Boundary-Layer Solvers for Binary Gases and a Five Species Air Model

by

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Table of Contents

List of Figures **7**

Abstract **10**

Nomenclature **11**

Nomenclature **11**

1. Introduction **13**

2. Equilibrium Properties of O2+O,N2+N, and Air **18**

3. Non-Equilibrium Gas Mixtures **21**

4. Boundary Layer Equations for Reacting Gases **24**

5. Numerical Method Description **28**

6. Results **33**

6.1 Binary Mixture 34

6.2 Five Species Air Model 44

6.2.1 Comparison with Binary Mixture of Oxygen 45

6.2.2 Comparison with Binary Mixture of Nitrogen 49

6.2.3 Tests for Five Species Air Model 53

7. Conclusion and Future Work **61**

References **62**

Appendix A Numerical Formulation **67**

Table of Contents—*Continued*

Appendix B The Iterative Algorithm for the Discretized Equations 85

Appendix C Block Elimination Method 140

List of Figures

6.1 $T_e = 2000$ K, $P_e = 0.01$ atm, $u_e = 4.273$ km/s, non-catalytic and adiabatic wall . . . 33

6.2 $T_e = 2000$ K, $P_e = 0.01$ atm, $u_e = 4.273$ km/s, non-catalytic and adiabatic wall . . . 34

6.3 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, $c_{wO}/c_{eO} = 0.3$ and $I_w/I_e = 0.8$ 35

6.4 $T_e = 3000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, $c_{wO}/c_{eO} = 0.3$ and $I_w/I_e = 0.8$. 36

6.5 $T_e = 300$ K, $P_e = 1$ atm, $u_e = 0.6607$ km/s, equilibrium wall and $(dI/dy)_w = 0$ . . . 37

6.6 $T_e = 300$ K, $P_e = 1$ atm, $u_e = 0.6607$ km/s, equilibrium wall and $(dI/dy)_w = 0$ . . . 37

6.7 $T_e = 3000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$ 38

6.8 $T_e = 5000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$ 38

6.9 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$ . . . 39

6.10 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$ . . . 39

6.11 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic and adiabatic wall . . . 40

6.12 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic and adiabatic wall . . . 40

6.13 $T_e = 3000$ K, $P_e = 0.001$ atm, $u_e = 2$ km/s, equilibrium wall and $(dI/dy)_w = 0$ . . . 41

6.14 $T_e = 5000$ K, $P_e = 0.001$ atm, $u_e = 2$ km/s, equilibrium wall and $(dI/dy)_w = 0$ . . . 41

List of Figures—*Continued*

6.15 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_w/I_e = 0.95$ 42
6.16 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_w/I_e = 0.95$ 42
6.17 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, T_w = 1000 K, and $c_{wO}/c_{eO} = 0.1$ 43
6.18 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, T_w = 1000 K, and $c_{wO}/c_{eO} = 0.1$ 43
6.19 T_e = 3000 K, P_e = 1 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$ 45
6.20 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$ 46
6.21 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic and adiabatic wall 46
6.22 T_e = 3000 K, P_e = 0.001 atm, u_e = 2 km/s, equilibrium wall and $(dI/dy)_w = 0$ 47
6.23 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_w/I_e = 0.95$ 48
6.24 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, $T_w = 1000K$, and $c_{wO}/c_{eO} = 0.1$ 48
6.25 T_e = 5000 K, P_e = 1 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$ 49
6.26 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$ 50
6.27 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic and adiabatic wall 51
6.28 T_e = 5000 K, P_e = 0.001 atm, u_e = 2 km/s, equilibrium wall and $(dI/dy)_w = 0$ 51

List of Figures—*Continued*

6.29 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_e/I_w = 0.95$ 52
6.30 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, T_w = 1000 K, and $c_{wN}/c_{eN} = 0.1$ 53
6.31 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$ 54
6.32 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic and adiabatic wall 56
6.33 T_e = 5000 K, P_e = 0.001 atm, u_e = 2 km/s, equilibrium wall and $(dI/dy)_w = 0$ 57
6.34 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_w/I_e = 0.95$ 59
6.35 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, T_w = 1000 K, and c_{wN}/c_{eN} = 0.1, $c_{wO}/c_{eO} = c_{wO_2}/c_{eO_2} = c_{wNO}/c_{eNO} = 0$ 60

Abstract

Boundary-layer solvers for binary gases and a five species air model have been developed. The boundary-layer equations are solved by using the Levy-Lees-Dorodnitsyn transformation. The transformed boundary-layer equations are written as a first order system by introducing new dependent variables. The equations are discretized using second order finite differences. Newton's method together with the block-elimination method is used to solve the non-linear algebraic equations. The energy equation is solved separately after the momentum equation and the equations for species conservation are solved. The effect of chemical reactions on the flow is explored for chemical equilibrium, frozen, and non-equilibrium gases. The reaction rates and transport properties of the gases are evaluated according to Gupta et al (1990) [1].

Nomenclature

c_s = mass fraction of species s

C_p = Specific heat at constant pressure

D_{sm} = diffusion coefficient of species s

e = internal energy per unit mass

$f = u/u_e$

$g = I/I_e$

h_s = enthalpy of species s

I = total enthalpy

k = thermal conductivity of mixture

k_b = backward reaction-rate coefficient

k_f = forward reaction-rate coefficient

K_{p-s} = equilibrium constant of species s

μ = viscosity of mixture

n_s = the number of moles of species s

p = pressure in the mixture

p_s = partial pressure of species s

$q = c_s/c_{es}$

q_s = mass fraction function of species s

$[s]$ = concentration of species s

u, v, w = velocity component of the mixture

u_s, v_s, w_s = velocity component of species s

$\overrightarrow{V}$ = velocity vector of mixture

W_s = source term of species s

x = coordinate along the surface

y = distance from the wall

τ_{ij} = shear stress tensor

ρ = density of mixture

ρ_s = density of specie s

Subscripts

b = backward reaction

e = boundary layer edge condition

f = forward reaction

m = mixture component

p = constant pressure

s = species index

w = wall condition

1. Introduction

With the rapid development of high-speed flight technology, the phenomena of high speed chemically reactive boundary layer flow is now of great interest. The boundary-layer is a thin layer of gas formed by the flow past a body where viscous and thermal conductivity effects are significant. Analysis of the boundary-layer is important for prediction of heat transfer between a body and the surrounding flow. In order to properly characterize and model the boundary-layer equations for reacting gases, one has to include and capture other processes occurring simultaneously with the dominant conduction and viscous shearing processes. These other processes include chemical reactions, thermal property changes, mass transfer interactions, along with the primary viscous fluid mechanics of boundary-layers.

Our analysis is most appropriate for boundary layers in the temperature range of 2500K-9000K where ionization does not play a significant role in the boundary-layer flow under assumption of thermal equilibrium.

As early as 1938, Prandtl formulated the boundary-layer concept. Following the concept, there has been a great development in understanding of the flow physics and in numerical techniques. So far, there have been three categories of numerical techniques which are difference-differential procedure, method of integral relations, and finite difference schemes.

In the difference-differential procedure, the derivatives along the surface are written with finite difference equations, and the partial differential equations are written as ordinary differential equations using distance from the wall as an independent variable. The solution has to satisfy the same boundary conditions at the wall and at the boundary-layer edge. In the integral relations method, the partial differential equations are reduced to a system of ordinary differential equations using the streamwise coordinate as the independent variable. In the finite difference method, all derivatives in the partial differential equations are approximated by finite differences, and a system of nonlinear algebraic equations are to be solved.

Hartree and Womersley [2] originally developed the difference-differential procedure for certain types of partial differential equations and Leight [3] and Manohar [4] applied this method to the laminar boundary-layer equations and steady boundary-layer flow equations, respectively. Smith and his colleagues[5] - [10] developed and applied this technique to the different types of problems such as incompressible laminar boundary-layer equations.

The method of integral relations is a special case of the weighted residuals method. It was considered and discussed by Finlayson and Scriven [11]. This method is due to Dorodnitsyn [12] and applied in the Russian papers [13] - [15]. The method was applied by Pallone and his colleagues [16] - [17], and considered further by Bethel [18] - [19]. Kendall and Bartlett [20] used the integral method to exclude the normal derivatives while the tangential derivatives were approximated by a finite difference method. Thus, the partial differential equations are recast as a system of nonlinear algebraic equations.

Finite difference techniques were used by Eichelbrenner and Flgge-Lotz [21] for the solution of the boundary-layer equations in the Crocco form. In the Crocco form, the continuity equation is discarded and the independent velocity variable u/u_e goes from zero to one. The velocity within the boundary layer should not be greater than the velocity at the edge in the Crocco form. Work done by Eichelbrenner and Flgge-Lotz was extended by Baxter and Flugge-Lotz [22] using finite difference method where the step size along the wall is strictly dependent on stability considerations. Kramer and Lieberstein [23] employed another finite difference technique in order to avoid the stability restrictions. Raetz [24] used this technique for solving the three-dimensional boundary-layer equations. The boundary-layer equations were solved by Mitchell and Thomson [25] using the von Mises transformation.

Then the development of the solution of the boundary-layer equations in non-transformed coordinates arose in the numerical techniques. Flugge-Lotz and Yu applied the finite difference method to the compressible equations in non-transformed coordinates. This approach ended unsuccessful because of the strict stability requirements and the problems that originated from replacement of the continuity equation. Wu [26] obtained more stable solution with a difference scheme. Chudov and Brailovskaya [27] also studied the solution of the boundary-layer equations in untransformed coordinates. Paskonov [28] developed another procedure into a standard program for equations of the boundary-layer type. In this procedure, coupling between the equations is initially neglected when the governing equations are recast with finite difference relations. Then, the accuracy of the dependent variables are found using the iteration procedure. Flugge-Lotz and Blottner [29] developed similar technique independently for the boundary-layer equations in untransformed coordinates. The difference between this work and Chudov and Brailovskaya is that coupling is allowed between the equations. Flugge-Lotz and Blottner also investigated the boundary-layer equations transformed with the Levy-Lees-Dorodnitsyn.

The boundary-layer equations are of parabolic type and then require an inflow conditions for the solutions. In all previous methods, the starting of the marching along the streamwise coordinate was a problem. Blottner [30] used ordinary differential equations in order to find inflow conditions for the boundary-layer equations. He [31] also applied this method to a binary gas mixture and to air boundary-layer flow with seven chemical species and finite reaction rates. Galowin and Gould [32] solved the chemically reacting boundary-layer using a finite difference scheme. In this work, the boundary-layer equations were transformed into the von Mises coordinates before the derivatives were replaced with finite difference relations.

Davis and Flugge-Lotz [33], Flugge-Lotz and Fannelop [34] made the application of the finite difference technique to the boundary-layer equations for axisymmetric and two-dimensional bodies. Fussell and Hellums [35] applied the finite difference method to the the boundary-layer equation written in a self-similar form. In this paper, an iteration procedure was used for obtaining solution of the nonlinear difference equations at the grid points. Kleinstein [36] used finite difference method to solve the boundary-layer equations in the von Mises coordinates. Lane, Liberman and Fox [37] used a finite difference technique to solve the compressible boundary-layer equation in untransformed coordinates.

Moore investigated a multi-component reacting gas with thermal diffusion effects included using a finite difference technique which was introduced by Farrington [38]. Schnauer [39] studied a finite difference scheme of the boundary-layer equations in nearly the Crocco form. The tangential velocity non-dimensionalized using velocity at the edge of the boundary layer, therefore the independent variable goes from zero to one. Shchennikov [40] introduced a method for constructing finite difference equations on the basis of the conservation laws. Patankar and Spalding [41] developed a finite difference technique for solving boundary-layer equation where the governing equations were transformed with a von Mises-type coordinate system and the stream function was an independent variable across the layer. Koh and Price [42] studied the boundary-layer flow on a rotating cone with a finite difference method. Solan, Cohen, Sibulkin, and Dispaux [43] used the finite difference procedure for the Rayleigh problem and a flat-plate boundary-layer flow with radiation effects. Rayleigh problem is basically when the governing equations become ordinary differential equations or similarity solution is available in the absence of radiation or at the leading edge of the flat plate. Douglas [44] solved nonlinear algebraic boundary-layer equation by using iterations and this method was applied to the Rayleigh problem. Levine [45] solved the boundary-layer equations for real equilibrium gases using a finite difference method. Sills [46] used a transformation that maps the infinite region of the boundary-layer flow into a finite interval. Blottner [47] used finite difference technique to solve the boundary-layer equations for a multi-component flow with finite chemical reactions on a sharp cone and hyperboloid at re-entry conditions.

In this work, the chemically reacted boundary-layer solver for five species air model and binary mixture of oxygen and nitrogen gases were studied by using the finite difference technique and the Levy-Lees-Dorodnitsyn transformation. We also studied the impact of real gas effects on the boundary-layer which forces the consideration of many other parameters rather than using calorically perfect gas.

2. Equilibrium Properties of O2+O,N2+N, and Air

A mixture of gases at an equilibrium state is defined by temperature and pressure of the mixture. The total energy of the reactants and products is constant and the total number of each chemical element (atoms of oxygen and nitrogen in this work) is also constant. With knowledge of these facts, one can determine the ratio of reactants and product using the equilibrium constant which can be found from experiments or calculated using statistical thermodynamics.

One can define the equilibrium constant using the ratio of partial pressures of the products and reactants of the reaction. For the reaction:

$$n_1 A + n_2 B \rightleftarrows n_3 C + n_4 D. \tag{2.1}$$

The equilibrium constant is defined using the partial pressures of the species:

$$K_p = \frac{p_C^{n_3} p_D^{n_4}}{p_A^{n_1} p_B^{n_2}}. \tag{2.2}$$

According to thermodynamics, equilibrium constants depend only on temperature of the flow.

The following three chemical reactions are considered in our work:

$$N_2 \rightleftarrows 2N, \tag{2.3}$$

$$O_2 \rightleftarrows 2O, \tag{2.4}$$

$$N + O \rightleftarrows NO. \tag{2.5}$$

For the binary mixtures of oxygen and nitrogen, only equations (2.3) and (2.4) are considered to determine the partial pressures. For 5 species air model at temperatures below 9000K, all of the three reactions above must be taken into account.

For the binary mixture, there are two equations for each case:

$$K_{p-N} = \frac{p_N^2}{p_{N_2}}, p = p_N + p_{N_2}, \tag{2.6}$$

$$K_{p-O} = \frac{p_O^2}{p_{O_2}}, p = p_O + p_{O_2}. \tag{2.7}$$

One can find the partial pressure of the species for the binary mixture of oxygen and nitrogen:

$$p_N = \frac{1}{2}\left(-K_p + \sqrt{{K_p}^2 + 4pK_p}\right), \tag{2.8}$$

$$p_{N_2} = p - p_N, \tag{2.9}$$

$$p_O = \frac{1}{2}\left(-K_p + \sqrt{{K_p}^2 + 4pK_p}\right), \tag{2.10}$$

$$p_{O_2} = p - p_O. \tag{2.11}$$

For the five species air model, there are three equilibrium constants, one for each reaction:

$$K_{p-N} = \frac{p_N^2}{p_{N_2}}, K_{p-O} = \frac{p_O^2}{p_{O_2}}, K_{p-NO} = \frac{p_N p_O}{p_{NO}}. \tag{2.12}$$

In addition, the pressure in the mixture can be determined as follows:

$$p = p_N + p_{N_2} + p_O + p_{O_2} + p_{NO}. \tag{2.13}$$

In order to have a complete set of equations, composition of air must be defined. We assumed that air is comprised of 21 percent oxygen and 79 percent nitrogen molar fraction. The number of chemical elements remains constant in the mixture when dissociation occurs. Therefore, we can write the mass-balance equation as:

$$\frac{2p_{O_2} + p_O + p_{NO}}{2p_{N_2} + p_N + p_{NO}} = \frac{0.21}{0.79}. \tag{2.14}$$

Using Eqs. (2.12), (2.13), and (2.14), one can derive the following:

$$p_N = -\frac{1}{4}K_{p-N} + \sqrt{\frac{K^2{}_{p-N}}{16} + \frac{\Psi K_{p-N}}{2}}, \tag{2.15}$$

$$p_{N_2} = \frac{p - \Psi - p_N}{2}, \tag{2.16}$$

$$p_O = -\frac{1}{4}K_{p-O} + \sqrt{\frac{K^2{}_{p-O}}{16} + \frac{\Psi K_{p-O}}{2}}, \tag{2.17}$$

$$p_{O_2} = \frac{\Psi - p_O}{2}, \tag{2.18}$$

$$p_{NO} = \frac{p_O p_N}{K_{p-NO}}. \tag{2.19}$$

where $\Psi = 0.21atm$.

The five equations for the air model stated above are solved numerically using Newtons iterations. When the partial pressures of each component are obtained, the equilibrium composition and the equilibrium gas mixture thermodynamic properties can be determined within the boundary-layer.

3. Non-Equilibrium Gas Mixtures

In the non-equilibrium state, there is a finite rate of change in time for concentration of species s. The concentration [s] is defined as the number of moles of species s per unit volume of the mixture.

For the binary mixtures of nitrogen and oxygen, the chemical reactions equation (2.3) and (2.4) are taken into account. These chemical reactions are written with their collision partners which are denoted as M. Collision partners are O and O_2 for oxygen, N and N_2 for nitrogen.

$$O_2 + M \rightleftarrows 2O + M, \tag{3.1}$$

$$N_2 + M \rightleftarrows 2N + M. \tag{3.2}$$

The time rates of formation for both molecules and atoms of binary mixtures of oxygen and nitrogen are:

$$\frac{d[O]}{dt} = 2k_f^1[O_2]\left([O_2]+[O]\right) - 2k_b^1[O]^2\left([O_2]+[O]\right), \tag{3.3}$$

$$\frac{d[O_2]}{dt} = -k_f^1[O_2]\left([O_2]+[O]\right) + k_b^1[O]^2\left([O_2]+[O]\right), \tag{3.4}$$

$$\frac{d[N]}{dt} = 2k_f^2[N_2][N_2] + 2k_f^3[N_2][N] - 2k_b^2[N]^2[N_2] - 2k_b^3[N]^2[N], \tag{3.5}$$

$$\frac{d[N_2]}{dt} = -k_f^2[N_2][N_2] - k_f^3[N_2][N] + k_b^2[N]^2[N_2] + k_b^3[N]^2[N]. \tag{3.6}$$

where superscripts determine the different forward and backward reaction-rate coefficients of the chemical reactions.

Unlikely oxygen, nitrogen has different forward and backward reaction rates with respect to the collision partners. Therefore, the time rates of formation for nitrogen molecules and atoms have to be written subject to the collision partners.

For the five species air model, the chemical reactions of nitrogen, oxygen and nitric oxide are taken into account and the collision partners are N, N_2, O, O_2, and NO. The chemical reaction mechanism for the five species air model is:

$$O_2 + M \rightleftarrows 2O + M, \tag{3.7}$$

$$N_2 + M \rightleftarrows 2N + M, \tag{3.8}$$

$$NO + M \rightleftarrows N + O + M, \tag{3.9}$$

$$NO + O \rightleftarrows O_2 + N, \tag{3.10}$$

$$N_2 + O \rightleftarrows NO + N. \tag{3.11}$$

There is one more extra reaction for the five species air model which is:

$$N_2 + O_2 \rightleftarrows 2NO. \tag{3.12}$$

This reaction does not play a significant role in the energy balance, and it is usually omitted from consideration.

The time rate of formation equations for all species are written as follows:

$$\begin{aligned}\frac{d[O]}{dt} &= 2k_f^{(1)}[O_2]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &-2k_b^{(1)}[O]^2\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &+k_f^{(4)}[NO]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &-k_b^{(4)}[N][O]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &-k_f^{(5)}[NO][O]+k_b^{(5)}[N][O_2]-k_f^{(6)}[N_2][O]+k_b^{(6)}[NO][N],\end{aligned} \tag{3.13}$$

$$\frac{d[O_2]}{dt} = -k_f^{(1)}[O_2]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)$$

$$+k_b^{(1)}[O]^2\left([O_2]+[O]+[N_2]+[N]+[NO]\right)+k_f^{(5)}[NO][O]-k_b^{(5)}[N][O_2], \tag{3.14}$$

$$\begin{aligned}\frac{d[N]}{dt} &= 2k_f^{(2)}[N_2]\left([O_2]+[O]+[N_2]+[NO]\right)+2k_f^{(3)}[N_2][N]\\ &-2k_b^{(2)}[N]^2\left([O_2]+[O]+[N_2]+[NO]\right)\\ &-2k_b^{(3)}[N]^2[N]+k_f^{(4)}[NO]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &-k_b^{(4)}[N][O]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &+k_f^{(5)}[NO][O]-k_b^{(}5)[N][O_2]+k_f^{(}6)[N_2][O]-k_b^{(6)}[NO][N],\end{aligned} \tag{3.15}$$

$$\begin{aligned}\frac{d[N_2]}{dt} &= -k_f^{(2)}[N_2]\left([O_2]+[O]+[N_2]+[NO]\right)-k_f^{(3)}[N_2][N]\\ &+k_b^{(2)}[N]^2\left([O_2]+[O]+[N_2]+[NO]\right)+k_b^{(3)}[N]^2[N]\\ &-k_f^{(6)}[N_2][O]+k_b^{(6)}[NO][N],\end{aligned} \tag{3.16}$$

$$\begin{aligned}\frac{d[NO]}{dt} &= -k_f^{(4)}[NO]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &+k_b^{(4)}[N][O]\left([O_2]+[O]+[N_2]+[N]+[NO]\right)\\ &-k_f^{(5)}[NO][O]+k_b^{(5)}[N][O_2]+k_f^{(6)}[N_2][O]-k_b^{(6)}[NO][N].\end{aligned} \tag{3.17}$$

These equations are needed for establishing the source term in the mass conservation equation for each species.

4. Boundary Layer Equations for Reacting Gases

The boundary layer thickness is very small in high-speed flow and the pressure distribution normal to the surface is considered constant. Therefore, it is always assumed that the derivative with respect to the flow direction is negligible comparing to the derivative with respect to the normal coordinate. In order to know the thermodynamic properties of the flow at a point in the flow, one has to get the distribution of each chemical species present in the flow. The mass fraction of each chemical species $c_s(x, y)$ can be calculated by solving boundary-layer equations for reacting gases, where x is the coordinate along the wall and y is the coordinate perpendicular to the wall.

According to the boundary-layer concept, viscosity and thermal conductivity do not have significant effect on the flow outside of a thin layer. So, the Euler equations are to be used to find flow characteristics outside the boundary-layer. The flow properties found from the solution of the Euler equation are used as boundary conditions at the edge of the boundary-layer. In the present work, we consider examples when flow outside the boundary layer is in chemical and thermal equilibrium.

Mass Conservation of Species

Mass conservation equation for two-dimensional and steady chemically reactive flow is:

$$\frac{\partial}{\partial x}\left[\rho_s\left(u+u_s\right)\right]+\frac{\partial}{\partial y}\left[\rho_s\left(v+v_s\right)\right]=W_s. \tag{4.1}$$

In a mixture, the diffusion of individual species takes place by three mechanisms which are ordinary diffusion, pressure (baro-) diffusion, and thermal diffusion. Neglecting thermo- and baro- diffusion, and applying Fick's Law for mass diffusion:

$$\rho_s u_s = -\rho D_{sm} \nabla c_s, \tag{4.2}$$

the equation is recast as

$$\frac{\partial}{\partial x}\left[\rho_s\left(u + \frac{D_{sm}}{c_s}\frac{\partial c_s}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[\rho_s\left(v + \frac{D_{sm}}{c_s}\frac{\partial c_s}{\partial y}\right)\right] = W_s. \tag{4.3}$$

Using the mass fraction $c_s = \rho_s/\rho$, one can derive the mass conservation equation in the boundary layer approximation as follows:

$$\rho u \frac{\partial c_s}{\partial x} + \rho v \frac{\partial c_s}{\partial y} = \frac{\partial}{\partial y}\left(\rho D_{sm}\frac{\partial c_s}{\partial y}\right) + W_s. \tag{4.4}$$

Momentum Equation

The x- and y-momentum equations are written in the differential form as follows:

$$\frac{\partial(\rho u)}{\partial x} + \nabla \cdot (\rho u \vec{V}) = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y}, \tag{4.5}$$

$$\nabla \cdot (\rho v \vec{V}) = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y}. \tag{4.6}$$

Stoke's hypothesis(the bulk viscosity is equal to zero) is utilized here to define the shear stress components as follows:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \lambda \frac{\partial u_k}{\partial x_k}\delta_{ij}, \tag{4.7}$$

where $\lambda = -(2/3)\mu$.

Using the boundary-layer approximation x- and y-momentum equations become:

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right), \tag{4.8}$$

$$\rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial x} = \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial y}\right). \tag{4.9}$$

Energy Equation

If the flow is a chemically reacting mixture, there should be an energy transport due to diffusion. For example, x-component of the energy flux due to diffusion of all species at a point can be written as:

$$\sum_s \rho_s u_s h_s, \tag{4.10}$$

Using Fick's Law, the final differential form of energy equation is obtained as:

$$\nabla \cdot \left[\rho\left(e + \frac{V^2}{2}\right)\vec{V}\right] = -\nabla \cdot \left[p\vec{V}\right] + \rho\left(-k\nabla T + \rho \sum_s D_{sm} h_s \nabla c_s\right) + \nabla \cdot \left(\tau \vec{V}\right). \tag{4.11}$$

Using the total enthalpy I, the energy equation in the boundary layer approximation is derived as follows:

$$\rho u \frac{\partial I}{\partial x} + \rho v \frac{\partial I}{\partial y} = \frac{\partial}{\partial y}\left[\frac{\mu}{\Pr}\frac{\partial I}{\partial y} + \mu\left(1 - \frac{1}{\Pr}\right)\frac{1}{2}\frac{\partial u^2}{\partial y}\right] -$$

$$\frac{\partial}{\partial y}\left[\sum_{s=1}^{ns}\left(\frac{1}{Le_s}-1\right)\rho D_{sm} h_s \frac{\partial c_s}{\partial y}\right], \qquad (4.12)$$

where $I = h + u^2/2$, $h = \sum_{s=1}^{ns} c_s h_s$, $Le_s = \rho D_{sm} C_{pf}/k$.

In our work, the viscosity μ is obtained using Wilke's rule [48] and the diffusion coefficient, D_{sm}, is then determined with the help of the approximation suggested in Ref [49].

