. (4.183) does not drop to a tolerable value, we set $m \rightarrow m+1$ and seek the additional search direction through the Arnoldi process described above.

GMRES works best when the eigenvalues of matrix A is clustered. To realize this we apply the preconditioning technique. For reasons described in [103], we choose the right preconditioning of the form

$$(AP^{-1})(P\phi) = F \quad (4.184)$$

The preconditioning matrix P is an approximation of A and clusters the eigenvectors of A around unity. It is worth noting that the only information we need for P is the products $a = P^{-1}b$ and this corresponds to that we solve $Aa = b$ approximately. Hence we can consider a number of relaxation schemes as a preconditioner and we applied the Gauss-Seidel line relaxation algorithm here.

The overall algorithm is summarized in ALGORITHM 4.3. For the practical implementation, it is confirmed that the matrix-vector product $\mathbf{A}\mathbf{v}$ can be evaluated at each point (i, j) by Eq. (4.168) with ϕ being $\mathbf{v}$. The L2-norm $\|\mathbf{r}\|$ is evaluated as

$$\|\mathbf{r}\|^2 = \sum_{i=1}^{imax} \sum_{j=1}^{jmax} r_{i,j}^2 \quad (4.185)$$

The detail of QR algorithm to solve the least squares problem Eq. (4.183) is found in Ref. [102]. Finally, the actual formulation of the preconditioning step $\mathbf{a} = \mathbf{P}^{-1}\mathbf{b}$ can be described as follows:

$$Aa_{i,j-1} + Ba_{i,j} + Ca_{i,j+1} = D \quad (4.186)$$

where

$$\begin{aligned} A &= -(\bar{A}\gamma)_{j-1/2} \\ B &= (\bar{A}\alpha)_{i+1/2} + (\bar{A}\alpha)_{i-1/2} + (\bar{A}\gamma)_{j+1/2} + (\bar{A}\gamma)_{j-1/2} \\ C &= -(\bar{A}\gamma)_{j+1/2} \\ D &= b_{i,j} + (\bar{A}\alpha)_{i-1/2}a_{i-1,j} + (\bar{A}\alpha)_{i+1/2}a_{i+1,j} \\ &\quad + (\bar{A}\beta)_{i-1/2}(a_{i,j+1} - a_{i,j-1} + a_{i-1,j+1} - a_{i-1,j-1})/4 \\ &\quad - (\bar{A}\beta)_{i+1/2}(a_{i,j+1} - a_{i,j-1} + a_{i+1,j+1} - a_{i+1,j-1})/4 \\ &\quad + (\bar{A}\beta)_{j-1/2}(a_{i+1,j} - a_{i-1,j} + a_{i+1,j-1} - a_{i-1,j-1})/4 \\ &\quad - (\bar{A}\beta)_{j+1/2}(a_{i+1,j} - a_{i-1,j} + a_{i+1,j+1} - a_{i-1,j+1})/4 \end{aligned}$$

The tridiagonal equation system Eq. (4.186) can be solved for $a_{i,j}$ by the standard Thomas algorithm.

Shown in Fig. 4.4 is the comparison of the present GMRES + Gauss-Seidel algorithm and the conventional Gauss-Seidel line relaxation method applied to the present electric field equation. The use of GMRES technique dramatically reduce the computational time. It has been shown that the residual is dropped to 10^{-5} with only 9 search directions or less.

It is also possible to apply GMRES in Eq. (4.150) to solve the flow field equations. However, this is less efficient since the time increment Δt is inevitably limited to small due to the strong nonlinearity of the thermochemical source term. The application of GMRES becomes advantageous only if the additional computational cost is compensated for by a reduction of the error associated with the approximate factorization for the LU-SGS scheme. In the case Δt is sufficiently small, the approximate factorization works well since the error is basically rounded of the order of $(\Delta t)^2$. Hence the advantage of GMRES will be lost.

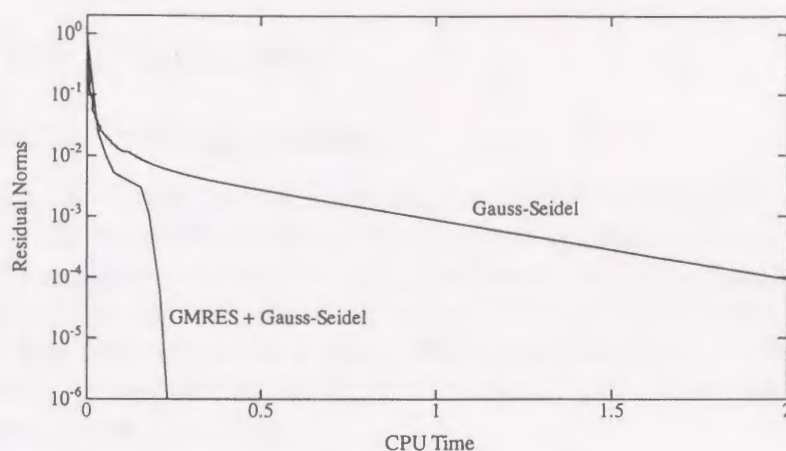


Figure 4.4: Comparison of residual histories using the preconditioned GMRES and Gauss-Seidel algorithms

4.7.3 Electric field boundary conditions

As for the boundary conditions on the electric field, no currents are allowed to pass through the inlet and the nozzle exit. This condition is implemented in the electric field solver so as to rigorously conserve the total current inside the computational domain,

$$[2\bar{y}(y_{\eta}j_x - x_{\eta}j_y)]_{i,j+1/2} = 0 \quad (4.187)$$

hence,

$$\left[\beta\phi_{\xi} - \alpha\phi_{\eta} + \frac{1}{en_e}(-\beta p_{e,\xi} + \alpha p_{e,\eta}) \right]_{i,j+1/2} = 0 \quad (4.188)$$

where $i = 1$ for the inlet and $i = imax$ for the nozzle exit. To treat the boundary conditions implicitly, Eq. (4.188) is included in the linear system of equation Eq. (4.175) and solved simultaneously with the electric field equation itself.

Mirror-condition is applied at the axisymmetric line, i.e. $\phi_{i,1} = \phi_{i,2}$.

Both anode and cathode are assumed to be at equi-potential, so that

$$\phi = \begin{cases} V & \text{(on the anode surface)} \\ 0 & \text{(on the cathode surface)} \end{cases} \quad (4.189)$$

and V can be evaluated from the total current.