5. Numerical Method Description

In the present work, 2D boundary-layer flows are considered. In order to have a general form for the boundary-layer equation, bodies of revolution are included into the consideration as well. For this reason, the Levy-Lees-Dorodnitsyn transformation is chosen. New variables ξ and η are used for new coordinate system instead of x-y coordinate system. The stream-function is [48]:

$$\psi(\xi,\eta) = N(\xi)\, f(\eta,\xi)\,, N(\xi) = \frac{\sqrt{2\xi}}{p_e r_0^k}, \tag{5.1}$$

where $\xi = \int\limits_0^x \rho_e u_e \mu_e r_0^{2j} ds$ and $\eta = \frac{r_0^{2j}\rho_e u_e}{\sqrt{2\xi}} \int\limits_0^y \frac{\rho}{\rho_e} dy$ subscript e indicates the flow parameters at the edge of the boundary-layer, an $r_0(x)$ stands for local radius of the body of revolution. The parameter k=0 is for case of 2D flow, and k=1 is for an axisymmetric flow, $f'(\xi,\eta) = u/u_e$, where $'$ is derivative with respect to η. Introduction of the stream function satisfies the continuity equation fot the mixture.

Applying the transformation, the governing equations are recast in the following form:

Mass Conservation of Species

$$2\xi\left(\frac{\partial q_s}{\partial \xi} f' - q'_s \frac{\partial f}{\partial \xi}\right) = \left(\frac{C}{Sm} q'_s\right)' + q'_s f - \frac{2\xi}{c_{se}}\frac{dc_{se}}{d\xi} f' + \frac{2\xi W_s}{\rho\rho_e u_e^2 \mu_e r_0^{2k} c_{se}} m, \tag{5.2}$$

where $Sm = \frac{\mu}{\rho D_{sm}}$, $C = \frac{\rho\mu}{\rho_e \mu_e}$, and $q_s(\xi,\eta) = c_s/c_{se}$.

In our analysis, we can exclude one mass conservation equation because we use the global mass conservation equation. In our five species air model work, nitrogen molecule species is excluded from the system of equations.

Momentum Equation

$$(Cf'')' + ff'' + \frac{2\xi}{u_e}\frac{du_e}{d\xi}\left[\frac{\rho_e}{\rho} - (f')^2\right] = 2\xi\left(f'\frac{\partial f'}{\partial \xi} - f''\frac{\partial f}{\partial \xi}\right). \tag{5.3}$$

Energy Equation

$$\left(\frac{C}{\mathrm{Pr}}g'\right)' + fg' = \frac{2\xi}{I_e}\frac{dI_e}{d\xi}gf' + \left[\sum_s \frac{C}{Sm_s}\left(\frac{1}{Le_s} - 1\right)\frac{h_s c_{se}}{I_e}{q_s}'\right]'$$
$$+\frac{u_e^2}{I_e}\left[\left(\frac{1}{\mathrm{Pr}} - 1\right)Cf'f''\right]' + 2\xi\left(f'\frac{\partial g}{\partial \xi} - g'\frac{\partial f}{\partial \xi}\right), \tag{5.4}$$

where $\mathrm{Pr} = \frac{\mu C_p}{k}$, $Le_i = \frac{\rho D_{im} C_p}{k}$, $g(\xi, \eta) = I/I_e$.

Having derived all the transformed governing equations, we set up the system as a system of equation of the first order along the lines of Cebeci method [50]. We introduced new depending variables in order to have first order system of equations. For five species air model, the system of equations are shown in Appendix-A from (A.6) to (A.11).

After setting up the system of equations of first order, we define the grid:

$$\xi^0 = 0, \xi^n = \xi^{n-1} + k_n, n = 1, 2, , N, \tag{5.5}$$

$$\eta_0 = 0, \eta_j = \eta_{j-1} + h_j, j = 1, 2, , J. \tag{5.6}$$

where k_n and h_j are the grid intervals.

In the numerical method, the equations are discretized using second order finite differences and written for the midpoint having coordinates $\xi^{n-1/2}, \eta_{j-1/2}$.

The discretized nonlinear system of algebraic equations is iterated using Newton's algorithm. The function is assumed to be:

$$Q^{(i)} = Q^{(i-1)} + \delta Q^{(i-1)} \tag{5.7}$$

where (i) indicates the iteration number, and $\delta Q^{(i-1)}$ is a correction to the solution from the previous iteration.

Boundary Conditions

In our work, the species indices are attributed to the chemical elements as follows:

1 - molecules of nitrogen,

2 - atoms of nitrogen,

3 - molecules of oxygen,

4 - atoms of oxygen,

5 - molecules of nitric oxide.

In order to outline the boundary conditions, we need to describe the new dependent variables. The new dependent variables Qs_j, Qd_j, F_j, and G_j are defined as follows:

$$q_2 = Qs_2,$$

$$q_3 = Qs_3,$$

$$q_4 = Qs_4,$$

$$q_5 = Qs_5,$$

$$q_2{}' = Qd_2,$$

$$q_3{}' = Qd_3,$$

$$q_4{}' = Qd_4,$$

$$q_5{}' = Qd_5,$$

$$f = F_1,$$

$$f' = F_2,$$

$$f'' = F_3,$$

$$g = G_1,$$

$$g' = G_2.$$

After having new notations, our boundary conditions can be written as follows:

$$\eta = 0 : F_{10}^n = F_{20}^n = 0, \gamma_0 G_{10}^n + \gamma_1 G_{20}^n = \gamma_2^n, \quad (5.8)$$

$$\eta = \eta_e : F_{2J}^n = G_{1J}^n = Qs_{2J}^n = Qs_{3J}^n = Qs_{4J}^n = Qs_{5J}^n = 1, \quad (5.9)$$

where γ_0 and γ_1 define the heat condition at the wall. If $\gamma_0 = 0$ and $\gamma_1 = 1$ the boundary condition corresponds to $g' = 0$. If $\gamma_0 = 1$ and $\gamma_1 = 0$ the boundary condition defines dimensionless total enthalpy at the wall.

In addition to these, we need a boundary condition on the wall for the concentrations.

Equilibrium Wall

Equilibrium wall for which chemical reactions are allowed to occur at the wall and so the species concentrations are at their equilibrium values.

$$c_{sw} = c_{sw,eq}. \quad (5.10)$$

Fully Catalytic Wall

At a fully catalytic wall, the atom concentrations are equal to zero (complete recombination of the atoms).

Non-Catalytic Wall

No chemical reactions are occurring at the non-catalytic wall so that the derivatives of the species concentrations are zero:

$$\frac{\partial c_s}{\partial \xi} = 0. \tag{5.11}$$

Partially Catalytic Wall

Chemical reactions occur at the wall, however recombination doesn't happen completely. So, there are still atom concentration at the wall. This type of wall is called "Partially Catalytic Wall".

Constant Mass Fraction

Mass fraction can be specified at the wall.

6. Results

We consider real gas effect in our consideration. There is a certain difference of velocity and temperature distribution between perfect gas mixture and real gas mixture. In order to illustrate that phenomena, we use an example of non-catalytic and adiabatic wall condition for oxygen binary mixture. The length of the flat plate is 2 m, and the total enthalpy of the outside boundary layer is 11.06 MJ/kg. The outside flow parameters are $p_e = 0.01$ atm, $u_e = 4.273$ km/s, and $T_e = 2000$ K.

Fig. 6.1 shows comparison of the velocity profile for binary mixture of oxygen with the solution for a perfect gas. One can see that the real gas effects decrease the boundary layer thickness.

In Fig. 6.1 and in what follows, we use the length scale $H = \frac{\sqrt{2\xi}}{\rho_e u_e}$.

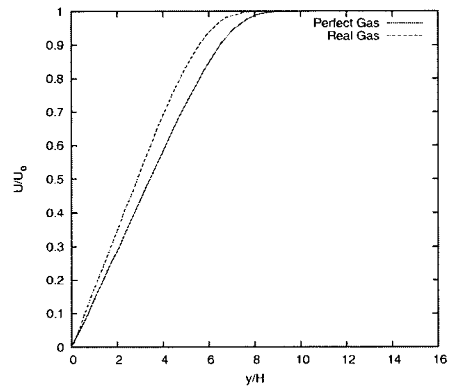


Figure 6.1 $T_e = 2000$ K, $P_e = 0.01$ atm, $u_e = 4.273$ km/s, non-catalytic and adiabatic wall

Fig. 6.2 shows comparison of the temperature profile for binary mixture of oxygen with the solution for a perfect gas. The temperature difference can be explained by the dependence of the specific heat change for calorically perfect gas and real gas. The temperature dramatically drops when real gas effects are taken into account.

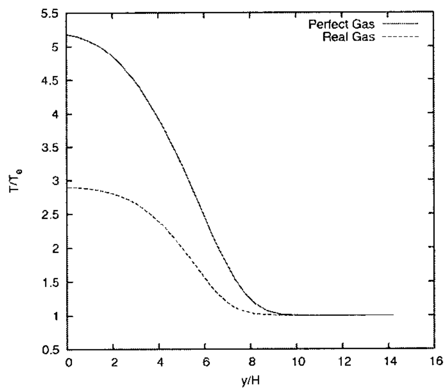


Figure 6.2 $T_e = 2000$ K, $P_e = 0.01$ atm, $u_e = 4.273$ km/s, non-catalytic and adiabatic wall

These comparisons illustrate importance of the real gas effects studies for high-speed flows.

6.1 Binary Mixture

Our initial step is comparing the boundary layer solver of binary mixture of oxygen with Probstein's integrals. If we consider the total enthalpy derivative with respect to x-coordinate to be zero, derivative of the mass fraction of the species at the edge to be zero, Prandtl and Schmidt numbers to be one, and frozen flow, the first Probstein's integral is [48]

$$q_s = q_{sw} + \left(\frac{1 - q_{sw}}{1 - g_w}\right)(g - g_w) \tag{6.1}$$

The parameters of the external flow at zero pressure gradient are $u_e = 2$ km/s, $p_e = 0.01$ atm, and $T_e = 3000$ K. The wall concentration of oxygen is $c_{wO}/c_O = 0.3$ and total enthalpy at the wall is defined as $I_w/I_e = 0.8$. The comparison of numerical and analytical results for mass fraction of atoms of oxygen is shown in Fig. 6.3. One can see good agreement of the numerical results with the Probstein's integtals in Fig. 6.3 and 6.4.

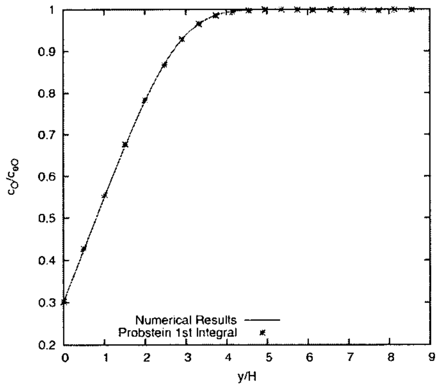


Figure 6.3 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, $c_{wO}/c_{eO} = 0.3$ and $I_w/I_e = 0.8$

If $du_e/dx = 0$, $dc_{ie}/d\xi = 0$, $Sm = 1$, and $W = 0$ (frozen flow), the second Probstein's integral is

$$q_s = q_{sw} + (1 - q_{sw})\, f'. \tag{6.2}$$

Using same boundary conditions and flow parameters as in the previous comparison, the comparison of numerical and analytical results for mass fraction of oxygen atoms is shown in Fig. 6.4.

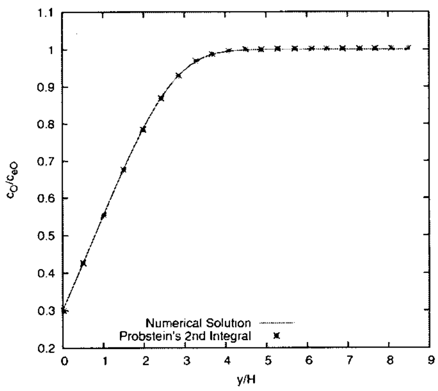


Figure 6.4 $T_e = 3000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, $c_{wO}/c_{eO} = 0.3$ and $I_w/I_e = 0.8$

Another test is illustrated by Figs. 6.5 and 6.6, where the self-similar solution was computed by solving a system of ordinary differential equations [48] for a boundary-layer past a flat plate at Mach number M=2, edge temperature $T_e = 300$ K, and Prandtl number $Pr = 0.7$. In order to compare the results from the new solver with the self-similar solution for a non-reacting calorically perfect gas, we adjusted the new solver to have a constant Prandtl number and defined the enthalpy according to constant specific heat. Additionally, we let the viscosity be given by Sutherland's viscosity as a function of temperature. One can see good agreement of the numerical results with the self similarity solution in Fig. 6.5 and 6.6.

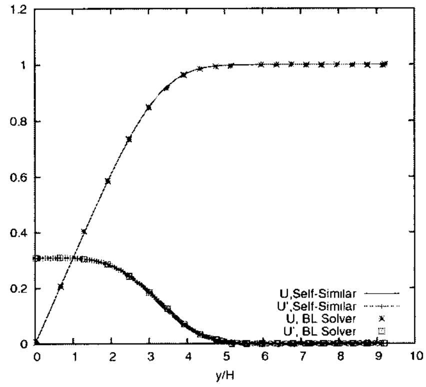


Figure 6.5 T_e = 300 K, P_e = 1 atm, u_e = 0.6607 km/s, equilibrium wall and $(dI/dy)_w = 0$

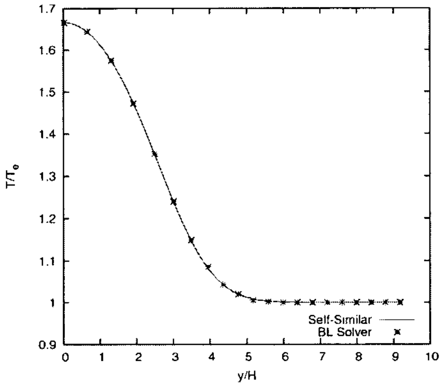


Figure 6.6 T_e = 300 K, P_e = 1 atm, u_e = 0.6607 km/s, equilibrium wall and $(dI/dy)_w = 0$

Now, we feel confident to examine our code with different tests to observe whether or not we can have physical meaning in our solution. In this example, we consider a flat plate[1] of 2m length using a grid with 800 intervals along the surface. The external flow parameters are u_e = 2 km/s, T_e = 3000 K for oxygen binary mixture, T_e = 5000 K for nitrogen binary mixture, and p_e = 1 atm. Mass fraction of the

[1]Actually we consider a flow with zero pressure gradient $dp_e/dy = 0$ and zero mass fraction gradient $dc_e/dx = 0$. For brevity we call such flow past "flat plate"

species at the boundary-layer edge are assumed to be in chemical equilibrium. We consider a non-catalytic wall, and the total enthalpy at the wall: $I_w/I_e = 0.8$. The atomic based mass fraction results for both nitrogen and oxygen are shown in Figs. 6.7 and 6.8.

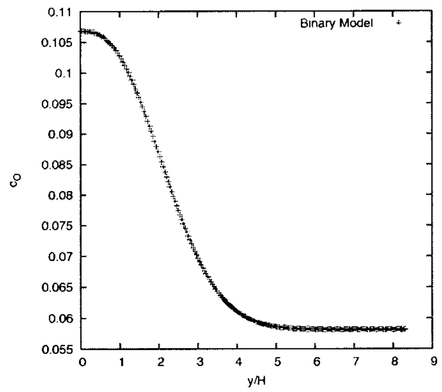


Figure 6.7 $T_e = 3000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$

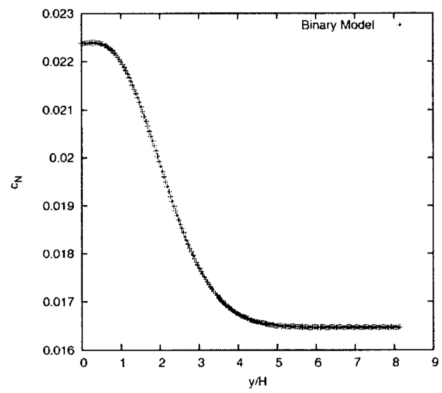


Figure 6.8 $T_e = 5000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$

In the next example, we have the flow same conditions as in the previous example except the pressure dropped to 0.01 atm.The atomic based mass fraction results for both nitrogen and oxygen are shown in Figs 6.9 and 6.10. One can see that variation of the mass fraction across the boundary-layer is very small.

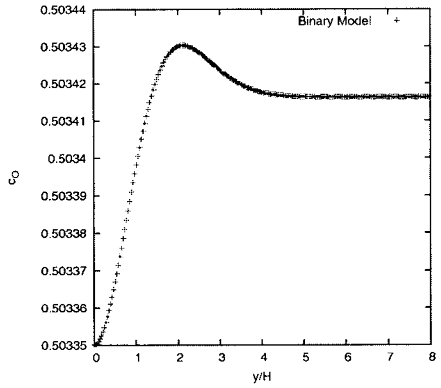


Figure 6.9 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$

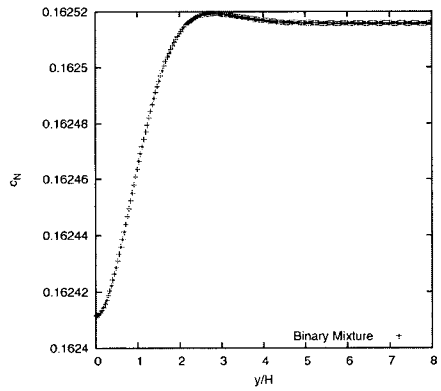


Figure 6.10 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$

In the next example, we consider an adiabatic and non-catalytic wall. The edge flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K for oxygen binary mixture, $T_e = 5000$ K for nitrogen binary mixture, and $p_e = 0.01$ atm. The atomic based mass fraction results for both nitrogen and oxygen are shown in Figs. 6.11 and 6.12.

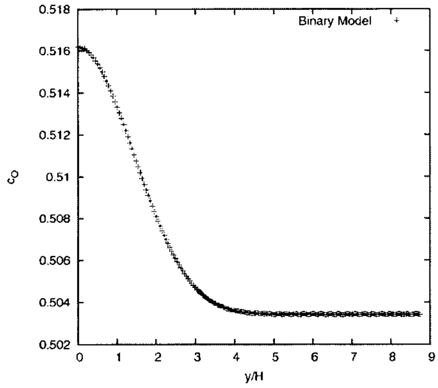


Figure 6.11 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic and adiabatic wall

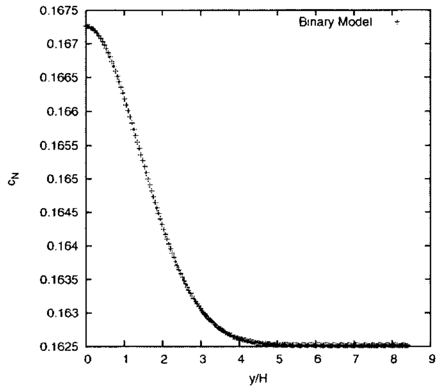


Figure 6.12 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic and adiabatic wall

In the next example, we examine flow past equilibrium and adiabatic wall. The edge flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K for oxygen case, $T_e = 5000$ K for nitrogen case, and $p_e = 0.001$ atm. The atomic based mass fraction results for both nitrogen and oxygen are shown 6.13 and 6.14. Because of the low pressure, the chemically equilibrium mixture at the edge of the boundary-layer is mainly composed of atoms (small fraction of molecules).

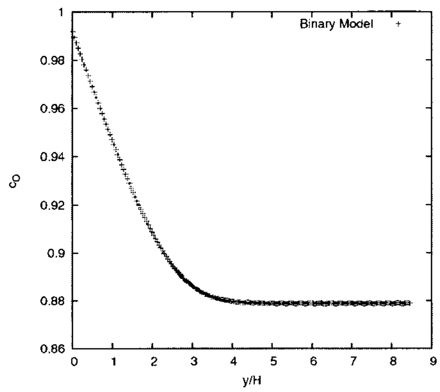


Figure 6.13 $T_e = 3000$ K, $P_e = 0.001$ atm, $u_e = 2$ km/s, equilibrium wall and $(dI/dy)_w = 0$

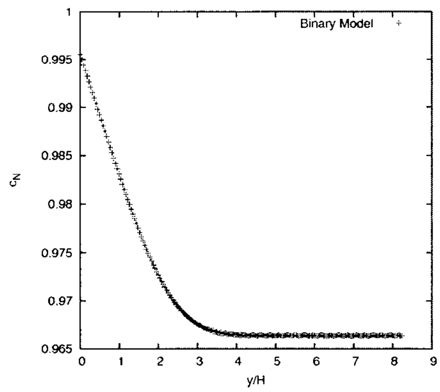


Figure 6.14 $T_e = 5000$ K, $P_e = 0.001$ atm, $u_e = 2$ km/s, equilibrium wall and $(dI/dy)_w = 0$

Here, we examine fully catalytic wall and temperature at the wall is formulated for total enthalpy: $I_w/I_e = 0.95$. The edge flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K for oxygen case, $T_e = 5000$ K for nitrogen case, and $p_e = 0.01$ atm. The atomic based mass fraction results for both nitrogen and oxygen are shown in Figs. 6.15 and 6.16. According to the boundary conditions, mass fractions of atoms at the wall are equal to zero.

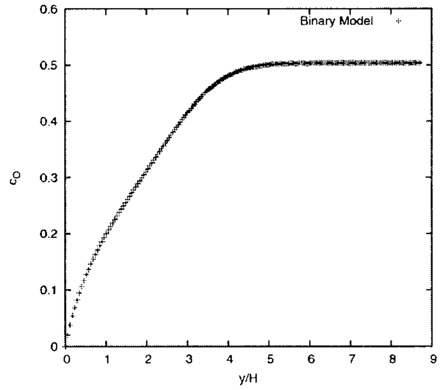


Figure 6.15 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, fully catalytic wall and $I_w/I_e = 0.95$

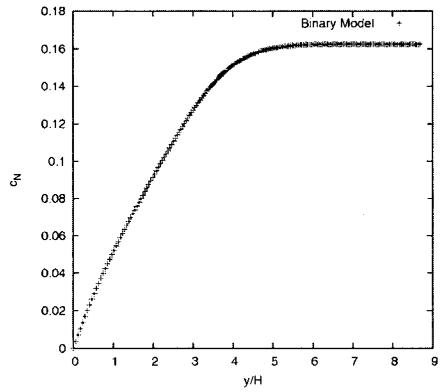


Figure 6.16 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, fully catalytic wall and $I_w/I_e = 0.95$

In the next example, we examine boundary layer flow at $T_w = 1000$ K and constant mass fractions at the wall using $c_{wO}/c_{eO} = 0.1$ for oxygen and $c_{wN}/c_{eN} = 0.1$ for nitrogen. The edge flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K for oxygen case, $T_e = 5000$ K for nitrogen case, and $p_e = 0.01$ atm. The atomic based mass fraction results for both nitrogen and oxygen are shown in Figs. 6.17 and 6.18.

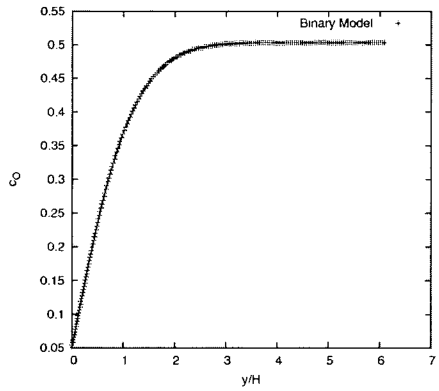


Figure 6.17 $T_e = 3000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, $T_w = 1000$ K, and $c_{wO}/c_{eO} = 0.1$

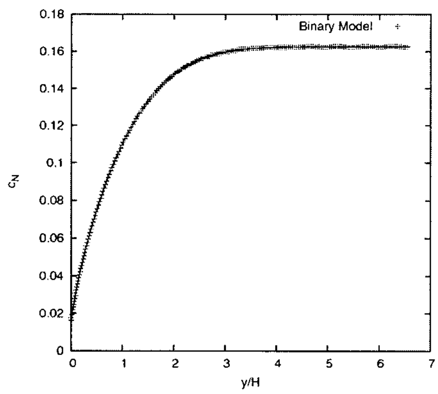


Figure 6.18 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, $T_w = 1000$ K, and $c_{wO}/c_{eO} = 0.1$

6.2 Five Species Air Model

In this part, we want to expand our study from binary mixture to a five species air model. The first step is comparing the air model solver with results obtained by solving the binary mixture equations.

6.2.1 Comparison with Binary Mixture of Oxygen

In order to compare results obtained using the five species air model solver with results obtained using the binary mixture solver, we needed to assign negligible mass fraction value at the edge for the chemical components which don't exist in the binary mixture model. In the five species solver, we assigned the edge mass fractions close to the values used in the binary mixture solver. The other mass fractions were chosen very small but the sum of mass fractions for all five species was kept equal to one. We consider a flat plate of 2 m length using a grid with 800 intervals along the surface. In this example, the external flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K, and $p_e = 1$ atm and $p_e = 0.01$ atm, respectively. Mass fraction of the species at the boundary-layer edge in the binary mixtures are assumed to be in chemical equilibrium. We consider a non-catalytic wall, and the total enthalpy at the wall: $I_w/I_e = 0.8$. One can see good agreement between the result obtained using the five species air model solver and obtained using the binary mixture solver for oxygen in Fig. 6.19 and 6.20.

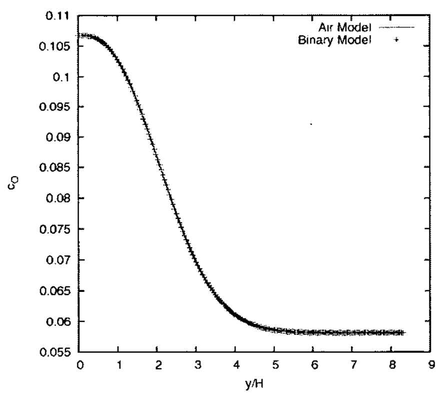


Figure 6.19 $T_e = 3000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$

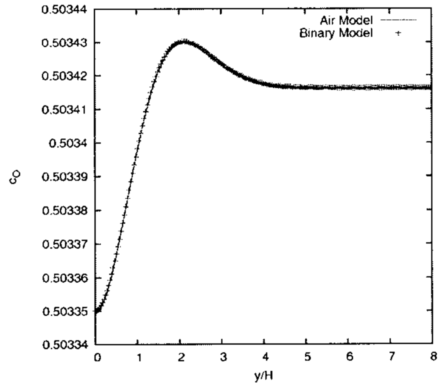


Figure 6.20 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$

In the next example, we consider an adiabatic and non-catalytic wall. The edge flow parameters are u_e = 2 km/s, T_e = 3000 K for oxygen binary mixture, and p_e = 0.01 atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for oxygen is shown in Fig. 6.21.

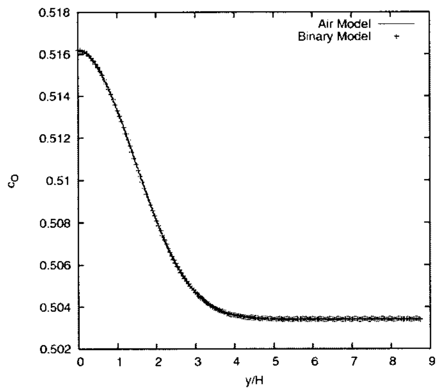


Figure 6.21 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic and adiabatic wall

In the next example, we examine flow past equilibrium and adiabatic wall. The edge flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K, and $p_e = 0.001$ atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for oxygen is shown in Fig. 6.22.

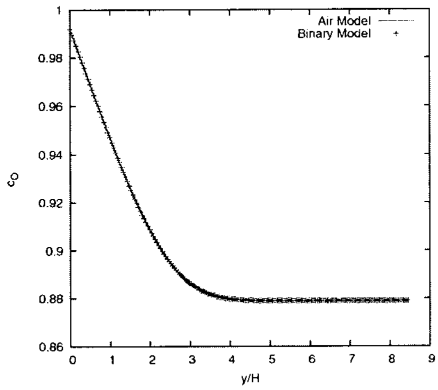


Figure 6.22 $T_e = 3000$ K, $P_e = 0.001$ atm, $u_e = 2$ km/s, equilibrium wall and $(dI/dy)_w = 0$

We examine fully catalytic wall and the temperature at the wall is formulated for total enthalpy: $I_w/I_e = 0.95$. The edge flow parameters are $u_e = 2$ km/s, $T_e = 3000$ K, and $p_e = 0.01$ atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for oxygen is shown in Fig. 6.23.

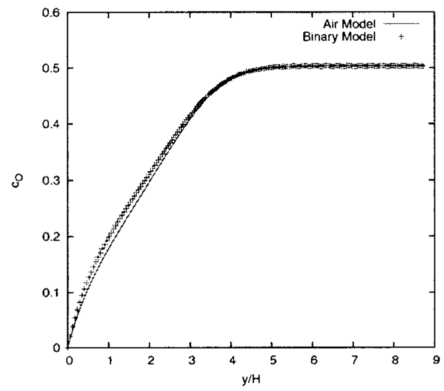


Figure 6.23 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_w/I_e = 0.95$

In the next example, we examine boundary layer flow at T_w = 1000 K and constant mass fractions at the wall using $c_{wO}/c_{eO} = 0.1$. The edge flow parameters are u_e = 2 km/s, T_e = 3000 K, and p_e = 0.01 atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for oxygen is shown in Fig. 6.24.

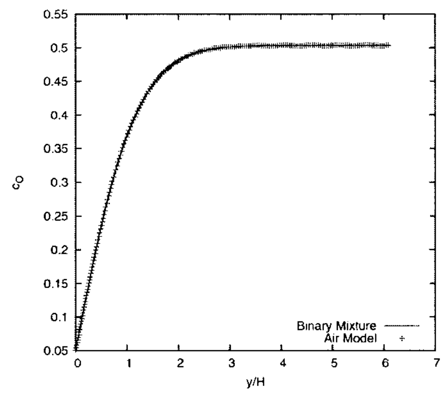


Figure 6.24 T_e = 3000 K, P_e = 0.01 atm, u_e = 2 km/s, $T_w = 1000K$, and c_{wO}/c_{eO} = 0.1

6.2.2 Comparison with Binary Mixture of Nitrogen

In this example, we consider a flat plate of 2m length using a grid with 800 intervals along the surface. The external flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K, and $p_e = 1$ atm and $p_e = 0.01$ atm, respectively. Mass fraction of the species at the boundary-layer edge are assumed to be in chemical equilibrium. We consider a non-catalytic wall, and the total enthalpy at the wall: $I_w/I_e = 0.8$. One can see good agreement between the result obtained using the five species air model solver and obtained using the binary mixture solver for nitrogen in Fig. 6.25 and 6.26.

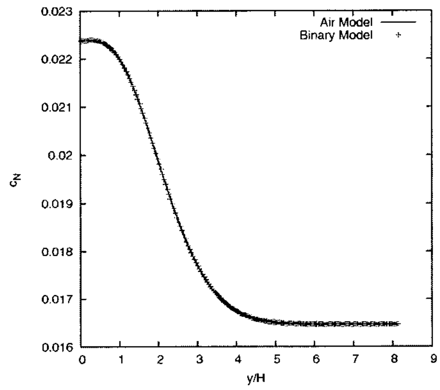


Figure 6.25 $T_e = 5000$ K, $P_e = 1$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e =$ 0.8

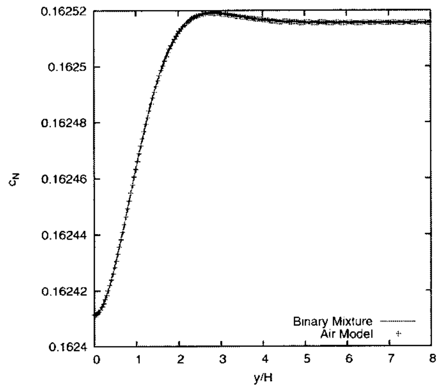


Figure 6.26 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic wall and $I_w/I_e = 0.8$

In the next example, we consider an adiabatic and non-catalytic wall. The edge flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K for nitrogen binary mixture, and $p_e = 0.01$ atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for nitrogen is shown in Fig. 6.27.

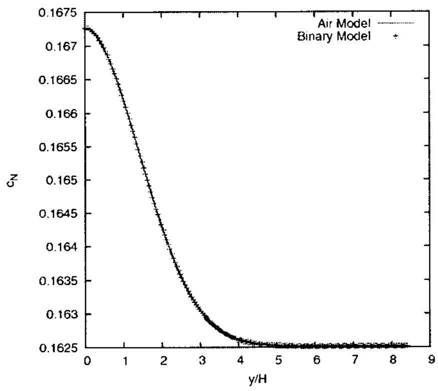


Figure 6.27 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic and adiabatic wall

In the next example, we examine flow past equilibrium and adiabatic wall. The edge flow parameters are u_e = 2 km/s, T_e = 5000 K, and p_e = 0.001 atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for nitrogen is shown in Fig. 6.28.

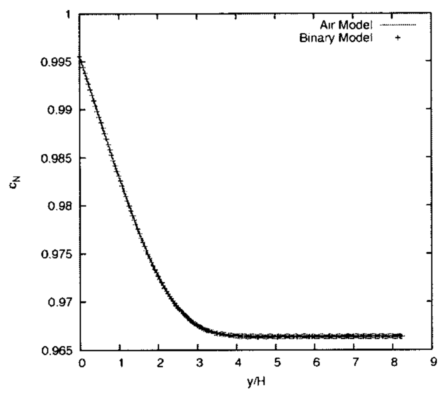


Figure 6.28 T_e = 5000 K, P_e = 0.001 atm, u_e = 2 km/s, equilibrium wall and $(dI/dy)_w = 0$

We examine fully catalytic wall and temperature at the wall is formulated for total enthalpy: $I_w/I_e = 0.95$. The edge flow parameters are u_e = 2 km/s, T_e = 5000

K, and $p_e = 0.01$ atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for nitrogen is shown in Fig. 6.29.

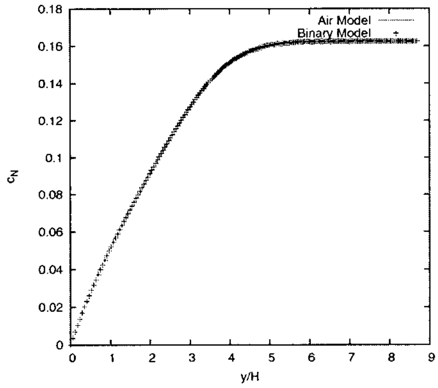


Figure 6.29 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, fully catalytic wall and $I_e/I_w = 0.95$

In the next example, we examine boundary layer flow at $T_w = 1000K$ and constant mass fractions at the wall using $c_{wO}/c_{eO} = 0.1$. The edge flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K, and $p_e = 0.001$ atm. Comparison of the result obtained using the five species air model solver with the result obtained using the binary mixture solver for nitrogen is shown in Fig. 6.30.

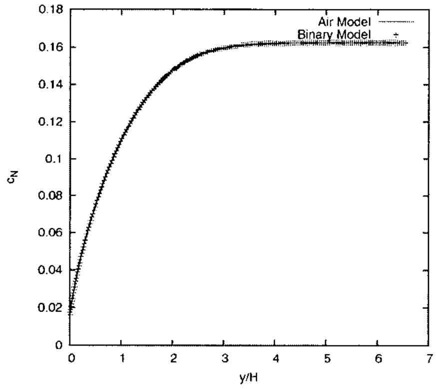


Figure 6.30 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, $T_w = 1000$ K, and $c_{wN}/c_{eN} = 0.1$

6.2.3 Tests for Five Species Air Model

Now, we explore the five species air model with equilibrium state of the air at the edge of the boundary layer. In this example, the external flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K, and $p_e = 0.01$ atm. Mass fraction of the species at the boundary-layer edge are assumed to be in chemical equilibrium. We consider a non-catalytic wall, and the total enthalpy at the wall: $I_w/I_e = 0.8$. Outside boundary-layer, one can see constant mass fraction of species, however we have some oscillation in the oxygen molecule mass fraction at the few last steps. This comes from a numerical error. The order of magnitude is "-5" which is negligible in this manner. The mass fractions of the chemical component of five species air model are shown in Fig. 6.31.

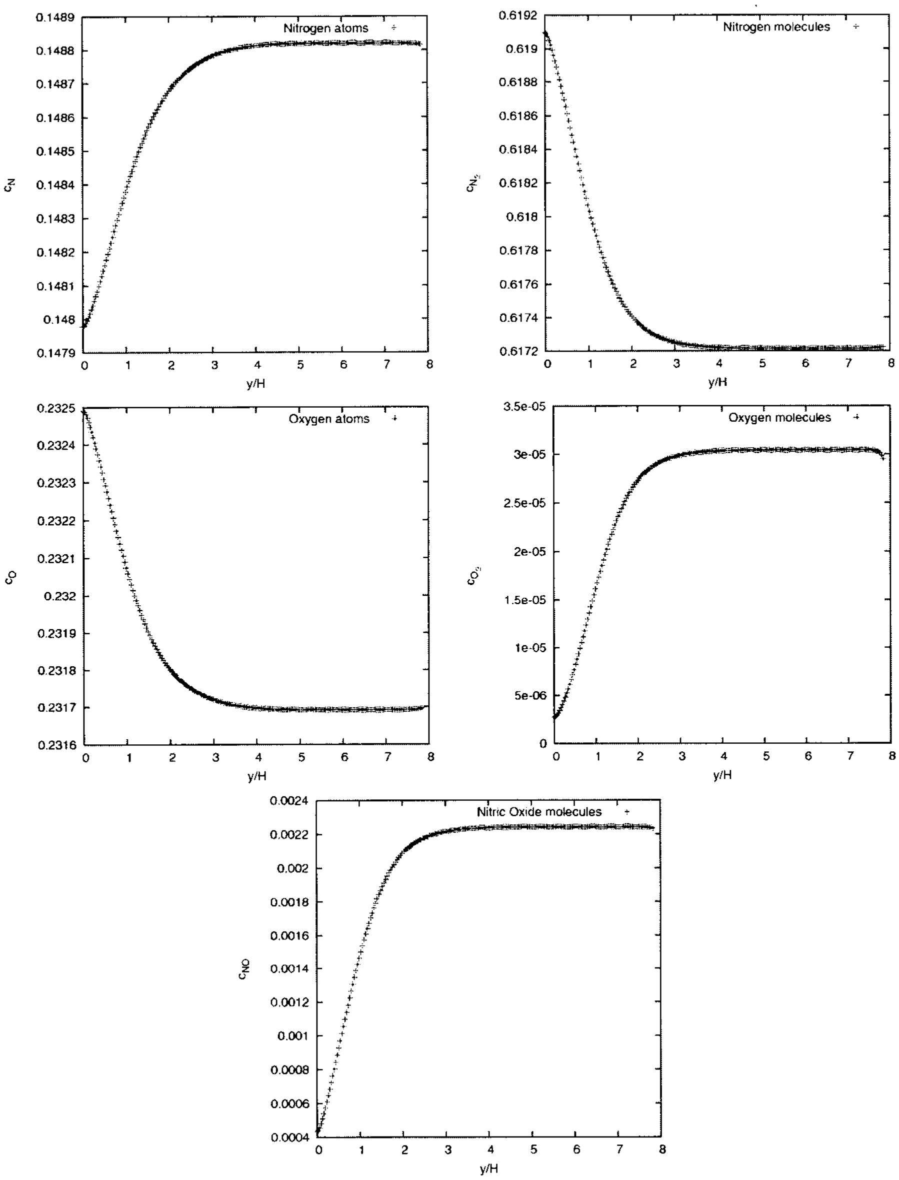
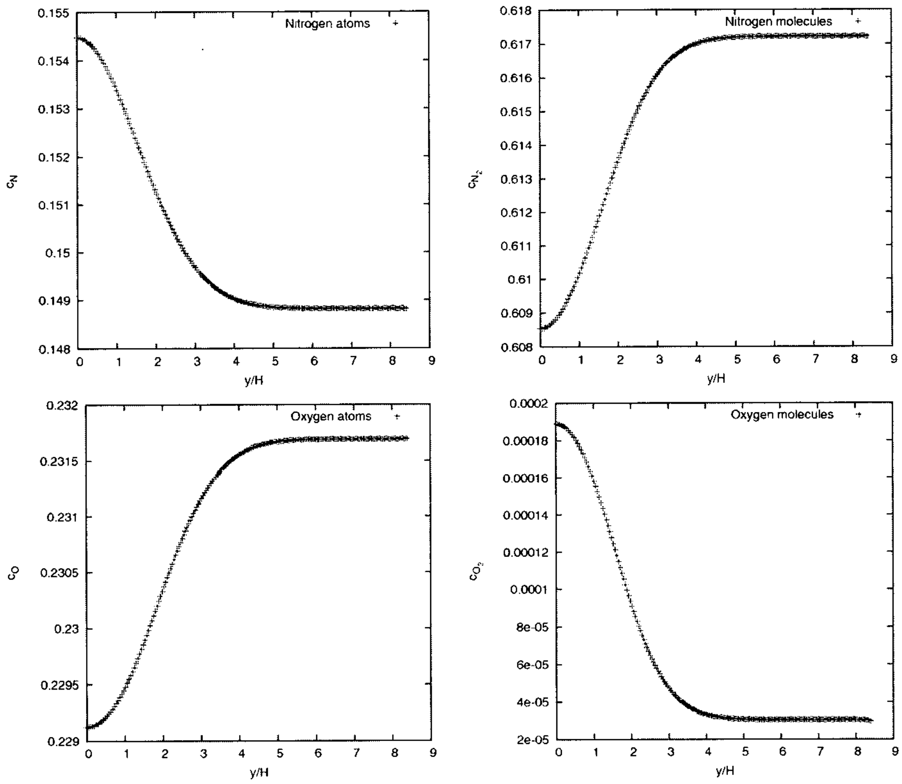


Figure 6.31 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, non-catalytic wall and $I_w/I_e = 0.8$

In the next example, we consider an adiabatic and non-catalytic wall. The edge flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K, and $p_e = 0.01$ atm. It can be still seen the numerical error in concentration of oxygen molecule at the last steps. The mass fractions of the chemical component of five species air model are shown in Fig. 6.32.



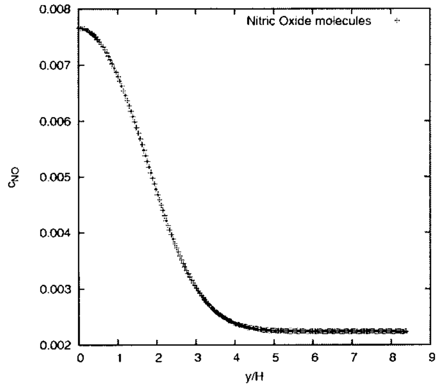


Figure 6.32 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, non-catalytic and adiabatic wall

In the next example, we examine the flow past equilibrium and adiabatic wall. The edge flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K, and $p_e = 0.001$ atm. Around 5000K, oxygen molecules dissociate and state as atoms. It is the reason that oxygen molecule has small order of magnitude and we can still observe oscillation at the last steps. From the mass conservation, we know that air contains around 23 percent of oxygen mass fraction in the air mixture. One can see that value from the mass fraction of oxygen atom figure. The mass fractions of the chemical component of five species air model are shown in Fig. 6.33.

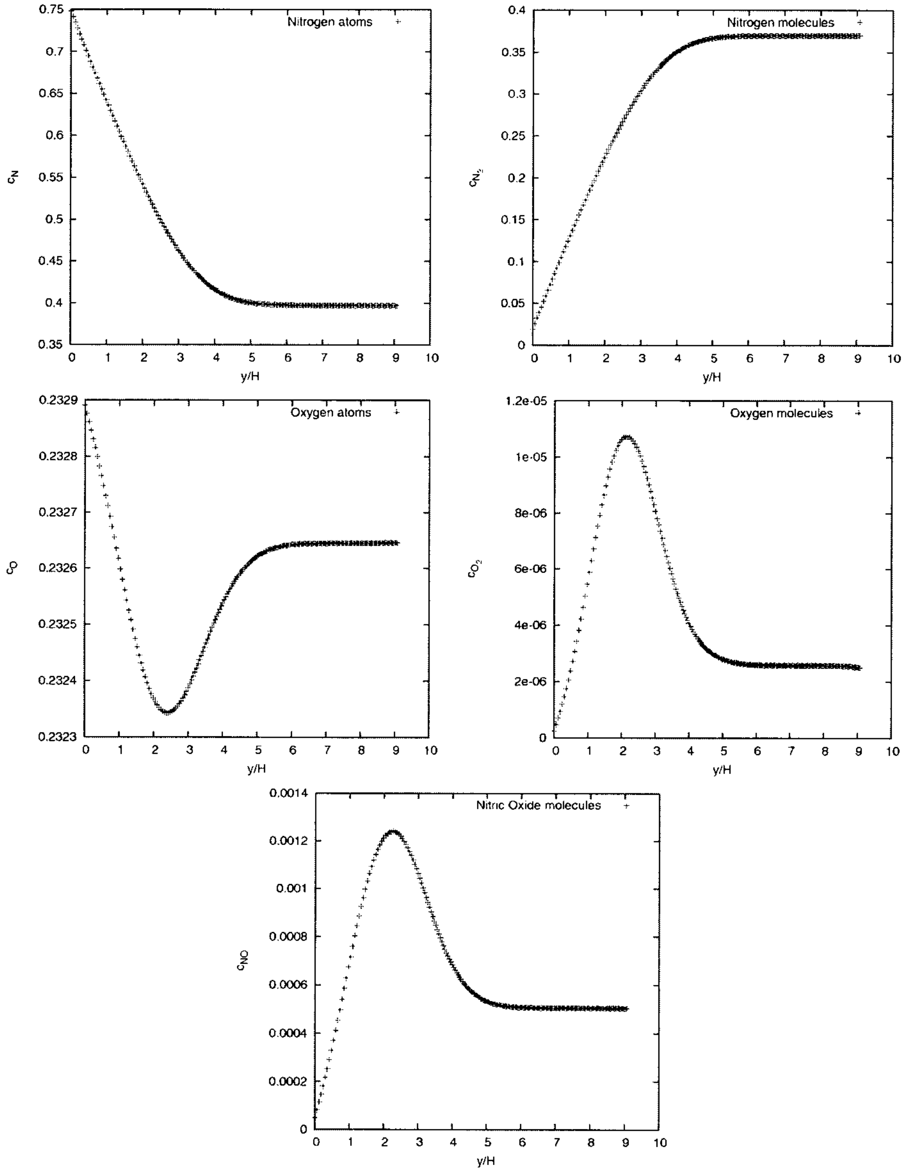
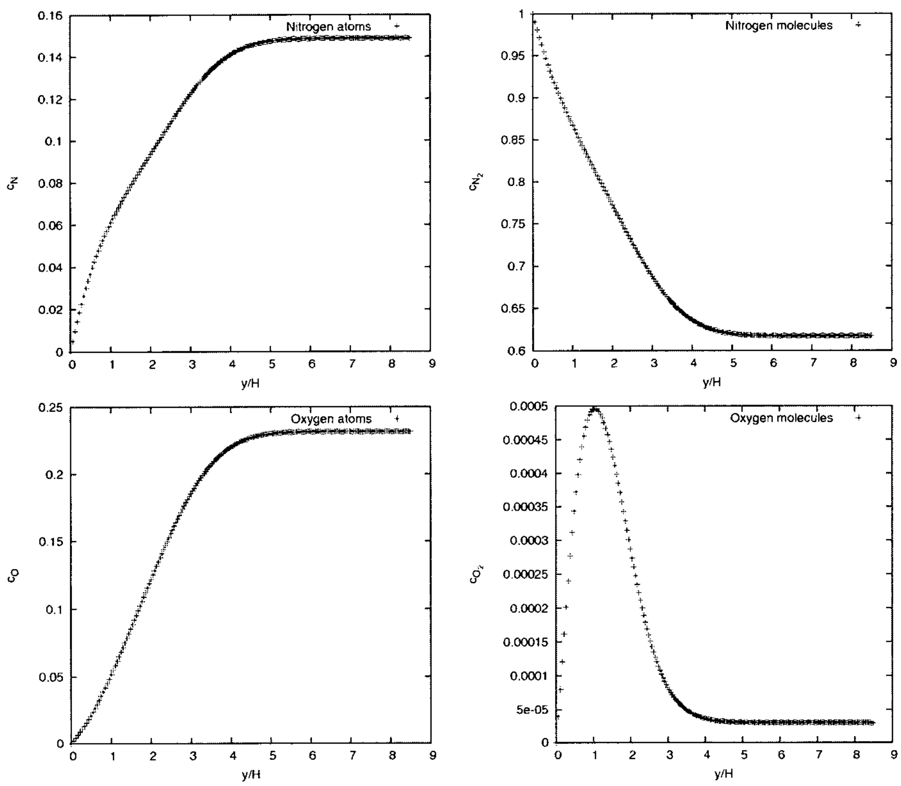


Figure 6.33 T_e = 5000 K, P_e = 0.001 atm, u_e = 2 km/s, equilibrium wall and $(dI/dy)_w = 0$

We examine fully catalytic wall and temperature at the wall is formulated for total enthalpy: $I_w/I_e = 0.95$. The edge flow parameters are $u_e = 2$ km/s, $T_e = 5000$ K, and $p_e = 0.01$ atm. The mass fractions of the chemical component of five species air model are shown in Fig. 6.34.



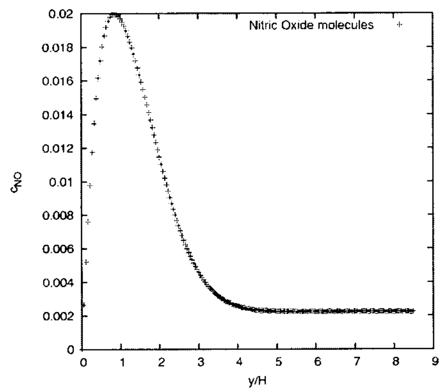
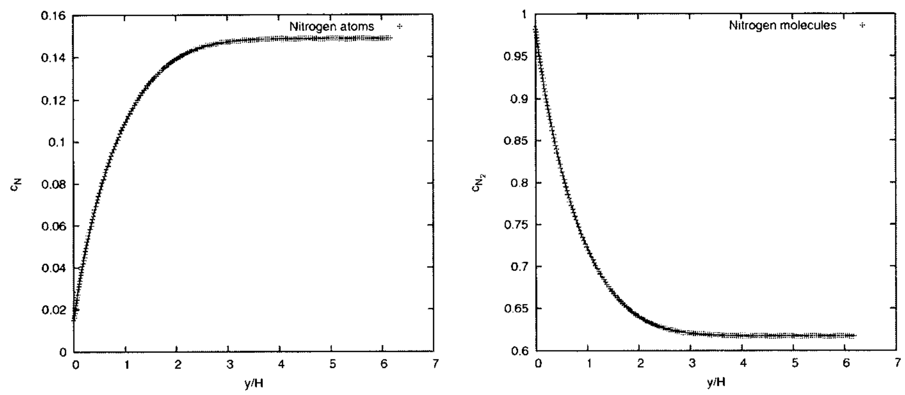


Figure 6.34 T_e = 5000 K, P_e = 0.01 atm, u_e = 2 km/s, fully catalytic wall and $I_w/I_e = 0.95$

In the next example, we examine boundary layer flow at T_w = 1000 K and constant mass fractions at the wall using $c_{wN}/c_{eN} = 0.1$, $c_{wO}/c_{eO} = c_{wO_2}/c_{eO_2} = c_{wNO}/c_{eNO} = 0$. The edge flow parameters are u_e = 2 km/s, T_e = 5000 K, and p_e = 0.01 atm. The mass fractions of the chemical component of five species air model are shown in Fig. 6.35.



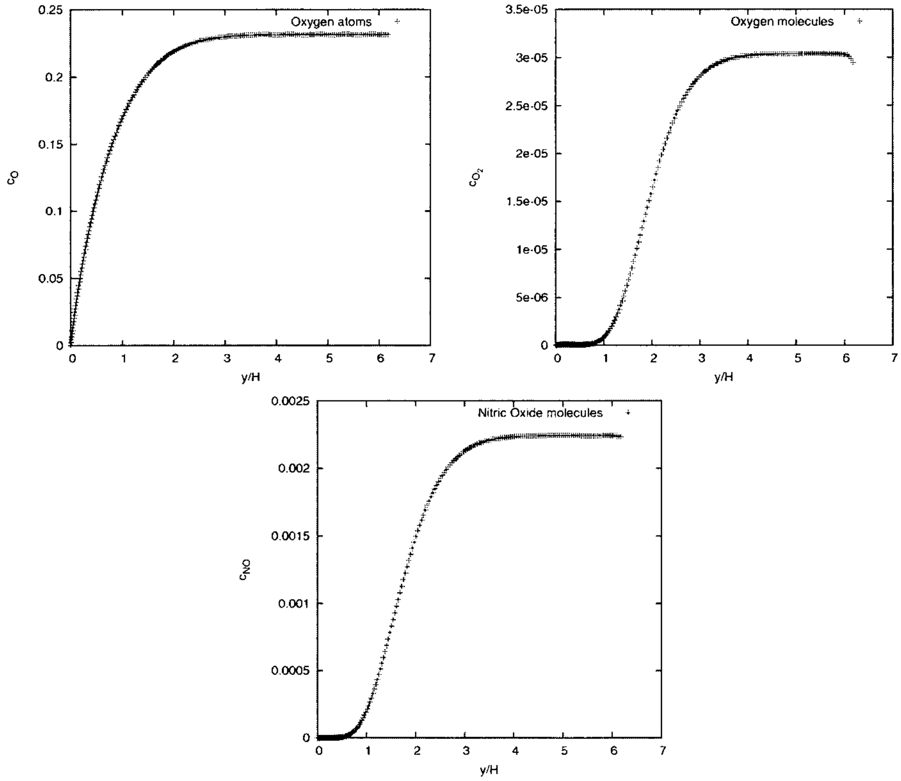


Figure 6.35 $T_e = 5000$ K, $P_e = 0.01$ atm, $u_e = 2$ km/s, $T_w = 1000$ K, and $c_{wN}/c_{eN} = 0.1$, $c_{wO}/c_{eO} = c_{wO_2}/c_{eO_2} = c_{wNO}/c_{eNO} = 0$

7. Conclusion and Future Work

We examined high-temperature chemically reacting boundary layer flow. We used the Levy-Lees-Dorodnitsyn transformation which allows for the consideration of different body shapes. First, we developed a numerical solver for binary mixtures of oxygen atoms and molecules and nitrogen atoms and molecules. We tested the solver by comparing its results with the Probstein's integrals and self-similarity solutions. This gave us confidence to expand our study to consider a five species air model. After writing a numerical solver for the five species air model, we compared its results with those of the binary mixture solver. We found good agreement between the two models. We then considered different boundary conditions. However, the five species solver has a problem at the edge of the computational domain (outside of the boundary layer). At some flow parameters, solution for mass fractions can possess oscillations. As part of our future work, we plan to resolve this issue.

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Appendix A: Numerical Formulation

The boundary layer equations are:

$$2\xi\left(\frac{\partial q_s}{\partial \xi}f' - q'_s\frac{\partial f}{\partial \xi}\right) = \left(\frac{C}{Sm_s}q'_s\right)' + q'_s f - \frac{2\xi}{c_{se}}\frac{dc_{se}}{d\xi}f' + \frac{2\xi W_s}{\rho\rho_e u_e^2\mu_e r_0^{2k}c_{se}}, \qquad \text{(A.1)}$$

$$(Cf'')' + ff'' + \beta\left[\frac{\rho_e}{\rho} - (f')^2\right] = 2\xi\left(f'\frac{\partial f'}{\partial \xi} - f''\frac{\partial f}{\partial \xi}\right), \qquad \text{(A.2)}$$

$$\left(\frac{C}{\mathrm{Pr}}g'\right)' + fg' = \frac{2\xi}{I_e}\frac{dI_e}{d\xi}gf' + \left[\sum_{s=1}^{ns}\frac{C}{Sm_s}\left(\frac{1}{Le_s} - 1\right)\frac{h_s c_{se}}{I_e}q_s'\right]' +$$

$$\frac{u_e^2}{I_e}\left[\left(\frac{1}{\mathrm{Pr}} - 1\right)Cf'f''\right]' + 2\xi\left(f'\frac{\partial g}{\partial \xi} - g'\frac{\partial f}{\partial \xi}\right). \qquad \text{(A.3)}$$

In our work, the species indices are attributed to the chemical elements as follows:

1 - molecules of nitrogen,

2 - atoms of nitrogen,

3 - molecules of oxygen,

4 - atoms of oxygen,

5 - molecules of nitric oxide.

As we know, summation of mass fraction for all species is 1. Therefore, we have:

$$c_{1e}q_1 + c_{2e}q_2 + c_{3e}q_3 + c_{4e}q_4 + c_{5e}q_5 = 1. \qquad \text{(A.4)}$$

Because we use the global mass conservation law for the mixture and introduced the stream function, we can exclude one of the species. In this work, we exclude nitrogen molecule and write mass fraction of nitrogen molecule by using mass fraction equation as following:

$$c_{1e}q_1 = 1 - (c_{2e}q_2 + c_{3e}q_3 + c_{4e}q_4 + c_{5e}q_5). \qquad \text{(A.5)}$$

We need to describe the new dependent variables. The new dependent variables Qs_j, Qd_j, F_j, and G_j are defined as follows:

$$q_2 = Qs_2,$$

$$q_3 = Qs_3,$$

$$q_4 = Qs_4,$$

$$q_5 = Qs_5,$$

$$q_2{}' = Qd_2,$$

$$q_3{}' = Qd_3,$$

$$q_4{}' = Qd_4,$$

$$q_5{}' = Qd_5,$$

$$f = F_1,$$

$$f' = F_2,$$

$$f'' = F_3,$$

$$g = G_1,$$

$$g' = G_2.$$

The boundary-layer equations are written as:

$$2\xi\left(\frac{\partial Qs_2}{\partial \xi}F_2 - Qd_2\frac{\partial F_1}{\partial \xi}\right) = \left(\frac{C}{Sm_2}Qd_2\right)' + Qd_2F_1 - \frac{2\xi}{c_{2e}}\frac{dc_{2e}}{d\xi}F_2 + \frac{2\xi W_N}{\rho\rho_e u_e^2 \mu_e r_0^{2k} c_{2e}}, \tag{A.6}$$

$$2\xi\left(\frac{\partial Qs_3}{\partial\xi}F_2 - Qd_3\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_3}Qd_3\right)' + Qd_3F_1 -$$
$$\frac{2\xi}{c_{3e}}\frac{dc_{3e}}{d\xi}F_2 + \frac{2\xi W_{O_2}}{\rho\rho_e u_e^2\mu_e r_0^{2k}c_{3e}}, \tag{A.7}$$

$$2\xi\left(\frac{\partial Qs_4}{\partial\xi}F_2 - Qd_4\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_4}Qd_4\right)' + Qd_4F_1 -$$
$$\frac{2\xi}{c_{4e}}\frac{dc_{4e}}{d\xi}F_2 + \frac{2\xi W_{O}}{\rho\rho_e u_e^2\mu_e r_0^{2k}c_{4e}}, \tag{A.8}$$

$$2\xi\left(\frac{\partial Qs_5}{\partial\xi}F_2 - Qd_5\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_5}Qd_5\right)' + Qd_5F_1 -$$
$$\frac{2\xi}{c_{5e}}\frac{dc_{5e}}{d\xi}F_2 + \frac{2\xi W_{NO}}{\rho\rho_e u_e^2\mu_e r_0^{2k}c_{5e}}, \tag{A.9}$$

$$(CF_3)' + F_1F_3 + \beta\left[\frac{\rho_e}{\rho} - F_2^2\right] = 2\xi\left(F_2\frac{\partial F_2}{\partial\xi} - F_3\frac{\partial F_1}{\partial\xi}\right), \tag{A.10}$$

$$\left(\frac{C}{\Pr}G_2\right)' + F_1G_2 = \frac{2\xi}{I_e}\frac{dI_e}{d\xi}G_1F_2 +$$
$$\left[\frac{C}{Sm_1}\left(\frac{1}{Le_1} - 1\right)\frac{(-c_{2e}Qd_2 - c_{3e}Qd_3 - c_{4e}Qd_4 - c_{5e}Qd_5)}{I_e}h_1\right]'$$
$$+\left[\frac{C}{Sm_2}\left(\frac{1}{Le_2} - 1\right)\frac{c_{2e}Qd_2}{I_e}h_2\right]' + \left[\frac{C}{Sm_3}\left(\frac{1}{Le_3} - 1\right)\frac{c_{3e}Qd_3}{I_e}h_3\right]'$$
$$+\left[\frac{C}{Sm_4}\left(\frac{1}{Le_4} - 1\right)\frac{c_{4e}Qd_4}{I_e}h_4\right]' + \left[\frac{C}{Sm_5}\left(\frac{1}{Le_5} - 1\right)\frac{c_{5e}Qd_5}{I_e}h_5\right]' \tag{A.11}$$
$$\frac{u_e^2}{I_e}\left[\left(\frac{1}{\Pr} - 1\right)CF_2F_3\right]' + 2\xi\left(F_2\frac{\partial G_1}{\partial\xi} - G_2\frac{\partial F_1}{\partial\xi}\right).$$

The definition of new notations leads to the following first-order equations:

$$Qs_2{}' = Qd_2,$$

$$Qs_3{}' = Qd_3,$$

$$Qs_4{}' = Qd_4,$$

$$Qs_5{}' = Qd_5,$$

$$F_1' = F_2,$$

$$F_2' = F_3,$$

$$G_1' = G_2,$$

The first order equations are discretized and written for the midpoint $\xi^n, \eta_{j-1/2}$ as follows:

$$\frac{Qs_{2j}^n - Qs_{2j-1}^n}{h_j} = \frac{Qd_{2j}^n + Qd_{2j-1}^n}{2} \equiv Qd_{2j-1/2}^n, \tag{A.12}$$

$$\frac{Qs_{3j}^n - Qs_{3j-1}^n}{h_j} = \frac{Qd_{3j}^n + Qd_{3j-1}^n}{2} \equiv Qd_{3j-1/2}^n, \tag{A.13}$$

$$\frac{Qs_{4j}^n - Qs_{4j-1}^n}{h_j} = \frac{Qd_{4j}^n + Qd_{4j-1}^n}{2} \equiv Qd_{4j-1/2}^n, \tag{A.14}$$

$$\frac{Qs_{5j}^n - Qs_{5j-1}^n}{h_j} = \frac{Qd_{5j}^n + Qd_{5j-1}^n}{2} \equiv Qd_{5j-1/2}^n, \tag{A.15}$$

$$\frac{F_{1j}^n - F_{1j-1}^n}{h_j} = \frac{F_{2j}^n + F_{2j-1}^n}{2} \equiv F_{2j-1/2}^n, \tag{A.16}$$

$$\frac{F_{2j}^n - F_{2j-1}^n}{h_j} = \frac{F_{3j}^n + F_{3j-1}^n}{2} \equiv F_{3j-1/2}^n, \tag{A.17}$$

$$\frac{G_{1j}^n - G_{1j-1}^n}{h_j} = \frac{G_{2j}^n + G_{2j-1}^n}{2} \equiv G_{2j-1/2}^n. \tag{A.18}$$

Equations of boundary layer are also written for midpoint $\xi^{n-1/2}, \eta_{j-1/2}$ as follows. We begin with the species conservation and write down the equation at the point $\xi^{n-1/2}$.

Mass Conservation Equations

Mass conservation equations for each species are:

$$2\xi\left(\frac{\partial Qs_2}{\partial\xi}F_2 - Qd_2\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_2}Qd_2\right)' + Qd_2F_1 - \frac{2\xi}{c_{2e}}\frac{dc_{2e}}{d\xi}F_2 + \frac{2\xi W_N}{\rho\rho_e u_e^2\mu_e r_0^{2k} c_{2e}}, \tag{A.19}$$

$$2\xi\left(\frac{\partial Qs_3}{\partial\xi}F_2 - Qd_3\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_3}Qd_3\right)' + Qd_3F_1 - \frac{2\xi}{c_{3e}}\frac{dc_{3e}}{d\xi}F_2 + \frac{2\xi W_{O_2}}{\rho\rho_e u_e^2\mu_e r_0^{2k} c_{3e}}, \tag{A.20}$$

$$2\xi\left(\frac{\partial Qs_4}{\partial\xi}F_2 - Qd_4\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_4}Qd_4\right)' + Qd_4F_1 - \frac{2\xi}{c_{4e}}\frac{dc_{4e}}{d\xi}F_2 + \frac{2\xi W_O}{\rho\rho_e u_e^2\mu_e r_0^{2k} c_{4e}}, \tag{A.21}$$

$$2\xi\left(\frac{\partial Qs_5}{\partial\xi}F_2 - Qd_5\frac{\partial F_1}{\partial\xi}\right) = \left(\frac{C}{Sm_5}Qd_5\right)' + Qd_5F_1 - \frac{2\xi}{c_{5e}}\frac{dc_{5e}}{d\xi}F_2 + \frac{2\xi W_{NO}}{\rho\rho_e u_e^2\mu_e r_0^{2k} c_{5e}}, \tag{A.22}$$

$$(CF_3)' + F_1F_3 + \beta\left[\frac{\rho_e}{\rho} - F_2^2\right] = 2\xi\left(F_2\frac{\partial F_2}{\partial\xi} - F_3\frac{\partial F_1}{\partial\xi}\right), \tag{A.23}$$

Before we begin to discretize the equations, we define the mass conservation equations as follows:

$$P_2 \equiv \left(\frac{C}{Sm_2}Qd_2\right)' + Qd_2F_1 - \frac{2\xi}{c_{2e}}\frac{dc_{2e}}{d\xi}F_2 + \frac{2\xi W_N}{\rho\rho_e u_e^2\mu_e r_0^{2k} c_{2e}} = 2\xi\left(\frac{\partial Qs_2}{\partial\xi}F_2 - Qd_2\frac{\partial F_1}{\partial\xi}\right), \tag{A.24}$$

$$P_3 \equiv \left(\frac{C}{Sm_3} Qd_3\right)' + Qd_3 F_1 - \frac{2\xi}{c_{3e}} \frac{dc_{3e}}{d\xi} F_2 + \frac{2\xi W_{O_2}}{\rho\rho_e u_e^2 \mu_e r_0^{2k} c_{3e}} =$$
$$2\xi \left(\frac{\partial Qs_3}{\partial \xi} F_2 - Qd_3 \frac{\partial F_1}{\partial \xi}\right), \tag{A.25}$$

$$P_4 \equiv \left(\frac{C}{Sm_4} Qd_4\right)' + Qd_4 F_1 - \frac{2\xi}{c_{4e}} \frac{dc_{4e}}{d\xi} F_2 + \frac{2\xi W_{O}}{\rho\rho_e u_e^2 \mu_e r_0^{2k} c_{4e}} =$$
$$2\xi \left(\frac{\partial Qs_4}{\partial \xi} F_2 - Qd_4 \frac{\partial F_1}{\partial \xi}\right), \tag{A.26}$$

$$P_5 \equiv \left(\frac{C}{Sm_5} Qd_5\right)' + Qd_5 F_1 - \frac{2\xi}{c_{5e}} \frac{dc_{5e}}{d\xi} F_2 + \frac{2\xi W_{NO}}{\rho\rho_e u_e^2 \mu_e r_0^{2k} c_{5e}} =$$
$$2\xi \left(\frac{\partial Qs_5}{\partial \xi} F_2 - Qd_5 \frac{\partial F_1}{\partial \xi}\right). \tag{A.27}$$

Discretize the equations for point $\xi^{n-1/2}$ as:

$$\frac{1}{2}\left(P_2^n + P_2^{n-1}\right) =$$
$$2\xi^{n-1/2}\left[\frac{\left(Qs_2^n - Qs_2^{n-1}\right)}{\left(\xi^n - \xi^{n-1}\right)} \frac{\left(F_2^n + F_2^{n-1}\right)}{2} - \frac{\left(Qd_2^n + Qd_2^{n-1}\right)}{2} \frac{\left(F_2^n - F_2^{n-1}\right)}{\left(\xi^n - \xi^{n-1}\right)}\right], \tag{A.28}$$

$$P_2^n - 2\xi^{n-1/2}\frac{Qs_2^nF_2^n + Qs_2^nF_2^{n-1} - Qs_2^{n-1}F_2^n - Qd_2^nF_2^n + Qd_2^nF_2^{n-1} - Qd_2^{n-1}F_2^n}{k_n} =$$

$$-2\xi^{n-1/2}\left(\frac{Qs_2^{n-1}F_2^{n-1} - Qd_2^{n-1}F_2^{n-1}}{k_n}\right) - P_2^{n-1}, \tag{A.29}$$

where $k_n = (\xi^n - \xi^{n-1})$.

The other equations for species are written as follows:

$$P_3^n - 2\xi^{n-1/2}\frac{Qs_3^nF_2^n + Qs_3^nF_2^{n-1} - Qs_3^{n-1}F_2^n - Qd_3^nF_2^n + Qd_3^nF_2^{n-1} - Qd_3^{n-1}F_2^n}{k_n} =$$

$$-2\xi^{n-1/2}\left(\frac{Qs_3^{n-1}F_2^{n-1} - Qd_3^{n-1}F_2^{n-1}}{k_n}\right) - P_3^{n-1}, \tag{A.30}$$

$$P_4^n - 2\xi^{n-1/2}\frac{Qs_4^nF_2^n + Qs_4^nF_2^{n-1} - Qs_4^{n-1}F_2^n - Qd_4^nF_2^n + Qd_4^nF_2^{n-1} - Qd_4^{n-1}F_2^n}{k_n} =$$

$$-2\xi^{n-1/2}\left(\frac{Qs_4^{n-1}F_2^{n-1} - Qd_4^{n-1}F_2^{n-1}}{k_n}\right) - P_4^{n-1}, \tag{A.31}$$

$$P_5^n - 2\xi^{n-1/2}\frac{Qs_5^nF_2^n + Qs_5^nF_2^{n-1} - Qs_5^{n-1}F_2^n - Qd_5^nF_2^n + Qd_5^nF_2^{n-1} - Qd_5^{n-1}F_2^n}{k_n} =$$

$$-2\xi^{n-1/2}\left(\frac{Qs_5^{n-1}F_2^{n-1} - Qd_5^{n-1}F_2^{n-1}}{k_n}\right) - P_5^{n-1}. \tag{A.32}$$

Next step is to write Eq. (A.29) at the point $\eta_{j-1/2}$.

$$P^n_{2j-1/2} - 2\xi^{n-1/2}\left(\frac{Qs^n_{2j-1/2}F^n_{2j-1/2} + Qs^n_{2j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{2j-1/2}F^n_{2j-1/2} - Qd^n_{2j-1/2}F^n_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{Qd^n_{2j-1/2}F^{n-1}_{2j-1/2} - Qd^{n-1}_{2j-1/2}F^n_{2j-1/2}}{k_n}\right) = \tag{A.33}$$
$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{2j-1/2}F^{n-1}_{2j-1/2} - Qd^{n-1}_{2j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right) - P^{n-1}_{2j-1/2},$$

Using same procedure, we obtain the discretized at the point $\eta_{j-1/2}$ mass conservation equations for other species as follows:

$$P^n_{3j-1/2} - 2\xi^{n-1/2}\left(\frac{Qs^n_{3j-1/2}F^n_{2j-1/2} + Qs^n_{3j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{3j-1/2}F^n_{2j-1/2} - Qd^n_{3j-1/2}F^n_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{Qd^n_{3j-1/2}F^{n-1}_{2j-1/2} - Qd^{n-1}_{3j-1/2}F^n_{2j-1/2}}{k_n}\right) = \tag{A.34}$$
$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{3j-1/2}F^{n-1}_{2j-1/2} - Qd^{n-1}_{3j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right) - P^{n-1}_{3j-1/2},$$

$$P^n_{4j-1/2} - 2\xi^{n-1/2}\left(\frac{Qs^n_{4j-1/2}F^n_{2j-1/2} + Qs^n_{4j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{4j-1/2}F^n_{2j-1/2} - Qd^n_{4j-1/2}F^n_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{Qd^{n}_{4j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{4j-1/2}F^{n}_{2j-1/2}}{k_n}\right)= \tag{A.35}$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{4j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{4j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)-P^{n-1}_{4j-1/2},$$

$$P^{n}_{5j-1/2}-2\xi^{n-1/2}\left(\frac{Qs^{n}_{5j-1/2}F^{n}_{2j-1/2}+Qs^{n}_{5j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{5j-1/2}F^{n}_{2j-1/2}-Qd^{n}_{5j-1/2}F^{n}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{Qd^{n}_{5j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{5j-1/2}F^{n}_{2j-1/2}}{k_n}\right)= \tag{A.36}$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{5j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{5j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)-P^{n-1}_{5j-1/2}.$$

From the definition Eqs. (A.24) through (A.27), we can also write the equations at the point $\eta_{j-1/2}$ as follows:

$$P^{n}_{2j-1/2}=\frac{\left(\frac{C}{Sm_2}\right)^{n}_{j}Qd^{n}_{2j}-\left(\frac{C}{Sm_2}\right)^{n}_{j-1}Qd^{n}_{2j-1}}{h_j}+$$

$$(Qd_2F_1)^{n}_{j-1/2}-ms^{n}_{2}F^{n}_{2j-1/2}+md^{n}_{2}\left(\frac{W_N}{\rho}\right)^{n}_{j-1/2}, \tag{A.37}$$

$$P^n_{3j-1/2} = \frac{\left(\frac{C}{Sm_3}\right)^n_j Qd^n_{3j} - \left(\frac{C}{Sm_3}\right)^n_{j-1} Qd^n_{3j-1}}{h_j} +$$

$$(Qd_3F_1)^n_{j-1/2} - ms^n_3 F^n_{2j-1/2} + md^n_3 \left(\frac{W_{O_2}}{\rho}\right)^n_{j-1/2}, \tag{A.38}$$

$$P^n_{4j-1/2} = \frac{\left(\frac{C}{Sm_4}\right)^n_j Qd^n_{4j} - \left(\frac{C}{Sm_4}\right)^n_{j-1} Qd^n_{4j-1}}{h_j} +$$

$$(Qd_4F_1)^n_{j-1/2} - ms^n_4 F^n_{2j-1/2} + md^n_4 \left(\frac{W_O}{\rho}\right)^n_{j-1/2}, \tag{A.39}$$

$$P^n_{5j-1/2} = \frac{\left(\frac{C}{Sm_5}\right)^n_j Qd^n_{5j} - \left(\frac{C}{Sm_5}\right)^n_{j-1} Qd^n_{5j-1}}{h_j} +$$

$$(Qd_5F_1)^n_{j-1/2} - ms^n_5 F^n_{2j-1/2} + md^n_5 \left(\frac{W_{NO}}{\rho}\right)^n_{j-1/2}, \tag{A.40}$$

where $ms_2 = \frac{2\xi}{c_{2e}}\frac{dc_{2e}}{d\xi}$, $ms_3 = \frac{2\xi}{c_{3e}}\frac{dc_{3e}}{d\xi}$, $ms_4 = \frac{2\xi}{c_{4e}}\frac{dc_{4e}}{d\xi}$, $ms_5 = \frac{2\xi}{c_{5e}}\frac{dc_{5e}}{d\xi}$, $md_2 = \frac{2\xi}{\rho_e u_e^2 \mu_e r_0^{2k} c_{2e}}$, $md_3 = \frac{2\xi}{\rho_e u_e^2 \mu_e r_0^{2k} c_{3e}}$, $md_4 = \frac{2\xi}{\rho_e u_e^2 \mu_e r_0^{2k} c_{4e}}$, $md_5 = \frac{2\xi}{\rho_e u_e^2 \mu_e r_0^{2k} c_{5e}}$.

Final form of the mass conservation equations are written as:

$$\frac{\left(\frac{C}{Sm_2}\right)^n_j Qd^n_{2j} - \left(\frac{C}{Sm_2}\right)^n_{j-1} Qd^n_{2j-1}}{h_j} +$$

$$(Qd_2F_1)^n_{j-1/2} - ms^n_2 F^n_{2j-1/2} + md^n_2 \left(\frac{W_N}{\rho}\right)^n_{j-1/2}$$

$$-2\xi^{n-1/2}\left(\frac{Qs^n_{2j-1/2}F^n_{2j-1/2} + Qs^n_{2j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{2j-1/2}F^{n}_{2j-1/2}-Qd^{n}_{2j-1/2}F^{n}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{Qd^{n}_{2j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{2j-1/2}F^{n}_{2j-1/2}}{k_n}\right)=$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{2j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{2j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-\frac{\left(\frac{C}{Sm_2}\right)^{n-1}_{j}Qd^{n-1}_{2j}+\left(\frac{C}{Sm_2}\right)^{n-1}_{j-1}Qd^{n-1}_{2j-1}}{h_j}-$$

$$(Qd_2F_1)^{n-1}_{j-1/2}+ms^{n-1}_2F^{n-1}_{2j-1/2}-md^{n-1}_2\left(\frac{W_N}{\rho}\right)^{n-1}_{j-1/2} \quad \text{(A.41)}$$

$$\frac{\left(\frac{C}{Sm_3}\right)^{n}_{j}Qd^{n}_{3j}-\left(\frac{C}{Sm_3}\right)^{n}_{j-1}Qd^{n}_{3j-1}}{h_j}+$$

$$(Qd_3F_1)^{n}_{j-1/2}-ms^{n}_3F^{n}_{2j-1/2}+md^{n}_3\left(\frac{W_{O_2}}{\rho}\right)^{n}_{j-1/2}$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n}_{3j-1/2}F^{n}_{2j-1/2}+Qs^{n}_{3j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{3j-1/2}F^{n}_{2j-1/2}-Qd^{n}_{3j-1/2}F^{n}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{Qd^{n}_{3j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{3j-1/2}F^{n}_{2j-1/2}}{k_n}\right)=$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{3j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{3j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-\frac{\left(\frac{C}{Sm_3}\right)^{n-1}_{j}Qd^{n-1}_{3j}+\left(\frac{C}{Sm_3}\right)^{n-1}_{j-1}Qd^{n-1}_{3j-1}}{h_j}-$$

$$(Qd_3F_1)^{n-1}_{j-1/2} + ms_3^{n-1}F^{n-1}_{2j-1/2} - md_3^{n-1}\left(\frac{W_{O_2}}{\rho}\right)^{n-1}_{j-1/2} \tag{A.42}$$

$$\frac{\left(\frac{C}{Sm_4}\right)^n_j Qd^n_{4j} - \left(\frac{C}{Sm_4}\right)^n_{j-1} Qd^n_{4j-1}}{h_j} +$$
$$(Qd_4F_1)^n_{j-1/2} - ms_4^nF^n_{2j-1/2} + md_4^n\left(\frac{W_O}{\rho}\right)^n_{j-1/2}$$
$$-2\xi^{n-1/2}\left(\frac{Qs^n_{4j-1/2}F^n_{2j-1/2} + Qs^n_{4j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{4j-1/2}F^n_{2j-1/2} - Qd^n_{4j-1/2}F^n_{2j-1/2}}{k_n}\right)$$
$$-2\xi^{n-1/2}\left(\frac{Qd^n_{4j-1/2}F^{n-1}_{2j-1/2} - Qd^{n-1}_{4j-1/2}F^n_{2j-1/2}}{k_n}\right) =$$
$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{4j-1/2}F^{n-1}_{2j-1/2} - Qd^{n-1}_{4j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$
$$-\frac{\left(\frac{C}{Sm_4}\right)^{n-1}_j Qd^{n-1}_{4j} + \left(\frac{C}{Sm_4}\right)^{n-1}_{j-1} Qd^{n-1}_{4j-1}}{h_j} -$$
$$(Qd_4F_1)^{n-1}_{j-1/2} + ms_4^{n-1}F^{n-1}_{2j-1/2} - md_4^{n-1}\left(\frac{W_O}{\rho}\right)^{n-1}_{j-1/2} \tag{A.43}$$

$$\frac{\left(\frac{C}{Sm_5}\right)^n_j Qd^n_{5j} - \left(\frac{C}{Sm_5}\right)^n_{j-1} Qd^n_{5j-1}}{h_j} +$$
$$(Qd_5F_1)^n_{j-1/2} - ms_5^nF^n_{2j-1/2} + md_5^n\left(\frac{W_{NO}}{\rho}\right)^n_{j-1/2}$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n}_{5j-1/2}F^{n}_{2j-1/2}+Qs^{n}_{5j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{-Qs^{n-1}_{5j-1/2}F^{n}_{2j-1/2}-Qd^{n}_{5j-1/2}F^{n}_{2j-1/2}}{k_n}\right)$$

$$-2\xi^{n-1/2}\left(\frac{Qd^{n}_{5j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{5j-1/2}F^{n}_{2j-1/2}}{k_n}\right)=$$

$$-2\xi^{n-1/2}\left(\frac{Qs^{n-1}_{5j-1/2}F^{n-1}_{2j-1/2}-Qd^{n-1}_{5j-1/2}F^{n-1}_{2j-1/2}}{k_n}\right)$$

$$-\frac{\left(\frac{C}{Sm_5}\right)^{n-1}_{j}Qd^{n-1}_{5j}+\left(\frac{C}{Sm_5}\right)^{n-1}_{j-1}Qd^{n-1}_{5j-1}}{h_j}-$$

$$(Qd_5F_1)^{n-1}_{j-1/2}+ms^{n-1}_5F^{n-1}_{2j-1/2}-md^{n-1}_5\left(\frac{W_{NO}}{\rho}\right)^{n-1}_{j-1/2} \qquad \text{(A.44)}$$

Momentum Equation

The momentum equation is written as:

$$(CF_3)' + F_1F_3 + \beta\left[\frac{\rho_e}{\rho} - F_2^2\right] = 2\xi\left(F_2\frac{\partial F_2}{\partial\xi} - F_3\frac{\partial F_1}{\partial\xi}\right). \tag{A.45}$$

Before we begin to discretize the momentum equation, we define the momentum equation as follows:

$$L \equiv (CF_3)' + F_1F_3 + \beta\left[\frac{\rho_e}{\rho} - F_2^2\right] = 2\xi\left(F_2\frac{\partial F_2}{\partial\xi} - F_3\frac{\partial F_1}{\partial\xi}\right). \tag{A.46}$$

The momentum equation is discretized at $\xi^{n-1/2}$ point as follows:

$$\frac{1}{2}\left(L^n + L^{n-1}\right) = 2\xi^{n-1/2}\left[\frac{\left(F_2^2\right)^n - \left(F_2^2\right)^{n-1}}{2\left(\xi^n - \xi^{n-1}\right)} - \frac{F_3^n + F_3^{n-1}}{2}\frac{F_1^n - F_1^{n-1}}{\left(\xi^n - \xi^{n-1}\right)}\right], \tag{A.47}$$

$$L^n - 2\xi^{n-1/2}\frac{\left(F_2^2\right)^n - F_3^nF_1^n + F_3^nF_1^{n-1} - F_3^{n-1}F_1^n}{k_n} = \frac{2\xi^{n-1/2}}{k_n}\left(-\left(F_2^2\right)^{n-1} + F_3^{n-1}F_1^{n-1}\right) - L^{n-1}. \tag{A.48}$$

The next step is to write the equation at the point $\eta_{j-1/2}$.

$$L_{j-1/2}^n - 2\xi^{n-1/2}\frac{\left(F_2^2\right)_{j-1/2}^n - F_{3j-1/2}^nF_{1j-1/2}^n + F_{3j-1/2}^nF_{1j-1/2}^{n-1} - F_{3j-1/2}^{n-1}F_{1j-1/2}^n}{k_n} = \frac{2\xi^{n-1/2}}{k_n}\left(-\left(F_2^2\right)_{j-1/2}^{n-1} + F_{3j-1/2}^{n-1}F_{1j-1/2}^{n-1}\right) - L_{j-1/2}^{n-1}. \tag{A.49}$$

Finally, we can obtain final version of the momentum equation;

$$\frac{C_j^nF_{3j}^n - C_{j-1}^nF_{3j-1}^n}{h_j} + \left(F_1F_3\right)_{j-1/2}^n + \beta^n\left[\left(\frac{\rho_e}{\rho}\right)_{j-1/2}^n - \left(F_2^2\right)_{j-1/2}^n\right] +$$

$$2\xi^{n-1/2}\frac{-\left(F_2^2\right)_{j-1/2}^{n}+F_{3j-1/2}^{n}F_{1j-1/2}^{n}-F_{3j-1/2}^{n}F_{1j-1/2}^{n-1}+F_{3j-1/2}^{n-1}F_{1j-1/2}^{n}}{k_n}=$$

$$\frac{2\xi^{n-1/2}}{k_n}\left(-\left(F_2^2\right)_{j-1/2}^{n-1}+F_{3j-1/2}^{n-1}F_{1j-1/2}^{n-1}\right)-$$

$$\frac{C_j^{n-1}F_{3j}^{n-1}-C_{j-1}^{n-1}F_{3j-1}^{n-1}}{h_j}-\left(F_1F_3\right)_{j-1/2}^{n-1}-\beta^{n-1}\left[\left(\frac{\rho_e}{\rho}\right)_{j-1/2}^{n-1}-\left(F_2^2\right)_{j-1/2}^{n-1}\right]. \quad \text{(A.50)}$$

Energy Equation

The energy equation is written as:

$$\left(\frac{C}{\Pr}G_2\right)' + F_1G_2 = \frac{2\xi}{I_e}\frac{dI_e}{d\xi}G_1F_2+$$
$$\left[\frac{C}{Sm_1}\left(\frac{1}{Le_1}-1\right)\frac{(-c_{2e}Qd_2 - c_{3e}Qd_3 - c_{4e}Qd_4 - c_{5e}Qd_5)}{I_e}h_1\right]'$$
$$+\left[\frac{C}{Sm_2}\left(\frac{1}{Le_2}-1\right)\frac{c_{2e}Qd_2}{I_e}h_2\right]' + \left[\frac{C}{Sm_3}\left(\frac{1}{Le_3}-1\right)\frac{c_{3e}Qd_3}{I_e}h_3\right]'$$
$$+\left[\frac{C}{Sm_4}\left(\frac{1}{Le_4}-1\right)\frac{c_{4e}Qd_4}{I_e}h_4\right]' + \left[\frac{C}{Sm_5}\left(\frac{1}{Le_5}-1\right)\frac{c_{5e}Qd_5}{I_e}h_5\right]'$$
$$\frac{u_e^2}{I_e}\left[\left(\frac{1}{\Pr}-1\right)CF_2F_3\right]' + 2\xi\left(F_2\frac{\partial G_1}{\partial \xi} - G_2\frac{\partial F_1}{\partial \xi}\right). \tag{A.51}$$

Before we begin to discretize the energy equation, we define the energy equation as follows:

$$T \equiv \left(\frac{C}{\Pr}G_2 - \frac{u_e^2}{I_e}\left(\frac{1}{\Pr}-1\right)CF_2F_3\right)' -$$
$$\left(\frac{C}{Sm_1}\left(\frac{1}{Le_1}-1\right)\frac{(-c_{2e}Qd_2 - c_{3e}Qd_3 - c_{4e}Qd_4 - c_{5e}Qd_5)}{I_e}h_1\right)' -$$
$$\left(\frac{C}{Sm_2}\left(\frac{1}{Le_2}-1\right)\frac{c_{2e}Qd_2}{I_e}h_2 + \frac{C}{Sm_3}\left(\frac{1}{Le_3}-1\right)\frac{c_{3e}Qd_3}{I_e}h_3\right)' -$$
$$\left(\frac{C}{Sm_4}\left(\frac{1}{Le_4}-1\right)\frac{c_{4e}Qd_4}{I_e}h_4 + \frac{C}{Sm_5}\left(\frac{1}{Le_5}-1\right)\frac{c_{5e}Qd_5}{I_e}h_5\right)' +$$
$$F_1G_2 - \frac{2\xi}{I_e}\frac{dI_e}{d\xi}G_1F_2 = 2\xi\left(F_2\frac{\partial G_1}{\partial \xi} - G_2\frac{\partial F_1}{\partial \xi}\right). \tag{A.52}$$

The next step is to write the equation at the point $\xi^{n-1/2}$.

$$T^n + T^{n-1} = \frac{2\xi^{n-1/2}}{k_n}\left(\left(F_2^n + F_2^{n-1}\right)\left(G_1^n - G_1^{n-1}\right)\right)$$

$$-\frac{2\xi^{n-1/2}}{k_n}\left(\left(G_2^n+G_2^{n-1}\right)\left(F_1^n-F_1^{n-1}\right)\right). \tag{A.53}$$

Then the point $\eta_{j-1/2}$ is written as follows:

$$T_{j-1/2}^n+T_{j-1/2}^{n-1}=\frac{2\xi^{n-1/2}}{k_n}\left(\left(F_{2j-1/2}^n+F_{2j-1/2}^{n-1}\right)\left(G_{1j-1/2}^n-G_{1j-1/2}^{n-1}\right)\right)-$$
$$\frac{2\xi^{n-1/2}}{k_n}\left(\left(G_{2j-1/2}^n+G_{2j-1/2}^{n-1}\right)\left(F_{1j-1/2}^n-F_{1j-1/2}^{n-1}\right)\right). \tag{A.54}$$

At the end, we can obtain discretized energy equation:

$$\frac{\left(\frac{C}{\Pr}\right)_j^n G_{2j}^n-\left(\frac{C}{\Pr}\right)_{j-1}^n G_{2j-1}^n}{h_j}+\left(\frac{u_e^2}{I_e}\right)^n\frac{\left(\frac{1}{\Pr}-1\right)_j^n C_j^n F_{2j}^n F_{3j}^n-\left(\frac{1}{\Pr}-1\right)_{j-1}^n C_{j-1}^n F_{2j-1}^n F_{3j-1}^n}{h_j}$$
$$+\frac{\left(\frac{C}{Sm_1}\right)_j^n\left(1-\frac{1}{Le_1}\right)_j^n\frac{(-c_{2e}^n Qd_{2j}^n-c_{3e}^n Qd_{3j}^n-c_{4e}^n Qd_{4j}^n-c_{5e}^n Qd_{5j}^n)}{I_e^n}h_{1j}^n}{h_j}$$
$$+\frac{\left(\frac{C}{Sm_2}\right)_j^n\left(1-\frac{1}{Le_2}\right)_j^n\frac{c_{2e}^n Qd_{2j}^n}{I_e^n}h_{2j}^n}{h_j}+\frac{\left(\frac{C}{Sm_3}\right)_j^n\left(1-\frac{1}{Le_3}\right)_j^n\frac{c_{3e}^n Qd_{3j}^n}{I_e^n}h_{3j}^n}{h_j}$$
$$+\frac{\left(\frac{C}{Sm_4}\right)_j^n\left(1-\frac{1}{Le_4}\right)_j^n\frac{c_{4e}^n Qd_{4j}^n}{I_e^n}h_{4j}^n}{h_j}+\frac{\left(\frac{C}{Sm_5}\right)_j^n\left(1-\frac{1}{Le_5}\right)_j^n\frac{c_{5e}^n Qd_{5j}^n}{I_e^n}h_{5j}^n}{h_j}$$
$$-\frac{\left(\frac{C}{Sm_1}\right)_{j-1}^n\left(1-\frac{1}{Le_1}\right)_{j-1}^n\frac{(-c_{2e}^n Qd_{2j-1}^n-c_{3e}^n Qd_{3j-1}^n-c_{4e}^n Qd_{4j-1}^n-c_{5e}^n Qd_{5j-1}^n)}{I_e^n}h_{1j-1}^n}{h_j}$$
$$-\frac{\left(\frac{C}{Sm_2}\right)_{j-1}^n\left(1-\frac{1}{Le_2}\right)_{j-1}^n\frac{c_{2e}^n Qd_{2j-1}^n}{I_e^n}h_{2j-1}^n}{h_j}-\frac{\left(\frac{C}{Sm_3}\right)_{j-1}^n\left(1-\frac{1}{Le_3}\right)_{j-1}^n\frac{c_{3e}^n Qd_{3j-1}^n}{I_e^n}h_{3j-1}^n}{h_j}$$
$$-\frac{\left(\frac{C}{Sm_4}\right)_{j-1}^n\left(1-\frac{1}{Le_4}\right)_{j-1}^n\frac{c_{4e}^n Qd_{4j}^n}{I_e^n}h_{4j-1}^n}{h_j}-\frac{\left(\frac{C}{Sm_5}\right)_{j-1}^n\left(1-\frac{1}{Le_5}\right)_{j-1}^n\frac{c_{5e}^n Qd_{5j-1}^n}{I_e^n}h_{5j-1}^n}{h_j}$$
$$+\left(F_1G_2\right)_{j-1/2}^n-\left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n\left(G_1F_2\right)_{j-1/2}^n$$

$$
\begin{aligned}
&-\frac{2\xi^{n-1/2}}{k_n}\left(F^{n}_{2j-1/2}G^{n}_{1j-1/2} - F^{n}_{2j-1/2}G^{n-1}_{1j-1/2} + F^{n-1}_{2j-1/2}G^{n}_{1j-1/2}\right) \\
&-\frac{2\xi^{n-1/2}}{k_n}\left(-G^{n}_{2j-1/2}F^{n}_{1j-1/2} + G^{n}_{2j-1/2}F^{n-1}_{1j-1/2} - G^{n-1}_{2j-1/2}F^{n}_{1j-1/2}\right) = \\
&T^{n-1}_{j-1/2} = \frac{\left(\frac{C}{\mathrm{Pr}}\right)^{n-1}_{j} G^{n-1}_{2j} - \left(\frac{C}{\mathrm{Pr}}\right)^{n-1}_{j-1} G^{n-1}_{2j-1}}{h_j} \\
&+\left(\frac{u_e^2}{I_e}\right)^{n-1}\frac{\left(\frac{1}{\mathrm{Pr}}-1\right)^{n-1}_{j} C^{n-1}_{j}F^{n-1}_{2j}F^{n-1}_{3j} - \left(\frac{1}{\mathrm{Pr}}-1\right)^{n-1}_{j-1} C^{n-1}_{j-1}F^{n-1}_{2j-1}F^{n-1}_{3j-1}}{h_j} \\
&+\frac{\left(\frac{C}{Sm_1}\right)^{n-1}_{j}\left(1-\frac{1}{Le_1}\right)^{n-1}_{j}\frac{(-c^{n-1}_{2e}Qd^{n-1}_{2j} - c^{n-1}_{3e}Qd^{n-1}_{3j} - c^{n-1}_{4e}Qd^{n-1}_{4j} - c^{n-1}_{5e}Qd^{n-1}_{5j})}{I^{n-1}_{e}} h^{n-1}_{1j}}{h_j} \\
&+\frac{\left(\frac{C}{Sm_2}\right)^{n-1}_{j}\left(1-\frac{1}{Le_2}\right)^{n-1}_{j}\frac{c^{n-1}_{2e}Qd^{n-1}_{2j}}{I^{n-1}_{e}} h^{n-1}_{2j}}{h_j} + \frac{\left(\frac{C}{Sm_3}\right)^{n-1}_{j}\left(1-\frac{1}{Le_3}\right)^{n-1}_{j}\frac{c^{n-1}_{3e}Qd^{n-1}_{3j}}{I^{n-1}_{e}} h^{n-1}_{3j}}{h_j} \\
&+\frac{\left(\frac{C}{Sm_4}\right)^{n-1}_{j}\left(1-\frac{1}{Le_4}\right)^{n-1}_{j}\frac{c^{n-1}_{4e}Qd^{n-1}_{4j}}{I^{n-1}_{e}} h^{n-1}_{4j}}{h_j} + \frac{\left(\frac{C}{Sm_5}\right)^{n-1}_{j}\left(1-\frac{1}{Le_5}\right)^{n-1}_{j}\frac{c^{n-1}_{5e}Qd^{n-1}_{5j}}{I^{n-1}_{e}} h^{n-1}_{5j}}{h_j} \\
&-\frac{\left(\frac{C}{Sm_1}\right)^{n-1}_{j-1}\left(1-\frac{1}{Le_1}\right)^{n-1}_{j-1}\frac{(-c^{n-1}_{2e}Qd^{n-1}_{2j-1} - c^{n-1}_{3e}Qd^{n-1}_{3j-1} - c^{n-1}_{4e}Qd^{n-1}_{4j-1} - c^{n-1}_{5e}Qd^{n-1}_{5j-1})}{I^{n-1}_{e}} h^{n-1}_{1j-1}}{h_j} \\
&-\frac{\left(\frac{C}{Sm_2}\right)^{n-1}_{j-1}\left(1-\frac{1}{Le_2}\right)^{n-1}_{j-1}\frac{c^{n-1}_{2e}Qd^{n-1}_{2j-1}}{I^{n-1}_{e}} h^{n-1}_{2j-1}}{h_j} - \frac{\left(\frac{C}{Sm_3}\right)^{n-1}_{j-1}\left(1-\frac{1}{Le_3}\right)^{n-1}_{j-1}\frac{c^{n-1}_{3e}Qd^{n-1}_{3j-1}}{I^{n-1}_{e}} h^{n-1}_{3j-1}}{h_j} \\
&-\frac{\left(\frac{C}{Sm_4}\right)^{n-1}_{j-1}\left(1-\frac{1}{Le_4}\right)^{n-1}_{j-1}\frac{c^{n-1}_{4e}Qd^{n-1}_{4j}}{I^{n-1}_{e}} h^{n-1}_{4j-1}}{h_j} - \frac{\left(\frac{C}{Sm_5}\right)^{n-1}_{j-1}\left(1-\frac{1}{Le_5}\right)^{n-1}_{j-1}\frac{c^{n-1}_{5e}Qd^{n-1}_{5j-1}}{I^{n-1}_{e}} h^{n-1}_{5j-1}}{h_j} \\
&+ (F_1G_2)^{n-1}_{j-1/2} - \left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^{n-1}(G_1F_2)^{n-1}_{j-1/2}\,. \qquad \text{(A.55)}
\end{aligned}
$$

Appendix B: The Iterative Algorithm for the Discretized Equations

First Equation

Using the iterative algorithm $Q^{(i)} = Q^{(i-1)} + \delta Q^{(i-1)}$, the linearized equations for $\delta Q^{(i-1)}$ are written as follows

$$\frac{\delta F_{1j}^n - \delta F_{1j-1}^n}{h_j} = \frac{\delta F_{2j}^n + \delta F_{2j-1}^n}{2} + \frac{F_{2j}^n + F_{2j-1}^n}{2} - \frac{F_{1j}^n - F_{1j-1}^n}{h_j}, \tag{B.1}$$

$$(r_1)_j = \delta F_{1j}^n - \delta F_{1j-1}^n - \frac{h_j}{2}\left(\delta F_{2j}^n + \delta F_{2j-1}^n\right), \tag{B.2}$$

where $(r_1)_j \equiv F_{1j} - F_{1j-1} + \frac{h_j}{2}(F_{2j} + F_{2j-1})$.

Second Equation

The second equation is the momentum equation. It has the same structure as in the case of non-reacting gas.

$$\begin{aligned}(r_2)_j = {} & \frac{C_j^n}{h_j}\delta F_{3j}^n - \frac{C_{j-1}^n}{h_j}\delta F_{3j-1}^n + \frac{\delta F_{1j}F_{3j} + \delta F_{1j-1}F_{3j-1}}{2} + \frac{F_{1j}\delta F_{3j} + F_{1j-1}\delta F_{3j-1}}{2} \\ & -\beta^n\left(F_{2j}\delta F_{2j} + F_{2j-1}\delta F_{2j-1}\right) - \frac{2\xi^{n-1/2}}{k_n}\left(F_{2j}\delta F_{2j} + F_{2j-1}\delta F_{2j-1}\right) + \\ & \frac{\xi^{n-1/2}}{k_n}\left(\delta F_{1j}F_{3j} + \delta F_{1j-1}F_{3j-1}\right) + \frac{\xi^{n-1/2}}{k_n}\left(F_{1j}\delta F_{3j} + F_{1j-1}\delta F_{3j-1}\right) + \\ & \frac{\xi^{n-1/2}}{k_n}F_{3j-1/2}^{n-1}\left(\delta F_{1j} + \delta F_{1j-1}\right) - \frac{\xi^{n-1/2}}{k_n}F_{1j-1/2}^{n-1}\left(\delta F_{3j} + \delta F_{3j-1}\right).\end{aligned} \tag{B.3}$$

The definition of $(r_2)_j$ is written as follows:

$$(r_2)_j \equiv \frac{C_j^n F_{3j}^n - C_{j-1}^n F_{3j-1}^n}{h_j} + (F_1 F_3)_{j-1/2}^n + \beta^n \left[\left(\frac{\rho_e}{\rho} \right)_{j-1/2}^n - \left(F_2^2 \right)_{j-1/2}^n \right] +$$

$$2\xi^{n-1/2} \frac{- \left(F_2^2 \right)_{j-1/2}^n + F_{3j-1/2}^n F_{1j-1/2}^n - F_{3j-1/2}^n F_{1j-1/2}^{n-1} + F_{3j-1/2}^{n-1} F_{1j-1/2}^n}{k_n}$$

We can recast the equation in the form of:

$$(r_2)_j = (s_1)_j \, \delta F_{3j} + (s_2)_j \, \delta F_{3j-1} + (s_3)_j \, \delta F_{1j} + (s_4)_j \, \delta F_{1j-1} + (s_5)_j \, \delta F_{2j} + (s_6)_j \, \delta F_{2j-1}. \tag{B.4}$$

The coefficients in (B.4) are defined as:

$$(s_1)_j = \frac{C_j^n}{h_j} + \frac{1}{2} F_{1j} + \frac{\xi^{n-1/2}}{k_n} F_{1j} - \frac{\xi^{n-1/2}}{k_n} F_{1j-1/2}^{n-1} = \frac{C_j^n}{h_j} + \frac{\alpha_1}{2} F_{1j} - \frac{\alpha^n}{2} F_{1j-1/2}^{n-1}, \tag{B.5}$$

where $\alpha_1 = 1 + \alpha^n$ and $\alpha^n = \frac{2\xi^{n-1/2}}{k_n}$,

$$(s_2)_j = -\frac{C_{j-1}^n}{h_j} + \frac{\alpha_1}{2} F_{1j-1} - \frac{\alpha^n}{2} F_{1j-1/2}^{n-1}, \tag{B.6}$$

$$(s_3)_j = \frac{1}{2} F_{3j} + \frac{\xi^{n-1/2}}{k_n} F_{3j} + \frac{\xi^{n-1/2}}{k_n} F_{3j-1/2}^{n-1} = \frac{\alpha_1}{2} F_{3j} + \frac{\alpha^n}{2} F_{3j-1/2}^{n-1}, \tag{B.7}$$

$$(s_3)_j = \frac{1}{2} F_{3j} + \frac{\xi^{n-1/2}}{k_n} F_{3j} + \frac{\xi^{n-1/2}}{k_n} F_{3j-1/2}^{n-1} = \frac{\alpha_1}{2} F_{3j} + \frac{\alpha^n}{2} F_{3j-1/2}^{n-1}, \tag{B.8}$$

$$(s_4)_j = \frac{\alpha_1}{2} F_{3j-1} + \frac{\alpha^n}{2} F^{n-1}_{3j-1/2}, \tag{B.9}$$

$$(s_5)_j = -\beta^n F_{2j} - \frac{2\xi^{n-1/2}}{k_n} F_{2j} = -\alpha_2 F_{2j}, \tag{B.10}$$

where $\alpha_2 = \beta^n + \alpha^n$,

$$(s_6)_j = -\beta^n F_{2j-1} - \frac{2\xi^{n-1/2}}{k_n} F_{2j-1} = -\alpha_2 F_{2j-1} \tag{B.11}$$

Third Equation

The third equation is energy equation. Structure of the equation will be similar to the equation in non-reacting gas with addition of two terms associated with concentration of species.

$$(r_3)_j = \frac{\left(\frac{C}{\Pr}\right)_j^n}{h_j}\delta G_{2j}^n - \frac{\left(\frac{C}{\Pr}\right)_{j-1}^n}{h_j}\delta G_{2j-1}^n + \left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_j^n C_j^n}{h_j}\delta F_{2j}^n F_{3j}^n +$$

$$\left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_j^n C_j^n}{h_j} F_{2j}^n \delta F_{3j}^n - \left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_{j-1}^n C_{j-1}^n}{h_j}\delta F_{2j-1}^n F_{3j-1}^n -$$

$$\left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_{j-1}^n C_{j-1}^n}{h_j} F_{2j-1}^n \delta F_{3j-1}^n + \tag{B.12}$$

$$\left(\frac{1}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)_j^n (-c_{2e}^n \delta Qd_{2j}^n - c_{3e}^n \delta Qd_{3j}^n - c_{4e}^n \delta Qd_{4j}^n - c_{5e}^n \delta Qd_{5j}^n) h_{1j}^n \frac{\left(\frac{C}{Sm_1}\right)_j^n}{h_j} +$$

$$\left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_2}\right)_j^n h_{2j}^n \frac{\left(\frac{C}{Sm_2}\right)_j^n}{h_j}\delta Qd_{2j}^n + \left(\frac{c_{3e}}{I_e}\right)^n \left(1-\frac{1}{Le_3}\right)_j^n h_{3j}^n \frac{\left(\frac{C}{Sm_3}\right)_j^n}{h_j}\delta Qd_{3j}^n +$$

$$\left(\frac{c_{4e}}{I_e}\right)^n \left(1-\frac{1}{Le_4}\right)_j^n h_{4j}^n \frac{\left(\frac{C}{Sm_4}\right)_j^n}{h_j}\delta Qd_{4j}^n + \left(\frac{c_{5e}}{I_e}\right)^n \left(1-\frac{1}{Le_5}\right)_j^n h_{5j}^n \frac{\left(\frac{C}{Sm_5}\right)_j^n}{h_j}\delta Qd_{5j}^n -$$

$$\left(\frac{1}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)_{j-1}^n (-c_{2e}^n \delta Qd_{2j}^n - c_{3e}^n \delta Qd_{3j}^n - c_{4e}^n \delta Qd_{4j}^n - c_{5e}^n \delta Qd_{5j}^n) h_{1j-1}^n \frac{\left(\frac{C}{Sm_1}\right)_{j-1}^n}{h_j} -$$

$$\left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_2}\right)_{j-1}^n h_{2j-1}^n \frac{\left(\frac{C}{Sm_2}\right)_{j-1}^n}{h_j}\delta Qd_{2j-1}^n - \left(\frac{c_{3e}}{I_e}\right)^n \left(1-\frac{1}{Le_3}\right)_{j-1}^n h_{3j-1}^n \frac{\left(\frac{C}{Sm_3}\right)_{j-1}^n}{h_j}\delta Qd_{3j-1}^n -$$

$$\left(\frac{c_{4e}}{I_e}\right)^n \left(1-\frac{1}{Le_4}\right)_{j-1}^n h_{4j-1}^n \frac{\left(\frac{C}{Sm_4}\right)_{j-1}^n}{h_j}\delta Qd_{4j-1}^n - \left(\frac{c_{5e}}{I_e}\right)^n \left(1-\frac{1}{Le_5}\right)_{j-1}^n h_{5j-1}^n \frac{\left(\frac{C}{Sm_5}\right)_{j-1}^n}{h_j}\delta Qd_{5j-1}^n +$$

$$(\delta F_1 G_2)_{j-1/2}^n + (F_1 \delta G_2)_{j-1/2}^n - \left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n (\delta G_1 F_2)_{j-1/2}^n - \left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n (G_1 \delta F_2)_{j-1/2}^n -$$

$$\alpha^n\left(\delta F_2 G_1\right)^n_{j-1/2} - \alpha^n\left(F_2\delta G_1\right)^n_{j-1/2} + \alpha^n\left(\delta F_1 G_2\right)^n_{j-1/2} + \alpha^n\left(F_1\delta G_2\right)^n_{j-1/2} -$$

$$\alpha^n\left(F^{n-1}_{2j-1/2}\delta G^n_{1j-1/2} - \delta F^n_{2j-1/2}G^{n-1}_{1j-1/2}\right) - \alpha^n\left(\delta G^n_{2j-1/2}F^{n-1}_{1j-1/2} - G^{n-1}_{2j-1/2}\delta F^n_{1j-1/2}\right),$$

The definition of $(r_3)_j$ is written as follows:

$$(r_3)_j \equiv \frac{\left(\frac{C}{\mathrm{Pr}}\right)^n_j}{h_j} G^n_{2j} - \frac{\left(\frac{C}{\mathrm{Pr}}\right)^n_{j-1}}{h_j} G^n_{2j-1} + \left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\mathrm{Pr}}-1\right)^n_j C^n_j}{h_j} F^n_{2j} F^n_{3j} -$$

$$\left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\mathrm{Pr}}-1\right)^n_{j-1} C^n_{j-1}}{h_j} F^n_{2j-1} F^n_{3j-1} +$$

$$\left(\frac{1}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)^n_j \left(-c^n_{2e}Qd^n_{2j} - c^n_{3e}Qd^n_{3j} - c^n_{4e}Qd^n_{4j} - c^n_{5e}Qd^n_{5j}\right) h^n_{1j} \frac{\left(\frac{C}{Sm_1}\right)^n_j}{h_j} +$$

$$\left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_2}\right)^n_j h^n_{2j} \frac{\left(\frac{C}{Sm_2}\right)^n_j}{h_j} Qd^n_{2j} + \left(\frac{c_{3e}}{I_e}\right)^n \left(1-\frac{1}{Le_3}\right)^n_j h^n_{3j} \frac{\left(\frac{C}{Sm_3}\right)^n_j}{h_j} Qd^n_{3j} +$$

$$\left(\frac{c_{4e}}{I_e}\right)^n \left(1-\frac{1}{Le_4}\right)^n_j h^n_{4j} \frac{\left(\frac{C}{Sm_4}\right)^n_j}{h_j} Qd^n_{4j} + \left(\frac{c_{5e}}{I_e}\right)^n \left(1-\frac{1}{Le_5}\right)^n_j h^n_{5j} \frac{\left(\frac{C}{Sm_5}\right)^n_j}{h_j} Qd^n_{5j} -$$

$$\left(\frac{1}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)^n_{j-1} \left(-c^n_{2e}Qd^n_{2j} - c^n_{3e}Qd^n_{3j} - c^n_{4e}Qd^n_{4j} - c^n_{5e}Qd^n_{5j}\right) h^n_{1j-1} \frac{\left(\frac{C}{Sm_1}\right)^n_{j-1}}{h_j} -$$

$$\left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_2}\right)^n_{j-1} h^n_{2j-1} \frac{\left(\frac{C}{Sm_2}\right)^n_{j-1}}{h_j} Qd^n_{2j-1} - \left(\frac{c_{3e}}{I_e}\right)^n \left(1-\frac{1}{Le_3}\right)^n_{j-1} h^n_{3j-1} \frac{\left(\frac{C}{Sm_3}\right)^n_{j-1}}{h_j} Qd^n_{3j-1} -$$

$$\left(\frac{c_{4e}}{I_e}\right)^n \left(1-\frac{1}{Le_4}\right)^n_{j-1} h^n_{4j-1} \frac{\left(\frac{C}{Sm_4}\right)^n_{j-1}}{h_j} Qd^n_{4j-1} - \left(\frac{c_{5e}}{I_e}\right)^n \left(1-\frac{1}{Le_5}\right)^n_{j-1} h^n_{5j-1} \frac{\left(\frac{C}{Sm_5}\right)^n_{j-1}}{h_j} Qd^n_{5j-1} +$$

$$\left(F_1 G_2\right)^n_{j-1/2} - \left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n \left(G_1 F_2\right)^n_{j-1/2} - \alpha^n\left(\left(F_2 G_1\right)^n_{j-1/2} - \left(F_1 G_2\right)^n_{j-1/2}\right) -$$

$$\alpha^n\left(F^n_{2j-1/2}G^n_{1j-1/2} - F^n_{2j-1/2}G^{n-1}_{1j-1/2}\right) - \alpha^n\left(G^n_{2j-1/2}F^{n-1}_{1j-1/2} - G^{n-1}_{2j-1/2}F^n_{1j-1/2}\right) = M^{n-1}_{j-1/2}$$

We can recast the equation in the form of:

$$(r_3)_j = (\beta_1)\,\delta G_{2j} + (\beta_2)\,\delta G_{2j-1} + (\beta_3)\,\delta F_{1j} + (\beta_4)\,\delta F_{1j-1} + (\beta_5)\,\delta F_{2j} + (\beta_6)\,\delta F_{2j-1} + (\beta_7)\,\delta G_{1j} +$$

$$(\beta_8)\,\delta G_{1j-1} + (\beta_9)\,\delta F_{3j} + (\beta_{10})\,\delta F_{3j-1} + (\beta_{11})\,\delta Qd_{2j} + (\beta_{12})\,\delta Qd_{2j-1} + (\beta_{13})\,\delta Qd_{3j} + (\beta_{14})\,\delta Qd_{3j-1} +$$

$$(\beta_{15})\,\delta Qd_{4j} + (\beta_{16})\,\delta Qd_{4j-1} + (\beta_{17})\,\delta Qd_{5j} + (\beta_{18})\,\delta Qd_{5j-1}. \qquad \text{(B.13)}$$

The coefficients in (B.13) are defined as:

$$(\beta_1)_j = \frac{\left(\frac{C}{\Pr}\right)_j^n}{h_j} + \frac{1}{2}(F_1)_j^n + \frac{\alpha^n}{2}(F_1)_j^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1} = \frac{\left(\frac{C}{\Pr}\right)_j^n}{h_j} + \frac{\alpha_1}{2}(F_1)_j^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}, \qquad \text{(B.14)}$$

$$(\beta_2)_j = -\frac{\left(\frac{C}{\Pr}\right)_j^n}{h_j} + \frac{\alpha_1}{2}(F_1)_{j-1}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}, \qquad \text{(B.15)}$$

$$(\beta_3)_j = \frac{1}{2}(G_2)_j^n + \frac{\alpha^n}{2}(G_2)_j^n + \frac{\alpha^n}{2}G_{2j-1/2}^{n-1} = \frac{\alpha_1}{2}(G_2)_j^n + \frac{\alpha^n}{2}G_{2j-1/2}^{n-1}, \qquad \text{(B.16)}$$

$$(\beta_4)_j = \frac{\alpha_1}{2}(G_2)_{j-1}^n + \frac{\alpha^n}{2}G_{2j-1/2}^{n-1}, \qquad \text{(B.17)}$$

$$(\beta_5)_j = \left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_j^n C_j^n}{h_j}F_{3j}^n - \frac{\alpha^n}{2}(G_1)_j^n + \frac{\alpha^n}{2}G_{1j-1/2}^{n-1} - \frac{1}{2}\left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n (G_1)_j^n, \qquad \text{(B.18)}$$

$$(\beta_6)_j = -\left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_{j-1}^n C_{j-1}^n}{h_j} F_{3j-1}^n - \frac{\alpha^n}{2}(G_1)_{j-1}^n + \frac{\alpha^n}{2} G_{1j-1/2}^{n-1} - \frac{1}{2}\left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n (G_1)_{j-1}^n, \tag{B.19}$$

$$(\beta_7)_j = -\frac{\alpha^n}{2}(F_2)_j^n - \frac{\alpha^n}{2} F_{2j-1/2}^{n-1} - \frac{1}{2}\left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n (F_2)_j^n, \tag{B.20}$$

$$(\beta_8)_j = -\frac{\alpha^n}{2}(F_2)_{j-1}^n - \frac{\alpha^n}{2} F_{2j-1/2}^{n-1} - \frac{1}{2}\left(\frac{2\xi}{I_e}\frac{dI_e}{d\xi}\right)^n (F_2)_{j-1}^n, \tag{B.21}$$

$$(\beta_9)_j = \left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_j^n C_j^n}{h_j} F_{2j}^n, \tag{B.22}$$

$$(\beta_{10})_j = \left(\frac{u_e^2}{I_e}\right)^n \frac{\left(\frac{1}{\Pr}-1\right)_{j-1}^n C_{j-1}^n}{h_j} F_{2j-1}^n, \tag{B.23}$$

$$(\beta_{11})_j = -\left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)_j^n h_{1j}^n \frac{\left(\frac{C}{Sm_1}\right)_j^n}{h_j} + \left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_2}\right)_j^n h_{2j}^n \frac{\left(\frac{C}{Sm_2}\right)_j^n}{h_j}, \tag{B.24}$$

$$(\beta_{12})_j = -\left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)_{j-1}^n h_{1j-1}^n \frac{\left(\frac{C}{Sm_1}\right)_{j-1}^n}{h_j} + \left(\frac{c_{2e}}{I_e}\right)^n \left(1-\frac{1}{Le_2}\right)_{j-1}^n h_{2j-1}^n \frac{\left(\frac{C}{Sm_2}\right)_{j-1}^n}{h_j}, \tag{B.25}$$

$$(\beta_{13})_j = -\left(\frac{c_{3e}}{I_e}\right)^n \left(1-\frac{1}{Le_1}\right)_j^n h_{1j}^n \frac{\left(\frac{C}{Sm_1}\right)_j^n}{h_j} + \left(\frac{c_{3e}}{I_e}\right)^n \left(1-\frac{1}{Le_3}\right)_j^n h_{3j}^n \frac{\left(\frac{C}{Sm_3}\right)_j^n}{h_j}, \tag{B.26}$$

$$(\beta_{14})_j = -\left(\frac{c_{3e}}{I_e}\right)^n\left(1-\frac{1}{Le_1}\right)^n_{j-1} h^n_{1j-1}\frac{\left(\frac{C}{Sm_1}\right)^n_{j-1}}{h_j}+\left(\frac{c_{3e}}{I_e}\right)^n\left(1-\frac{1}{Le_3}\right)^n_{j-1} h^n_{3j-1}\frac{\left(\frac{C}{Sm_3}\right)^n_{j-1}}{h_j}, \tag{B.27}$$

$$(\beta_{15})_j = -\left(\frac{c_{4e}}{I_e}\right)^n\left(1-\frac{1}{Le_1}\right)^n_{j} h^n_{1j}\frac{\left(\frac{C}{Sm_1}\right)^n_{j}}{h_j}+\left(\frac{c_{4e}}{I_e}\right)^n\left(1-\frac{1}{Le_4}\right)^n_{j} h^n_{4j}\frac{\left(\frac{C}{Sm_4}\right)^n_{j}}{h_j}, \tag{B.28}$$

$$(\beta_{16})_j = -\left(\frac{c_{4e}}{I_e}\right)^n\left(1-\frac{1}{Le_1}\right)^n_{j-1} h^n_{1j-1}\frac{\left(\frac{C}{Sm_1}\right)^n_{j-1}}{h_j}+\left(\frac{c_{4e}}{I_e}\right)^n\left(1-\frac{1}{Le_4}\right)^n_{j-1} h^n_{4j-1}\frac{\left(\frac{C}{Sm_4}\right)^n_{j-1}}{h_j}, \tag{B.29}$$

$$(\beta_{17})_j = -\left(\frac{c_{5e}}{I_e}\right)^n\left(1-\frac{1}{Le_1}\right)^n_{j} h^n_{1j}\frac{\left(\frac{C}{Sm_1}\right)^n_{j}}{h_j}+\left(\frac{c_{5e}}{I_e}\right)^n\left(1-\frac{1}{Le_5}\right)^n_{j} h^n_{5j}\frac{\left(\frac{C}{Sm_5}\right)^n_{j}}{h_j}, \tag{B.30}$$

$$(\beta_{18})_j = -\left(\frac{c_{5e}}{I_e}\right)^n\left(1-\frac{1}{Le_1}\right)^n_{j-1} h^n_{1j-1}\frac{\left(\frac{C}{Sm_1}\right)^n_{j-1}}{h_j}+\left(\frac{c_{5e}}{I_e}\right)^n\left(1-\frac{1}{Le_5}\right)^n_{j-1} h^n_{5j-1}\frac{\left(\frac{C}{Sm_5}\right)^n_{j-1}}{h_j}. \tag{B.31}$$

Forth Equation

The forth equation is conservation for specie of Nitrogen atom. In order to solve boundary layer equations numerically, we need to discard one of the species in the mixture and use the global mass conservation equation. In this work, the nitrogen molecule is discarded. Therefore, we will have four conservation of species equation for five species air model.

$$(r_4)_j = \frac{\left(\frac{C}{Sm_2}\right)^n_j}{h_j}\delta Qd^n_{2j} - \frac{\left(\frac{C}{Sm_2}\right)^n_{j-1}}{h_j}\delta Qd^n_{2j-1} + (\delta Qd_2F_1)^n_{j-1/2} + (Qd_2\delta F_1)^n_{j-1/2} - ms^n_2\delta F^n_{2j-1/2} +$$

$$2md^n_2\left(k^2_f\rho\right)^n_{j-1/2}\frac{M_N}{M_{N_2}}\left(-\left(c^n_{2e}\delta Qs^n_{2j-1/2} + c^n_{3e}\delta Qs^n_{3j-1/2} + c^n_{4e}\delta Qs^n_{4j-1/2} + c^n_{5e}\delta Qs^n_{5j-1/2}\right)\right)$$

$$\left[\frac{c^n_{4e}Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e}Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e}Qs^n_{5j-1/2}}{M_{NO}}\right] +$$

$$2md^n_2\left(k^2_f\rho\right)^n_{j-1/2}\frac{M_N}{M_{N_2}}\left(-\left(c^n_{2e}\delta Qs^n_{2j-1/2} + c^n_{3e}\delta Qs^n_{3j-1/2} + c^n_{4e}\delta Qs^n_{4j-1/2} + c^n_{5e}\delta Qs^n_{5j-1/2}\right)\right)$$

$$\frac{\left(1 - \left(c^n_{2e}Qs^n_{2j-1/2} + c^n_{3e}Qs^n_{3j-1/2} + c^n_{4e}Qs^n_{4j-1/2} + c^n_{5e}Qs^n_{5j-1/2}\right)\right)}{M_{N_2}} +$$

$$2md^n_2\left(k^2_f\rho\right)^n_{j-1/2}\frac{M_N}{M_{N_2}}\left(1 - \left(c^n_{2e}Qs^n_{2j-1/2} + c^n_{3e}Qs^n_{3j-1/2} + c^n_{4e}Qs^n_{4j-1/2} + c^n_{5e}Qs^n_{5j-1/2}\right)\right)$$

$$\left[\frac{c^n_{4e}\delta Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e}\delta Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e}\delta Qs^n_{5j-1/2}}{M_{NO}}\right] +$$

$$2md^n_2\left(k^2_f\rho\right)^n_{j-1/2}\frac{M_N}{M_{N_2}}\left(1 - \left(c^n_{2e}Qs^n_{2j-1/2} + c^n_{3e}Qs^n_{3j-1/2} + c^n_{4e}Qs^n_{4j-1/2} + c^n_{5e}Qs^n_{5j-1/2}\right)\right)$$

$$\frac{\left(-\left(c^n_{2e}\delta Qs^n_{2j-1/2} + c^n_{3e}\delta Qs^n_{3j-1/2} + c^n_{4e}\delta Qs^n_{4j-1/2} + c^n_{5e}\delta Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}$$

$$-2md^n_2\left(k^2_b\rho^2\right)^n_{j-1/2}\frac{1}{M_N}\left(c^n_{2e}\right)^2\left(Qs^n_{2j-1/2}\right)^2$$

$$\left[\frac{c^n_{4e}\delta Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e}\delta Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e}\delta Qs^n_{5j-1/2}}{M_{NO}}\right]$$

$$-2md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j-1/2}^n\right)^2$$

$$\frac{\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-2md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n\right)^2 2\left(Qs_2^n\delta Qs_2^n\right)_{j-1/2}$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}\right]$$

$$-2md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n\right)^2 2\left(Qs_2^n\delta Qs_2^n\right)_{j-1/2}$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+2md_2^n\left(k_f^3\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)$$

$$+2md_2^n\left(k_f^3\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)$$

$$\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)$$

$$-2md_2^n\left(k_b^3\rho^2\right)_{j-1/2}^n\frac{1}{\left(M_N\right)^2}\left(c_{2e}^n\right)^3 3\left(Qs_2^n\right)_{j-1/2}^2\delta Qs_{2j-1/2}^n+$$

$$md_2^n\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}\right]+$$

$$md_2^n\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+md_2^n\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n \delta Qs_{4j-1/2}^n}{M_O} + \frac{c_{2e}^n \delta Qs_{2j-1/2}^n}{M_N} + \frac{c_{3e}^n \delta Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n \delta Qs_{5j-1/2}^n}{M_{NO}}\right]$$

$$+md_2^n \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}} \left(c_{5e}^n Qs_{5j-1/2}^n\right)$$

$$\frac{\left(-\left(c_{2e}^n \delta Qs_{2j-1/2}^n + c_{3e}^n \delta Qs_{3j-1/2}^n + c_{4e}^n \delta Qs_{4j-1/2}^n + c_{5e}^n \delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_2^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n \delta Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1/2}^n}{M_O} + \frac{c_{2e}^n Qs_{2j-1/2}^n}{M_N} + \frac{c_{3e}^n Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1/2}^n}{M_{NO}}\right]$$

$$-md_2^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n \delta Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_2^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j-1/2}^n\right) \left(c_{2e}^n \delta Qs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1/2}^n}{M_O} + \frac{c_{2e}^n Qs_{2j-1/2}^n}{M_N} + \frac{c_{3e}^n Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1/2}^n}{M_{NO}}\right]$$

$$-md_2^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j-1/2}^n\right) \left(c_{2e}^n \delta Qs_{2j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_2^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n \delta Qs_{4j-1/2}^n}{M_O} + \frac{c_{2e}^n \delta Qs_{2j-1/2}^n}{M_N} + \frac{c_{3e}^n \delta Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n \delta Qs_{5j-1/2}^n}{M_{NO}}\right]$$

$$-md_2^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\frac{\left(-\left(c_{2e}^n \delta Qs_{2j-1/2}^n + c_{3e}^n \delta Qs_{3j-1/2}^n + c_{4e}^n \delta Qs_{4j-1/2}^n + c_{5e}^n \delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$md_2^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}M_O}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)\left(c_{4e}^nQs_{4j-1/2}^n\right)+$$
$$md_2^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}M_O}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{4e}^n\delta Qs_{4j-1/2}^n\right)-$$
$$md_2^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_{O_2}}\left(c_{3e}^n\delta Qs_{3j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)-$$
$$md_2^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)+$$
$$md_2^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n\delta Qs_{4j-1/2}^n\right)$$
$$\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)+$$
$$md_2^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}M_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)$$
$$\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)-$$
$$md_2^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)-$$
$$md_2^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)-$$
$$\alpha^n\left[\left(\delta Qs_2F_2\right)_{j-1/2}^n+\left(Qs_2\delta F_2\right)_{j-1/2}^n\right]+\alpha^n\left[\left(\delta Qd_2F_1\right)_{j-1/2}^n+\left(Qd_2\delta F_1\right)_{j-1/2}^n\right]-$$
$$\alpha^n\left[\delta Qs_{2j-1/2}^nF_{2j-1/2}^{n-1}-Qs_{2j-1/2}^{n-1}\delta F_{2j-1/2}^n+\delta Qd_{2j-1/2}^nF_{1j-1/2}^{n-1}-Qd_{2j-1/2}^{n-1}\delta F_{1j-1/2}^n\right],\tag{B.32}$$

The definition of $(r_4)_j$ is written as follows:

$$(r_4)_j\equiv\frac{\left(\frac{C}{Sm_2}\right)_j^nQd_{2j}^n-\left(\frac{C}{Sm_2}\right)_{j-1}^nQd_{2j-1}^n}{h_j}+\left(Qd_2F_1\right)_{j-1/2}^n-ms_2^nF_{2j-1/2}^n+$$
$$2md_2^n\left(k_f^2\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}}\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)$$

$$\left[\frac{c_{4e}^{n}Qs_{4j-1/2}^{n}}{M_{O}}+\frac{c_{3e}^{n}Qs_{3j-1/2}^{n}}{M_{O_2}}+\frac{c_{5e}^{n}Qs_{5j-1/2}^{n}}{M_{NO}}\right]+$$

$$2md_2^n\left(k_f^2\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}}\left(1-\left(c_{2e}^{n}Qs_{2j-1/2}^{n}+c_{3e}^{n}Qs_{3j-1/2}^{n}+c_{4e}^{n}Qs_{4j-1/2}^{n}+c_{5e}^{n}Qs_{5j-1/2}^{n}\right)\right)$$

$$\frac{\left(1-\left(c_{2e}^{n}Qs_{2j-1/2}^{n}+c_{3e}^{n}Qs_{3j-1/2}^{n}+c_{4e}^{n}Qs_{4j-1/2}^{n}+c_{5e}^{n}Qs_{5j-1/2}^{n}\right)\right)}{M_{N_2}}-$$

$$2md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j-1/2}^n\right)^2$$

$$\left[\frac{c_{4e}^{n}Qs_{4j-1/2}^{n}}{M_{O}}+\frac{c_{3e}^{n}Qs_{3j-1/2}^{n}}{M_{O_2}}+\frac{c_{5e}^{n}Qs_{5j-1/2}^{n}}{M_{NO}}\right]-$$

$$2md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j-1/2}^n\right)^2$$

$$\frac{\left(1-\left(c_{2e}^{n}Qs_{2j-1/2}^{n}+c_{3e}^{n}Qs_{3j-1/2}^{n}+c_{4e}^{n}Qs_{4j-1/2}^{n}+c_{5e}^{n}Qs_{5j-1/2}^{n}\right)\right)}{M_{N_2}}$$

$$+2md_2^n\left(k_f^3\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\left(1-\left(c_{2e}^{n}Qs_{2j-1/2}^{n}+c_{3e}^{n}Qs_{3j-1/2}^{n}+c_{4e}^{n}Qs_{4j-1/2}^{n}+c_{5e}^{n}Qs_{5j-1/2}^{n}\right)\right)$$

$$-2md_2^n\left(k_b^3\rho^2\right)_{j-1/2}^n\frac{1}{\left(M_N\right)^2}\left(c_{2e}^n\right)^3\left(Qs_{2j-1/2}^n\right)^3+$$

$$md_2^n\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^{n}Qs_{4j-1/2}^{n}}{M_{O}}+\frac{c_{3e}^{n}Qs_{3j-1/2}^{n}}{M_{O_2}}+\frac{c_{5e}^{n}Qs_{5j-1/2}^{n}}{M_{NO}}\right]+\frac{c_{2e}^{n}Qs_{2j-1/2}^{n}}{M_{N}}+$$

$$md_2^n\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^{n}Qs_{2j-1/2}^{n}+c_{3e}^{n}Qs_{3j-1/2}^{n}+c_{4e}^{n}Qs_{4j-1/2}^{n}+c_{5e}^{n}Qs_{5j-1/2}^{n}\right)\right)}{M_{N_2}}-$$

$$md_2^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^{n}Qs_{4j-1/2}^{n}}{M_{O}}+\frac{c_{3e}^{n}Qs_{3j-1/2}^{n}}{M_{O_2}}+\frac{c_{5e}^{n}Qs_{5j-1/2}^{n}}{M_{NO}}\right]+\frac{c_{2e}^{n}Qs_{2j-1/2}^{n}}{M_{N}}-$$

$$md_2^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)$$
$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}+$$
$$md_2^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}M_O}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{4e}^nQs_{4j-1/2}^n\right)-$$
$$md_2^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)+$$
$$md_2^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}M_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)$$
$$\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)-$$
$$md_2^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)-$$
$$2\xi^{n-1/2}\frac{\left(Qs_{2j-1/2}^nF_{2j-1/2}^n+Qs_{2j-1/2}^nF_{2j-1/2}^{n-1}-Qs_{2j-1/2}^{n-1}F_{2j-1/2}^n\right)}{k_n}-$$
$$2\xi^{n-1/2}\frac{\left(-Qd_{2j-1/2}^nF_{1j-1/2}^n+Qd_{2j-1/2}^nF_{1j-1/2}^{n-1}-Qd_{2j-1/2}^{n-1}F_{1j-1/2}^n\right)}{k_n}=$$
$$-2\xi^{n-1/2}\frac{Qs_{2j-1/2}^{n-1}F_{2j-1/2}^{n-1}}{k_n}+2\xi^{n-1/2}\frac{Qd_{2j-1/2}^{n-1}F_{1j-1/2}^{n-1}}{k_n}-P_{2j-1/2}^{n-1}$$

We can recast the equation in the form of:

$$(r_4)_j=(e_1)_j\,\delta F_{1j}+(e_5)_j\,\delta F_{1j-1}+(e_9)_j\,\delta F_{2j}+(e_{13})_j\,\delta F_{2j-1}+(e_{17})_j\,\delta Qs_{2j}+(e_{18})_j\,\delta Qs_{2j-1}+$$
$$(e_{19})_j\,\delta Qs_{3j}+(e_{20})_j\,\delta Qs_{3j-1}+(e_{21})_j\,\delta Qs_{4j}+(e_{22})_j\,\delta Qs_{4j-1}+(e_{23})_j\,\delta Qs_{5j}+$$
$$(e_{24})_j\,\delta Qs_{5j-1}+(e_{49})_j\,\delta Qd_{2j}+(e_{50})_j\,\delta Qd_{2j-1}. \qquad \text{(B.33)}$$

The coefficients in (B.33) are defined as:

$$(e_1)_j = \frac{1}{2}Qd_{2j}^n + \frac{\alpha^n}{2}Qd_{2j}^n + \frac{\alpha^n}{2}Qd_{2j-1/2}^{n-1} = \frac{\alpha_1}{2}Qd_{2j}^n + \frac{\alpha^n}{2}Qd_{2j-1/2}^{n-1}, \tag{B.34}$$

$$(e_5)_j = \frac{1}{2}Qd_{2j-1}^n + \frac{\alpha^n}{2}Qd_{2j-1}^n + \frac{\alpha^n}{2}Qd_{2j-1/2}^{n-1} = \frac{\alpha_1}{2}Qd_{2j-1}^n + \frac{\alpha^n}{2}Qd_{2j-1/2}^{n-1}, \tag{B.35}$$

$$(e_9)_j = -\frac{ms_2^n}{2} - \frac{\alpha^n}{2}Qs_{2j}^n + \frac{\alpha^n}{2}Qs_{2j-1/2}^{n-1}, \tag{B.36}$$

$$(e_{13})_j = -\frac{ms_2^n}{2} - \frac{\alpha^n}{2}Qs_{2j-1}^n + \frac{\alpha^n}{2}Qs_{2j-1/2}^{n-1}, \tag{B.37}$$

$$(e_{17})_j = md_2^n \left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}} \left(-c_{2e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}\right]$$

$$+md_2^n \left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}} \left(-c_{2e}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}} +$$

$$md_2^n \left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}} \left(1 - \left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right) \frac{\left(-c_{2e}^n\right)}{M_{N_2}} -$$

$$md_2^n \left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{2e}^n\right)^2 \left(Qs_{2j}^n\right)^2 \frac{\left(-c_{2e}^n\right)}{M_{N_2}} -$$

$$2md_2^n \left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{2e}^n\right)^2 Qs_{2j}^n$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}\right]$$

$$-2md_2^n \left(k_b^2 \rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{2e}^n\right)^2 Qs_{2j}^n$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}} +$$

$$md_2^n \left(k_f^3 \rho\right)_{j-1/2}^n \frac{1}{M_{N_2}} \left(-c_{2e}^n\right) \left(c_{2e}^n Qs_{2j}^n\right) +$$

$$md_2^n \left(k_f^3 \rho\right)_{j-1/2}^n \frac{1}{M_{N_2}} \left(c_{2e}^n\right)$$

$$\left(1 - \left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right) -$$

$$md_2^n \left(k_b^3 \rho^2\right)_{j-1/2}^n \frac{1}{\left(M_N\right)^2} \left(c_{2e}^n\right)^3 3 \left(Qs_2^n\right)_j^2 +$$

$$\frac{md_2^n}{2} \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}} \left(c_{5e}^n Qs_{5j}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$

$$\frac{md_2^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j}^n\right) \left(c_{2e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j}^n}{M_N}\right] -$$

$$\frac{md_2^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j}^n\right) \left(c_{2e}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}} +$$

$$\frac{md_2^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{5e}^n Qs_{5j}^n\right) \left(c_{2e}^n Qs_{2j}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$

$$\frac{md_2^n}{2} \left(k_b^5 \rho\right)_{j-1/2}^n \frac{1}{M_{O_2}} \left(c_{3e}^n Qs_{3j}^n\right) \left(c_{2e}^n\right) +$$

$$\frac{md_2^n}{2} \left(k_f^6 \rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2} M_O} \left(c_{4e}^n Qs_{4j}^n\right) \left(-c_{2e}^n\right) -$$

$$\frac{md_2^n}{2} \left(k_b^6 \rho\right)_{j-1/2}^n \frac{1}{M_{NO}} \left(c_{5e}^n Qs_{5j}^n\right) \left(c_{2e}^n\right) - \frac{\alpha^n}{2} F_{2j}^n - \frac{\alpha^n}{2} F_{2j-1/2}^{n-1}, \tag{B.38}$$

$$(e_{18})_j = md_2^n \left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}} \left(-c_{2e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}}\right] +$$

$$md_2^n \left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}} \left(-c_{2e}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}} +$$

$$md_2^n \left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}} \left(1 - \left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right) \frac{\left(-c_{2e}^n\right)}{M_{N_2}} -$$

$$md_2^n \left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{2e}^n\right)^2 \left(Qs_{2j-1}^n\right)^2 \frac{\left(-c_{2e}^n\right)}{M_{N_2}} -$$

$$2md_2^n \left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{2e}^n\right)^2 Qs_{2j-1}^n$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}}\right] -$$

$$2md_2^n \left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{2e}^n\right)^2 Qs_{2j-1}^n$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}} +$$

$$md_2^n \left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}} \left(-c_{2e}^n\right) \left(c_{2e}^n Qs_{2j-1}^n\right) +$$

$$md_2^n \left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}} \left(1 - \left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right) \left(c_{2e}^n\right) -$$

$$md_2^n \left(k_b^3\rho^2\right)_{j-1/2}^n \frac{1}{\left(M_N\right)^2} \left(c_{2e}^n\right)^3 3 \left(Qs_2^n\right)_{j-1}^2 +$$

$$\frac{md_2^n}{2} \left(k_f^4\rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}} \left(c_{5e}^n Qs_{5j-1}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$

$$\frac{md_2^n}{2} \left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n Qs_{4j-1}^n\right) \left(c_{2e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j-1}^n}{M_N}\right] -$$

$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}} +$$

$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{5e}^n Qs_{5j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$

$$\frac{md_2^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{1}{M_{O_2}}\left(c_{3e}^n Qs_{3j-1}^n\right)\left(c_{2e}^n\right) +$$

$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{2e}^n\right) -$$

$$\frac{md_2^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n \frac{1}{M_{NO}}\left(c_{5e}^n Qs_{5j-1}^n\right)\left(c_{2e}^n\right) - \frac{\alpha^n}{2}F_{2j-1}^n - \frac{\alpha^n}{2}F_{2j-1/2}^{n-1}, \tag{B.39}$$

$$(e_{19})_j = md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{3e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}\right]$$

$$+md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{3e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}} +$$

$$md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(1-\left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)$$

$$\left[\frac{c_{3e}^n}{M_{O_2}} - \frac{c_{3e}^n}{M_{N_2}}\right] -$$

$$md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j}^n\right)^2\left[\frac{c_{3e}^n}{M_{O_2}} - \frac{c_{3e}^n}{M_{N_2}}\right] +$$

$$md_2^n\left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(-c_{3e}^n\right)\left(c_{2e}^n Qs_{2j}^n\right) +$$

$$\frac{md_2^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^nQs_{5j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^nQs_{4j}^n\right)\left(c_{2e}^nQs_{2j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_{O_2}}\left(c_{2e}^nQs_{2j}^n\right)\left(c_{3e}^n\right)+$$
$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}M_O}\left(c_{4e}^nQs_{4j}^n\right)\left(-c_{3e}^n\right), \tag{B.40}$$

$$\left(e_{20}\right)_j=md_2^n\left(k_f^2\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}}\left(-c_{3e}^n\right)$$
$$\left[\frac{c_{4e}^nQs_{4j-1}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1}^n}{M_{NO}}\right]$$
$$+md_2^n\left(k_f^2\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}}\left(-c_{3e}^n\right)$$
$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1}^n+c_{3e}^nQs_{3j-1}^n+c_{4e}^nQs_{4j-1}^n+c_{5e}^nQs_{5j-1}^n\right)\right)}{M_{N_2}}+$$
$$md_2^n\left(k_f^2\rho\right)_{j-1/2}^n\frac{M_N}{M_{N_2}}$$
$$\left(1-\left(c_{2e}^nQs_{2j-1}^n+c_{3e}^nQs_{3j-1}^n+c_{4e}^nQs_{4j-1}^n+c_{5e}^nQs_{5j-1}^n\right)\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j-1}^n\right)^2\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$md_2^n\left(k_f^3\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(-c_{3e}^n\right)\left(c_{2e}^nQs_{2j-1}^n\right)+$$
$$\frac{md_2^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_N}{M_{NO}}\left(c_{5e}^nQs_{5j-1}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^nQs_{4j-1}^n\right)\left(c_{2e}^nQs_{2j-1}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_{O_2}}\left(c_{2e}^nQs_{2j-1}^n\right)\left(c_{3e}^n\right)+$$

$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{3e}^n\right), \tag{B.41}$$

$$\left(e_{21}\right)_j = md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{4e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O}+\frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}\right]$$

$$+md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{4e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}}+$$

$$md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}$$

$$\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j}^n\right)^2\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]+$$

$$md_2^n\left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(-c_{4e}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)+$$

$$\frac{md_2^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}}\left(c_{5e}^n Qs_{5j}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O}+\frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}+\frac{c_{2e}^n Qs_{2j}^n}{M_N}\right]$$

$$-\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}}+$$

$$\frac{md_2^n}{2}\left(k_f^5\rho^2\right)_{j-1/2}^n \frac{M_N}{M_{NO}M_O}\left(c_{5e}^n Qs_{5j}^n\right)\left(c_{4e}^n\right)+$$
$$\frac{md_2^n}{2}\left(k_f^6\rho^2\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n\right)$$
$$\left(1-\left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)+$$
$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(-c_{4e}^n\right), \tag{B.42}$$

$$\left(e_{22}\right)_j = md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{4e}^n\right)$$
$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}}\right]$$
$$+md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{4e}^n\right)$$
$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}}+$$
$$md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}$$
$$\left(1-\left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right]-$$
$$md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j-1}^n\right)^2\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right]+$$
$$md_2^n\left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(-c_{4e}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)+$$
$$\frac{md_2^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}}\left(c_{5e}^n Qs_{5j-1}^n\right)\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)$$
$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j-1}^n}{M_N}\right]$$

$$-\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)$$
$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}}+$$
$$\frac{md_2^n}{2}\left(k_f^5\rho^2\right)_{j-1/2}^n \frac{M_N}{M_{NO}M_O}\left(c_{5e}^n Qs_{5j-1}^n\right)\left(c_{4e}^n\right)+$$
$$\frac{md_2^n}{2}\left(k_f^6\rho^2\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n\right)$$
$$\left(1-\left(c_{2e}^n Qs_{2j-1}^n+c_{3e}^n Qs_{3j-1}^n+c_{4e}^n Qs_{4j-1}^n+c_{5e}^n Qs_{5j-1}^n\right)\right)+$$
$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{4e}^n\right), \tag{B.43}$$

$$\left(e_{23}\right)_j = md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{5e}^n\right)$$
$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O}+\frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}\right]$$
$$+md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{5e}^n\right)$$
$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}}+$$
$$md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}$$
$$\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$
$$md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j}^n\right)^2\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$
$$md_2^n\left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(-c_{5e}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)+$$
$$\frac{md_2^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}}\left(c_{5e}^n Qs_{5j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$
$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$

$$\frac{md_2^n}{2}\left(k_f^5\rho^2\right)_{j-1/2}^n \frac{M_N}{M_{NO}M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{5e}^n\right)+$$

$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(-c_{5e}^n\right)-$$

$$\frac{md_2^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n \frac{1}{M_{NO}}\left(c_{2e}^n Qs_{2j}^n\right)\left(c_{5e}^n\right), \tag{B.44}$$

$$\left(e_{24}\right)_j = md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{5e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O}+\frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}}\right]$$

$$+md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}\left(-c_{5e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1}^n+c_{3e}^n Qs_{3j-1}^n+c_{4e}^n Qs_{4j-1}^n+c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}}+$$

$$md_2^n\left(k_f^2\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}}$$

$$\left(1-\left(c_{2e}^n Qs_{2j-1}^n+c_{3e}^n Qs_{3j-1}^n+c_{4e}^n Qs_{4j-1}^n+c_{5e}^n Qs_{5j-1}^n\right)\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$md_2^n\left(k_b^2\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{2e}^n\right)^2\left(Qs_{2j-1}^n\right)^2\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$

$$md_2^n\left(k_f^3\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(-c_{5e}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)+$$

$$\frac{md_2^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_N}{M_{NO}}\left(c_{5e}^n Qs_{5j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$\frac{md_2^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$

$$\frac{md_2^n}{2}\left(k_f^5\rho^2\right)_{j-1/2}^n \frac{M_N}{M_{NO}M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{5e}^n\right)+$$

$$\frac{md_2^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_N}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{5e}^n\right)-$$

$$\frac{md_2^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n \frac{1}{M_{NO}}\left(c_{2e}^n Q s_{2j-1}^n\right)\left(c_{5e}^n\right), \tag{B.45}$$

$$(e_{49})_j = \frac{\left(\frac{C}{Sm_2}\right)_j^n}{h_j} + \frac{1}{2}F_{1j}^n + \frac{\alpha^n}{2}F_{1j}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}, \tag{B.46}$$

$$(e_{50})_j = \frac{\left(\frac{C}{Sm_2}\right)_{j-1}^n}{h_j} + \frac{1}{2}F_{1j-1}^n + \frac{\alpha^n}{2}F_{1j-1}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}. \tag{B.47}$$

Fifth Equation

$$(r_5)_j = \frac{\left(\frac{C}{Sm_3}\right)^n_j}{h_j}\delta Qd^n_{3j} - \frac{\left(\frac{C}{Sm_3}\right)^n_{j-1}}{h_j}\delta Qd^n_{3j-1} + (\delta Qd_3F_1)^n_{j-1/2} + (Qd_3\delta F_1)^n_{j-1/2} - ms^n_3\delta F^n_{2j-1/2}$$

$$-md^n_3\left(k^1_f\rho\right)^n_{j-1/2}\left(c^n_{3e}\delta Qs^n_{3j-1/2}\right)$$

$$\left[\frac{c^n_{4e}Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e}Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e}Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e}Qs^n_{2j-1/2}}{M_N}\right]$$

$$-md^n_3\left(k^1_f\rho\right)^n_{j-1/2}\left(c^n_{3e}\delta Qs^n_{3j-1/2}\right)$$

$$\frac{\left(1 - \left(c^n_{2e}Qs^n_{2j-1/2} + c^n_{3e}Qs^n_{3j-1/2} + c^n_{4e}Qs^n_{4j-1/2} + c^n_{5e}Qs^n_{5j-1/2}\right)\right)}{M_{N_2}} \tag{B.48}$$

$$-md^n_3\left(k^1_f\rho\right)^n_{j-1/2}\left(c^n_{3e}Qs^n_{3j-1/2}\right)$$

$$\left[\frac{c^n_{4e}\delta Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e}\delta Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e}\delta Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e}\delta Qs^n_{2j-1/2}}{M_N}\right.$$

$$-md^n_3\left(k^1_f\rho\right)^n_{j-1/2}\left(c^n_{3e}Qs^n_{3j-1/2}\right)$$

$$\frac{\left(-\left(c^n_{2e}\delta Qs^n_{2j-1/2} + c^n_{3e}\delta Qs^n_{3j-1/2} + c^n_{4e}\delta Qs^n_{4j-1/2} + c^n_{5e}\delta Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}$$

$$+md^n_3\left(k^1_b\rho^2\right)^n_{j-1/2}\frac{M_{O_2}}{M^2_O}\left(c^n_{4e}\right)^2 2\left(Qs^n_{4j-1/2}\delta Qs^n_{4j-1/2}\right)$$

$$\left[\frac{c^n_{4e}Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e}Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e}Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e}Qs^n_{2j-1/2}}{M_N}\right]$$

$$+md^n_3\left(k^1_b\rho^2\right)^n_{j-1/2}\frac{M_{O_2}}{M^2_O}\left(c^n_{4e}\right)^2 2\left(Qs^n_{4j-1/2}\delta Qs^n_{4j-1/2}\right)$$

$$\frac{\left(1 - \left(c^n_{2e}Qs^n_{2j-1/2} + c^n_{3e}Qs^n_{3j-1/2} + c^n_{4e}Qs^n_{4j-1/2} + c^n_{5e}Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}$$

$$+md^n_3\left(k^1_b\rho^2\right)^n_{j-1/2}\frac{M_{O_2}}{M^2_O}\left(c^n_{4e}\right)^2\left(Qs^n_{4j-1/2}\right)^2$$

$$\left[\frac{c_{4e}^n \delta Q s_{4j-1/2}^n}{M_O} + \frac{c_{3e}^n \delta Q s_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n \delta Q s_{5j-1/2}^n}{M_{NO}} + \frac{c_{2e}^n \delta Q s_{2j-1/2}^n}{M_N}\right.$$

$$+md_3^n \left(k_b^1 \rho^2\right)_{j-1/2}^n \frac{M_{O_2}}{M_O^2} \left(c_{4e}^n\right)^2 \left(Q s_{4j-1/2}^n\right)^2$$

$$\frac{\left(-\left(c_{2e}^n \delta Q s_{2j-1/2}^n + c_{3e}^n \delta Q s_{3j-1/2}^n + c_{4e}^n \delta Q s_{4j-1/2}^n + c_{5e}^n \delta Q s_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$md_3^n \left(k_f^5 \rho\right)_{j-1/2}^n \frac{M_{O_2}}{M_{NO} M_O} \left(c_{5e}^n \delta Q s_{5j-1/2}^n\right) \left(c_{4e}^n Q s_{4j-1/2}^n\right) +$$

$$md_3^n \left(k_f^5 \rho\right)_{j-1/2}^n \frac{M_{O_2}}{M_{NO} M_O} \left(c_{5e}^n Q s_{5j-1/2}^n\right) \left(c_{4e}^n \delta Q s_{4j-1/2}^n\right) -$$

$$md_3^n \left(k_b^5 \rho\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{3e}^n \delta Q s_{3j-1/2}^n\right) \left(c_{2e}^n Q s_{2j-1/2}^n\right) -$$

$$md_3^n \left(k_b^5 \rho\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{3e}^n Q s_{3j-1/2}^n\right) \left(c_{2e}^n \delta Q s_{2j-1/2}^n\right) -$$

$$\alpha^n \left[\left(\delta Q s_3 F_2\right)_{j-1/2}^n + \left(Q s_3 \delta F_2\right)_{j-1/2}^n\right] + \alpha^n \left[\left(\delta Q d_3 F_1\right)_{j-1/2}^n + \left(Q d_3 \delta F_1\right)_{j-1/2}^n\right] -$$

$$\alpha^n \left[\delta Q s_{3j-1/2}^n F_{2j-1/2}^{n-1} - Q s_{3j-1/2}^{n-1} \delta F_{2j-1/2}^n + \delta Q d_{3j-1/2}^n F_{1j-1/2}^{n-1} - Q d_{3j-1/2}^{n-1} \delta F_{1j-1/2}^n\right].$$

The definition of $(r_5)_j$ is written as follows:

$$(r_5)_j \equiv \frac{\left(\frac{C}{Sm_3}\right)_j^n Q d_{3j}^n - \left(\frac{C}{Sm_3}\right)_{j-1}^n Q d_{3j-1}^n}{h_j} + \left(Q d_3 F_1\right)_{j-1/2}^n - m s_3^n F_{2j-1/2}^n$$

$$-md_3^n \left(k_f^1 \rho\right)_{j-1/2}^n \left(c_{3e}^n Q s_{3j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n Q s_{4j-1/2}^n}{M_O} + \frac{c_{3e}^n Q s_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n Q s_{5j-1/2}^n}{M_{NO}} + \frac{c_{2e}^n Q s_{2j-1/2}^n}{M_N}\right]$$

$$-md_3^n \left(k_f^1 \rho\right)_{j-1/2}^n \left(c_{3e}^n Q s_{3j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Q s_{2j-1/2}^n + c_{3e}^n Q s_{3j-1/2}^n + c_{4e}^n Q s_{4j-1/2}^n + c_{5e}^n Q s_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+md_3^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}(c_{4e}^n)^2\left(Qs_{4j-1/2}^n\right)^2$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}\right]$$

$$+md_3^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}(c_{4e}^n)^2\left(Qs_{4j-1/2}^n\right)^2$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+md_3^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_{O_2}}{M_{NO}M_O}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{4e}^nQs_{4j-1/2}^n\right)$$

$$-md_3^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{3e}^nQs_{3j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)-$$

$$2\xi^{n-1/2}\frac{\left(Qs_{3j-1/2}^nF_{2j-1/2}^n+Qs_{3j-1/2}^nF_{2j-1/2}^{n-1}-Qs_{3j-1/2}^{n-1}F_{2j-1/2}^n\right)}{k_n}-$$

$$2\xi^{n-1/2}\frac{\left(-Qd_{3j-1/2}^nF_{1j-1/2}^n+Qd_{3j-1/2}^nF_{1j-1/2}^{n-1}-Qd_{3j-1/2}^{n-1}F_{1j-1/2}^n\right)}{k_n}$$

We can recast the equation in the form of:

$$(r_5)_j=(e_2)_j\,\delta F_{1j}+(e_6)_j\,\delta F_{1j-1}+(e_{10})_j\,\delta F_{2j}+(e_{14})_j\,\delta F_{2j-1}+(e_{25})_j\,\delta Qs_{2j}+(e_{26})_j\,\delta Qs_{2j-1}+$$
$$(e_{27})_j\,\delta Qs_{3j}+(e_{28})_j\,\delta Qs_{3j-1}+(e_{29})_j\,\delta Qs_{4j}+(e_{30})_j\,\delta Qs_{4j-1}+(e_{31})_j\,\delta Qs_{5j}+$$
$$(e_{32})_j\,\delta Qs_{5j-1}+(e_{51})_j\,\delta Qd_{3j}+(e_{52})_j\,\delta Qd_{3j-1}. \qquad \text{(B.49)}$$

The coefficients in (B.49) are defined as:

$$(e_2)_j = \frac{1}{2}Qd_{3j}^n + \frac{\alpha^n}{2}Qd_{3j}^n + \frac{\alpha^n}{2}Qd_{3j-1/2}^{n-1} = \frac{\alpha_1}{2}Qd_{3j}^n + \frac{\alpha^n}{2}Qd_{3j-1/2}^{n-1}, \tag{B.50}$$

$$(e_6)_j = \frac{1}{2}Qd_{3j-1}^n + \frac{\alpha^n}{2}Qd_{3j-1}^n + \frac{\alpha^n}{2}Qd_{3j-1/2}^{n-1} = \frac{\alpha_1}{2}Qd_{3j-1}^n + \frac{\alpha^n}{2}Qd_{3j-1/2}^{n-1}, \tag{B.51}$$

$$(e_{10})_j = -\frac{ms_3^n}{2} - \frac{\alpha^n}{2}Qs_{3j}^n + \frac{\alpha^n}{2}Qs_{3j-1/2}^{n-1}, \tag{B.52}$$

$$(e_{14})_j = -\frac{ms_3^n}{2} - \frac{\alpha^n}{2}Qs_{3j-1}^n + \frac{\alpha^n}{2}Qs_{3j-1/2}^{n-1}, \tag{B.53}$$

$$(e_{25})_j = -\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n Qs_{3j}^n\right)\left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right]$$
$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n \frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)^2\left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$
$$\frac{md_3^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{3e}^n Qs_{3j}^n\right)\left(c_{2e}^n\right), \tag{B.54}$$

$$(e_{26})_j = -\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n Qs_{3j-1}^n\right)\left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right]$$
$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n \frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$
$$\frac{md_3^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{3e}^n Qs_{3j-1}^n\right)\left(c_{2e}^n\right), \tag{B.55}$$

$$(e_{27})_j = -\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n\right)$$
$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j}^n}{M_N}\right]$$

$$-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j}^n+c_{3e}^nQs_{3j}^n+c_{4e}^nQs_{4j}^n+c_{5e}^nQs_{5j}^n\right)\right)}{M_{N_2}}$$

$$-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^nQs_{3j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)^2\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$

$$\frac{md_3^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^nQs_{2j}^n\right)\left(c_{3e}^n\right)-\frac{\alpha^n}{2}F_{2j}^n-\frac{\alpha^n}{2}F_{2j-1/2}^{n-1}, \qquad \text{(B.56)}$$

$$\left(e_{28}\right)_j=-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1}^n}{M_N}\right]$$

$$-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1}^n+c_{3e}^nQs_{3j-1}^n+c_{4e}^nQs_{4j-1}^n+c_{5e}^nQs_{5j-1}^n\right)\right)}{M_{N_2}}$$

$$-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^nQs_{3j-1}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$

$$\frac{md_3^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^nQs_{2j-1}^n\right)\left(c_{3e}^n\right)-\frac{\alpha^n}{2}F_{2j-1}^n-\frac{\alpha^n}{2}F_{2j-1/2}^{n-1}, \qquad \text{(B.57)}$$

$$\left(e_{29}\right)_j=-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^nQs_{3j}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j}^n}{M_O}+\frac{c_{3e}^nQs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j}^n}{M_N}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j}^n+c_{3e}^nQs_{3j}^n+c_{4e}^nQs_{4j}^n+c_{5e}^nQs_{5j}^n\right)\right)}{M_{N_2}}$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)^2\left[\frac{c_{4e}^n}{M_{O_2}}-\frac{c_{4e}^n}{M_{N_2}}\right]+$$

$$\frac{md_3^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_{O_2}}{M_OM_{NO}}\left(c_{5e}^nQs_{5j}^n\right)\left(c_{4e}^n\right), \tag{B.58}$$

$$\left(e_{30}\right)_j=-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^nQs_{3j-1}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1}^n}{M_N}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1}^n+c_{3e}^nQs_{3j-1}^n+c_{4e}^nQs_{4j-1}^n+c_{5e}^nQs_{5j-1}^n\right)\right)}{M_{N_2}}$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{4e}^n}{M_{O_2}}-\frac{c_{4e}^n}{M_{N_2}}\right]+$$

$$\frac{md_3^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_{O_2}}{M_OM_{NO}}\left(c_{5e}^nQs_{5j-1}^n\right)\left(c_{4e}^n\right), \tag{B.59}$$

$$\left(e_{31}\right)_j=-\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^nQs_{3j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)^2\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$

$$\frac{md_3^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_{O_2}}{M_OM_{NO}}\left(c_{4e}^nQs_{4j}^n\right)\left(c_{5e}^n\right), \tag{B.60}$$

$$(e_{32})_j = -\frac{md_3^n}{2}\left(k_f^1\rho\right)_{j-1/2}^n\left(c_{3e}^n Qs_{3j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}} - \frac{c_{5e}^n}{M_{N_2}}\right]$$

$$+\frac{md_3^n}{2}\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{M_{O_2}}{M_O^2}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{5e}^n}{M_{NO}} - \frac{c_{5e}^n}{M_{N_2}}\right] +$$

$$\frac{md_3^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{M_{O_2}}{M_O M_{NO}}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{5e}^n\right), \tag{B.61}$$

$$(e_{51})_j = \frac{\left(\frac{C}{Sm_3}\right)_j^n}{h_j} + \frac{1}{2}F_{1j}^n + \frac{\alpha^n}{2}F_{1j}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}, \tag{B.62}$$

$$(e_{52})_j = \frac{\left(\frac{C}{Sm_3}\right)_{j-1}^n}{h_j} + \frac{1}{2}F_{1j-1}^n + \frac{\alpha^n}{2}F_{1j-1}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}. \tag{B.63}$$

Sixth Equation

$$(r_6)_j = \frac{\left(\frac{C}{Sm_4}\right)_j^n \delta Qd_{4j}^n - \left(\frac{C}{Sm_4}\right)_{j-1}^n \delta Qd_{4j-1}^n}{h_j} + (\delta Qd_4F_1)_{j-1/2}^n + (Qd_4\delta F_1)_{j-1/2}^n - ms_4^n\delta F_{2j-1/2}^n$$

$$+2md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^n\delta Qs_{3j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}\right]$$

$$+2md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^n\delta Qs_{3j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+2md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right) \tag{B.64}$$

$$\left[\frac{c_{4e}^n\delta Qs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^n\delta Qs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^n\delta Qs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^n\delta Qs_{2j-1/2}^n}{M_N}\right.$$

$$+2md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)$$

$$\frac{\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-2md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2 2\left(Qs_{4j-1/2}^n\delta Qs_{4j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}\right]$$

$$-2md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2 2\left(Qs_{4j-1/2}^n\delta Qs_{4j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j-1/2}^n\right)^2$$

$$\left[\frac{c_{4e}^n \delta Qs_{4j-1/2}^n}{M_O} + \frac{c_{3e}^n \delta Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n \delta Qs_{5j-1/2}^n}{M_{NO}} + \frac{c_{2e}^n \delta Qs_{2j-1/2}^n}{M_N}\right.$$

$$-md_4^n \left(k_b^1 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n\right)^2 \left(Qs_{4j-1/2}^n\right)^2$$

$$\frac{\left(-\left(c_{2e}^n \delta Qs_{2j-1/2}^n + c_{3e}^n \delta Qs_{3j-1/2}^n + c_{4e}^n \delta Qs_{4j-1/2}^n + c_{5e}^n \delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+md_4^n \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n \delta Qs_{5j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1/2}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1/2}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j-1/2}^n}{M_N}\right]$$

$$+md_4^n \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n \delta Qs_{5j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+md_4^n \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n Qs_{5j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n \delta Qs_{4j-1/2}^n}{M_O} + \frac{c_{3e}^n \delta Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n \delta Qs_{5j-1/2}^n}{M_{NO}} + \frac{c_{2e}^n \delta Qs_{2j-1/2}^n}{M_N}\right.$$

$$+md_4^n \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n Qs_{5j-1/2}^n\right)$$

$$\frac{\left(-\left(c_{2e}^n \delta Qs_{2j-1/2}^n + c_{3e}^n \delta Qs_{3j-1/2}^n + c_{4e}^n \delta Qs_{4j-1/2}^n + c_{5e}^n \delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_4^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{4e}^n \delta Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1/2}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1/2}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1/2}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j-1/2}^n}{M_N}\right]$$

$$-md_4^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{4e}^n \delta Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_4^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}\right]$$

$$-md_4^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_4^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n\delta Qs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^n\delta Qs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^n\delta Qs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^n\delta Qs_{2j-1/2}^n}{M_N}\right.$$

$$-md_4^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\frac{\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_4^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)\left(c_{4e}^nQs_{4j-1/2}^n\right)$$

$$-md_4^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{4e}^n\delta Qs_{4j-1/2}^n\right)+$$

$$md_4^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{M_O}{M_NM_{O_2}}\left(c_{3e}^n\delta Qs_{3j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)+$$

$$md_4^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{M_O}{M_NM_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)-$$

$$md_4^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}c_{4e}^nQs_{4j-1/2}^n$$

$$\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)$$

$$-md_4^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}c_{4e}^n\delta Qs_{4j-1/2}^n$$

$$\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)$$

$$+md_4^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}M_N}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)+$$

$$md_4^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}M_N}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)-$$

$$\alpha^n\left[\left(\delta Qs_4F_2\right)_{j-1/2}^n+\left(Qs_4\delta F_2\right)_{j-1/2}^n\right]+\alpha^n\left[\left(\delta Qd_4F_1\right)_{j-1/2}^n+\left(Qd_4\delta F_1\right)_{j-1/2}^n\right]-$$

$$\alpha^n\left[\delta Qs_{4j-1/2}^nF_{2j-1/2}^{n-1}-Qs_{4j-1/2}^{n-1}\delta F_{2j-1/2}^n+\delta Qd_{4j-1/2}^nF_{1j-1/2}^{n-1}-Qd_{4j-1/2}^{n-1}\delta F_{1j-1/2}^n\right],$$

The definition of $(r_6)_j$ is written as follows:

$$(r_6)_j\equiv\frac{\left(\frac{C}{Sm_4}\right)_j^nQd_{4j}^n-\left(\frac{C}{Sm_4}\right)_{j-1}^nQd_{4j-1}^n}{h_j}+\left(Qd_4F_1\right)_{j-1/2}^n-ms_4^nF_{2j-1/2}^n+$$

$$2md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}\right]+$$

$$2md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}-$$

$$2md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j-1/2}^n\right)^2$$

$$\left[\frac{c_{4e}^nQs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1/2}^n}{M_N}\right]-$$

$$2md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j-1/2}^n\right)^2$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}+$$

$$md_4^n\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^nQs_{5j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^{n} Qs_{4j-1/2}^{n}}{M_O} + \frac{c_{3e}^{n} Qs_{3j-1/2}^{n}}{M_{O_2}} + \frac{c_{5e}^{n} Qs_{5j-1/2}^{n}}{M_{NO}} + \frac{c_{2e}^{n} Qs_{2j-1/2}^{n}}{M_N}\right] +$$

$$md_4^n \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n Qs_{5j-1/2}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right)}{M_{N_2}} -$$

$$md_4^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{4e}^n Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^{n} Qs_{4j-1/2}^{n}}{M_O} + \frac{c_{3e}^{n} Qs_{3j-1/2}^{n}}{M_{O_2}} + \frac{c_{5e}^{n} Qs_{5j-1/2}^{n}}{M_{NO}} + \frac{c_{2e}^{n} Qs_{2j-1/2}^{n}}{M_N}\right] -$$

$$md_4^n \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{4e}^n Qs_{4j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_4^n \left(k_f^5 \rho\right)_{j-1/2}^n \frac{1}{M_{NO}} \left(c_{5e}^n Qs_{5j-1/2}^n\right) \left(c_{4e}^n Qs_{4j-1/2}^n\right) +$$

$$md_4^n \left(k_b^5 \rho\right)_{j-1/2}^n \frac{M_O}{M_N M_{O_2}} \left(c_{3e}^n Qs_{3j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right) -$$

$$md_4^n \left(k_f^6 \rho\right)_{j-1/2}^n \frac{1}{M_{N_2}} c_{4e}^n Qs_{4j-1/2}^n$$

$$\left(1 - \left(c_{2e}^n Qs_{2j-1/2}^n + c_{3e}^n Qs_{3j-1/2}^n + c_{4e}^n Qs_{4j-1/2}^n + c_{5e}^n Qs_{5j-1/2}^n\right)\right) c_{4e}^n Qs_{4j-1/2}^n +$$

$$md_4^n \left(k_b^6 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO} M_N} \left(c_{5e}^n Qs_{5j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right) -$$

$$2\xi^{n-1/2} \frac{\left(Qs_{4j-1/2}^n F_{2j-1/2}^n + Qs_{4j-1/2}^n F_{2j-1/2}^{n-1} - Qs_{4j-1/2}^{n-1} F_{2j-1/2}^n\right)}{k_n} -$$

$$2\xi^{n-1/2} \frac{\left(-Qd_{4j-1/2}^n F_{1j-1/2}^n + Qd_{4j-1/2}^n F_{1j-1/2}^{n-1} - Qd_{4j-1/2}^{n-1} F_{1j-1/2}^n\right)}{k_n}$$

We can recast the equation in the form of:

$$(r_6)_j = (e_3)_j\,\delta F_{1j} + (e_7)_j\,\delta F_{1j-1} + (e_{11})_j\,\delta F_{2j} + (e_{15})_j\,\delta F_{2j-1} + (e_{33})_j\,\delta Qs_{2j} + (e_{34})_j\,\delta Qs_{2j-1} +$$
$$(e_{35})_j\,\delta Qs_{3j} + (e_{36})_j\,\delta Qs_{3j-1} + (e_{37})_j\,\delta Qs_{4j} + (e_{38})_j\,\delta Qs_{4j-1} + (e_{39})_j\,\delta Qs_{5j} +$$
$$(e_{40})_j\,\delta Qs_{5j-1} + (e_{53})_j\,\delta Qd_{4j} + (e_{54})_j\,\delta Qd_{4j-1}. \quad \text{(B.65)}$$

The coefficients in (B.65) are defined as:

$$(e_3)_j = \frac{1}{2}Qd_{4j}^n + \frac{\alpha^n}{2}Qd_{4j}^n + \frac{\alpha^n}{2}Qd_{4j-1/2}^{n-1} = \frac{\alpha_1}{2}Qd_{4j}^n + \frac{\alpha^n}{2}Qd_{4j-1/2}^{n-1}, \quad \text{(B.66)}$$

$$(e_7)_j = \frac{1}{2}Qd_{4j-1}^n + \frac{\alpha^n}{2}Qd_{4j-1}^n + \frac{\alpha^n}{2}Qd_{4j-1/2}^{n-1} = \frac{\alpha_1}{2}Qd_{4j-1}^n + \frac{\alpha^n}{2}Qd_{4j-1/2}^{n-1}, \quad \text{(B.67)}$$

$$(e_{11})_j = -\frac{ms_4^n}{2} - \frac{\alpha^n}{2}Qs_{4j}^n + \frac{\alpha^n}{2}Qs_{4j-1/2}^{n-1}, \quad \text{(B.68)}$$

$$(e_{15})_j = -\frac{ms_4^n}{2} - \frac{\alpha^n}{2}Qs_{4j-1}^n + \frac{\alpha^n}{2}Qs_{4j-1/2}^{n-1}, \quad \text{(B.69)}$$

$$(e_{33})_j = md_4^n \left(k_f^1\rho\right)_{j-1/2}^n \frac{M_O}{M_{O_2}} \left(c_{3e}^n Qs_{3j}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$
$$md_4^n \left(k_b^1\rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n\right)^2 \left(Qs_{4j}^n\right)^2 \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] +$$
$$\frac{md_4^n}{2} \left(k_f^4\rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n Qs_{5j}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] -$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O}+\frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}+\frac{c_{2e}^n Qs_{2j}^n}{M_N}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}}-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)\left[\frac{c_{2e}^n}{M_N}-\frac{c_{2e}^n}{M_{N_2}}\right]+$$

$$\frac{md_4^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{M_O}{M_N M_{O_2}}\left(c_{3e}^n Qs_{3j}^n\right)\left(c_{2e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(c_{4e}^n Qs_{4j}^n\right)\left(-c_{2e}^n\right)+$$

$$\frac{md_4^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}M_N}\left(c_{5e}^n Qs_{5j}^n\right)\left(c_{2e}^n\right), \tag{B.70}$$

$$(e_{34})_j = md_4^n\left(k_f^1\rho\right)_{j-1/2}^n \frac{M_O}{M_{O_2}}\left(c_{3e}^n Qs_{3j-1}^n\right)\left[\frac{c_{2e}^n}{M_N}-\frac{c_{2e}^n}{M_{N_2}}\right]-$$

$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{2e}^n}{M_N}-\frac{c_{2e}^n}{M_{N_2}}\right]+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}}\left(c_{5e}^n Qs_{5j-1}^n\right)\left[\frac{c_{2e}^n}{M_N}-\frac{c_{2e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O}+\frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}}+\frac{c_{2e}^n Qs_{2j-1}^n}{M_N}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1}^n+c_{3e}^n Qs_{3j-1}^n+c_{4e}^n Qs_{4j-1}^n+c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}}-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j-1}^n\right)\left(c_{2e}^nQs_{2j-1}^n\right)\left[\frac{c_{2e}^n}{M_N}-\frac{c_{2e}^n}{M_{N_2}}\right]+$$
$$\frac{md_4^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n\frac{M_O}{M_NM_{O_2}}\left(c_{3e}^nQs_{3j-1}^n\right)\left(c_{2e}^n\right)-$$
$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{4e}^nQs_{4j-1}^n\right)\left(-c_{2e}^n\right)+$$
$$\frac{md_4^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}M_N}\left(c_{5e}^nQs_{5j-1}^n\right)\left(c_{2e}^n\right), \tag{B.71}$$

$$(e_{35})_j=md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^n\right)$$
$$\left[\frac{c_{4e}^nQs_{4j}^n}{M_O}+\frac{c_{3e}^nQs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j}^n}{M_N}\right]+$$
$$md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^n\right)$$
$$\frac{\left(1-\left(c_{2e}^nQs_{2j}^n+c_{3e}^nQs_{3j}^n+c_{4e}^nQs_{4j}^n+c_{5e}^nQs_{5j}^n\right)\right)}{M_{N_2}}-$$
$$md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)^2\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^nQs_{5j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]-$$
$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j}^n\right)\left(c_{2e}^nQs_{2j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$\frac{md_4^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n\frac{M_O}{M_NM_{O_2}}\left(c_{2e}^nQs_{2j}^n\right)\left(c_{3e}^n\right)-$$
$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{4e}^nQs_{4j}^n\right)\left(-c_{3e}^n\right), \tag{B.72}$$

$$(e_{36})_j=md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j-1}^n}{M_N}\right] +$$

$$md_4^n \left(k_f^1 \rho\right)_{j-1/2}^n \frac{M_O}{M_{O_2}} \left(c_{3e}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j-1}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}} -$$

$$md_4^n \left(k_f^1 \rho\right)_{j-1/2}^n \frac{M_O}{M_{O_2}} \left(c_{3e}^n Qs_{3j-1}^n\right) \left[\frac{c_{3e}^n}{M_{O_2}} - \frac{c_{3e}^n}{M_{N_2}}\right] -$$

$$md_4^n \left(k_b^1 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n\right)^2 \left(Qs_{4j-1}^n\right)^2 \left[\frac{c_{3e}^n}{M_{O_2}} - \frac{c_{3e}^n}{M_{N_2}}\right] +$$

$$\frac{md_4^n}{2} \left(k_f^4 \rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}} \left(c_{5e}^n Qs_{5j-1}^n\right) \left[\frac{c_{3e}^n}{M_{O_2}} - \frac{c_{3e}^n}{M_{N_2}}\right] -$$

$$\frac{md_4^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{4e}^n Qs_{4j-1}^n\right) \left(c_{2e}^n Qs_{2j-1}^n\right) \left[\frac{c_{3e}^n}{M_{O_2}} - \frac{c_{3e}^n}{M_{N_2}}\right] +$$

$$\frac{md_4^n}{2} \left(k_b^5 \rho\right)_{j-1/2}^n \frac{M_O}{M_N M_{O_2}} \left(c_{2e}^n Qs_{2j-1}^n\right) \left(c_{3e}^n\right) -$$

$$\frac{md_4^n}{2} \left(k_f^6 \rho\right)_{j-1/2}^n \frac{1}{M_{N_2}} \left(c_{4e}^n Qs_{4j-1}^n\right) \left(-c_{3e}^n\right), \tag{B.73}$$

$$(e_{37})_j = md_4^n \left(k_f^1 \rho\right)_{j-1/2}^n \frac{M_O}{M_{O_2}} \left(c_{3e}^n Qs_{3j}^n\right) \left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right] -$$

$$md_4^n \left(k_b^1 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n\right)^2 2 \left(Qs_{4j}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j}^n}{M_N}\right] -$$

$$md_4^n \left(k_b^1 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n\right)^2 2 \left(Qs_{4j}^n\right)$$

$$\frac{\left(1 - \left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}} -$$

$$md_4^n \left(k_b^1 \rho^2\right)_{j-1/2}^n \frac{1}{M_O} \left(c_{4e}^n\right)^2 \left(Qs_{4j}^n\right)^2 \left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right] +$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^nQs_{5j}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^n\right)\left(c_{2e}^nQs_{2j}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j}^n}{M_O}+\frac{c_{3e}^nQs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j}^n}{M_N}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^n\right)\left(c_{2e}^nQs_{2j}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j}^n+c_{3e}^nQs_{3j}^n+c_{4e}^nQs_{4j}^n+c_{5e}^nQs_{5j}^n\right)\right)}{M_{N_2}}-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j}^n\right)\left(c_{2e}^nQs_{2j}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{5e}^nQs_{5j}^n\right)\left(c_{4e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{4e}^nQs_{4j}^n\right)\left(-c_{4e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{4e}^n\right)\left(1-\left(c_{2e}^nQs_{2j}^n+c_{3e}^nQs_{3j}^n+c_{4e}^nQs_{4j}^n+c_{5e}^nQs_{5j}^n\right)\right)$$

$$-\frac{\alpha^n}{2}F_{2j}^n-\frac{\alpha^n}{2}F_{2j-1/2}^{n-1}, \tag{B.74}$$

$$(e_{38})_j=md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j-1}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2 2\left(Qs_{4j-1}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1}^n}{M_N}\right]-$$

$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2 2\left(Qs_{4j-1}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1}^n+c_{3e}^nQs_{3j-1}^n+c_{4e}^nQs_{4j-1}^n+c_{5e}^nQs_{5j-1}^n\right)\right)}{M_{N_2}}-$$

$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}}\left(c_{5e}^n Qs_{5j-1}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O}+\frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}}+\frac{c_{2e}^n Qs_{2j-1}^n}{M_N}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j-1}^n+c_{3e}^n Qs_{3j-1}^n+c_{4e}^n Qs_{4j-1}^n+c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}}-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n \frac{1}{M_{NO}}\left(c_{5e}^n Qs_{5j-1}^n\right)\left(c_{4e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{4e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{1}{M_{N_2}}\left(c_{4e}^n\right)\left(1-\left(c_{2e}^n Qs_{2j-1}^n+c_{3e}^n Qs_{3j-1}^n+c_{4e}^n Qs_{4j-1}^n+c_{5e}^n Qs_{5j-1}^n\right)\right)$$

$$-\frac{\alpha^n}{2}F_{2j-1}^n-\frac{\alpha^n}{2}F_{2j-1/2}^{n-1}, \qquad \text{(B.75)}$$

$$\left(e_{39}\right)_j = md_4^n\left(k_f^1\rho\right)_{j-1/2}^n \frac{M_O}{M_{O_2}}\left(c_{3e}^n Qs_{3j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j}^n\right)^2\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}}\left(c_{5e}^n\right)$$

$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O}+\frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}+\frac{c_{2e}^n Qs_{2j}^n}{M_N}\right]+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \frac{M_O}{M_{NO}}\left(c_{5e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n+c_{3e}^n Qs_{3j}^n+c_{4e}^n Qs_{4j}^n+c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}}+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^nQs_{5j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j}^n\right)\left(c_{2e}^nQs_{2j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{4e}^nQs_{4j}^n\right)\left(c_{5e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{4e}^nQs_{4j}^n\right)\left(-c_{5e}^n\right)+$$

$$\frac{md_4^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}M_N}\left(c_{2e}^nQs_{2j}^n\right)\left(c_{5e}^n\right), \tag{B.76}$$

$$\left(e_{40}\right)_j=md_4^n\left(k_f^1\rho\right)_{j-1/2}^n\frac{M_O}{M_{O_2}}\left(c_{3e}^nQs_{3j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$md_4^n\left(k_b^1\rho^2\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n\right)^2\left(Qs_{4j-1}^n\right)^2\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^n\right)$$

$$\left[\frac{c_{4e}^nQs_{4j-1}^n}{M_O}+\frac{c_{3e}^nQs_{3j-1}^n}{M_{O_2}}+\frac{c_{5e}^nQs_{5j-1}^n}{M_{NO}}+\frac{c_{2e}^nQs_{2j-1}^n}{M_N}\right]+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1}^n+c_{3e}^nQs_{3j-1}^n+c_{4e}^nQs_{4j-1}^n+c_{5e}^nQs_{5j-1}^n\right)\right)}{M_{N_2}}+$$

$$\frac{md_4^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}}\left(c_{5e}^nQs_{5j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{4e}^nQs_{4j-1}^n\right)\left(c_{2e}^nQs_{2j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$

$$\frac{md_4^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_{NO}}\left(c_{4e}^nQs_{4j-1}^n\right)\left(c_{5e}^n\right)-$$

$$\frac{md_4^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{1}{M_{N_2}}\left(c_{4e}^nQs_{4j-1}^n\right)\left(-c_{5e}^n\right)+$$

$$\frac{md_4^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n\frac{M_O}{M_{NO}M_N}\left(c_{2e}^nQs_{2j-1}^n\right)\left(c_{5e}^n\right), \tag{B.77}$$

$$(e_{53})_j = \frac{\left(\frac{C}{Sm_4}\right)_j^n}{h_j} + \frac{1}{2}F_{1j}^n + \frac{\alpha^n}{2}F_{1j}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}, \tag{B.78}$$

$$(e_{54})_j = \frac{\left(\frac{C}{Sm_4}\right)_{j-1}^n}{h_j} + \frac{1}{2}F_{1j-1}^n + \frac{\alpha^n}{2}F_{1j-1}^n - \frac{\alpha^n}{2}F_{1j-1/2}^{n-1}. \tag{B.79}$$

Seventh Equation

$$(r_7)_j = \frac{\left(\frac{C}{Sm_5}\right)^n_j \delta Qd^n_{5j} - \left(\frac{C}{Sm_5}\right)^n_{j-1} \delta Qd^n_{5j-1}}{h_j} + (\delta Qd_5 F_1)^n_{j-1/2} + (Qd_5 \delta F_1)^n_{j-1/2} - ms^n_5 \delta F^n_{2j-1/2}$$

$$-md^n_5 \left(k^4_f \rho\right)^n_{j-1/2} \left(c^n_{5e} \delta Qs^n_{5j-1/2}\right)$$

$$\left[\frac{c^n_{4e} Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e} Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e} Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e} Qs^n_{2j-1/2}}{M_N}\right]$$

$$-md^n_5 \left(k^4_f \rho\right)^n_{j-1/2} \left(c^n_{5e} \delta Qs^n_{5j-1/2}\right)$$

$$\frac{\left(1 - \left(c^n_{2e} Qs^n_{2j-1/2} + c^n_{3e} Qs^n_{3j-1/2} + c^n_{4e} Qs^n_{4j-1/2} + c^n_{5e} Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}$$

$$-md^n_5 \left(k^4_f \rho\right)^n_{j-1/2} \left(c^n_{5e} Qs^n_{5j-1/2}\right) \tag{B.80}$$

$$\left[\frac{c^n_{4e} \delta Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e} \delta Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e} \delta Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e} \delta Qs^n_{2j-1/2}}{M_N}\right.$$

$$-md^n_5 \left(k^4_f \rho\right)^n_{j-1/2} \left(c^n_{5e} Qs^n_{5j-1/2}\right)$$

$$\frac{\left(-\left(c^n_{2e} \delta Qs^n_{2j-1/2} + c^n_{3e} \delta Qs^n_{3j-1/2} + c^n_{4e} \delta Qs^n_{4j-1/2} + c^n_{5e} \delta Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}$$

$$+md^n_5 \left(k^4_b \rho^2\right)^n_{j-1/2} \frac{M_{NO}}{M_N M_O} \left(c^n_{4e} \delta Qs^n_{4j-1/2}\right) \left(c^n_{2e} Qs^n_{2j-1/2}\right)$$

$$\left[\frac{c^n_{4e} Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e} Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e} Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e} Qs^n_{2j-1/2}}{M_N}\right]$$

$$+md^n_5 \left(k^4_b \rho^2\right)^n_{j-1/2} \frac{M_{NO}}{M_N M_O} \left(c^n_{4e} \delta Qs^n_{4j-1/2}\right) \left(c^n_{2e} Qs^n_{2j-1/2}\right)$$

$$\frac{\left(1 - \left(c^n_{2e} Qs^n_{2j-1/2} + c^n_{3e} Qs^n_{3j-1/2} + c^n_{4e} Qs^n_{4j-1/2} + c^n_{5e} Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}$$

$$+md^n_5 \left(k^4_b \rho^2\right)^n_{j-1/2} \frac{M_{NO}}{M_N M_O} \left(c^n_{4e} Qs^n_{4j-1/2}\right) \left(c^n_{2e} \delta Qs^n_{2j-1/2}\right)$$

$$\left[\frac{c^n_{4e} Qs^n_{4j-1/2}}{M_O} + \frac{c^n_{3e} Qs^n_{3j-1/2}}{M_{O_2}} + \frac{c^n_{5e} Qs^n_{5j-1/2}}{M_{NO}} + \frac{c^n_{2e} Qs^n_{2j-1/2}}{M_N}\right]$$

$$+md_5^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{M_{NO}}{M_NM_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)$$

$$\frac{\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$+md_5^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{M_{NO}}{M_NM_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\left[\frac{c_{4e}^n\delta Qs_{4j-1/2}^n}{M_O}+\frac{c_{3e}^n\delta Qs_{3j-1/2}^n}{M_{O_2}}+\frac{c_{5e}^n\delta Qs_{5j-1/2}^n}{M_{NO}}+\frac{c_{2e}^n\delta Qs_{2j-1/2}^n}{M_N}\right.$$

$$+md_5^n\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{M_{NO}}{M_NM_O}\left(c_{4e}^nQs_{4j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)$$

$$\frac{\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)}{M_{N_2}}$$

$$-md_5^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)\left(c_{4e}^nQs_{4j-1/2}^n\right)-$$

$$md_5^n\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{4e}^n\delta Qs_{4j-1/2}^n\right)+$$

$$md_5^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{M_{NO}}{M_NM_{O_2}}\left(c_{3e}^n\delta Qs_{3j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)+$$

$$md_5^n\left(k_b^5\rho\right)_{j-1/2}^n\frac{M_{NO}}{M_NM_{O_2}}\left(c_{3e}^nQs_{3j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)+$$

$$md_5^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_{NO}}{M_{N_2}M_O}c_{4e}^n\delta Qs_{4j-1/2}^n$$

$$\left(1-\left(c_{2e}^nQs_{2j-1/2}^n+c_{3e}^nQs_{3j-1/2}^n+c_{4e}^nQs_{4j-1/2}^n+c_{5e}^nQs_{5j-1/2}^n\right)\right)+$$

$$md_5^n\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_{NO}}{M_{N_2}M_O}c_{4e}^nQs_{4j-1/2}^n$$

$$\left(-\left(c_{2e}^n\delta Qs_{2j-1/2}^n+c_{3e}^n\delta Qs_{3j-1/2}^n+c_{4e}^n\delta Qs_{4j-1/2}^n+c_{5e}^n\delta Qs_{5j-1/2}^n\right)\right)-$$

$$md_5^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{5e}^n\delta Qs_{5j-1/2}^n\right)\left(c_{2e}^nQs_{2j-1/2}^n\right)-$$

$$md_5^n\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{5e}^nQs_{5j-1/2}^n\right)\left(c_{2e}^n\delta Qs_{2j-1/2}^n\right)-$$

$$\alpha^n\left[\left(\delta Qs_5F_2\right)_{j-1/2}^n+\left(Qs_5\delta F_2\right)_{j-1/2}^n\right]+\alpha^n\left[\left(\delta Qd_5F_1\right)_{j-1/2}^n+\left(Qd_5\delta F_1\right)_{j-1/2}^n\right]-$$

$$\alpha^n\left[\delta Qs^n_{5j-1/2}F^{n-1}_{2j-1/2}-Qs^{n-1}_{5j-1/2}\delta F^n_{2j-1/2}+\delta Qd^n_{5j-1/2}F^{n-1}_{1j-1/2}-Qd^{n-1}_{5j-1/2}\delta F^n_{1j-1/2}\right],$$

The definition of $(r_7)_j$ is written as follows:

$$(r_7)_j \equiv \frac{\left(\frac{C}{Sm_5}\right)^n_j Qd^n_{5j}-\left(\frac{C}{Sm_5}\right)^n_{j-1} Qd^n_{5j-1}}{h_j}+(Qd_5F_1)^n_{j-1/2}-ms^n_5F^n_{2j-1/2}$$

$$-md^n_5\left(k^4_f\rho\right)^n_{j-1/2}\left(c^n_{5e}Qs^n_{5j-1/2}\right)$$

$$\left[\frac{c^n_{4e}Qs^n_{4j-1/2}}{M_O}+\frac{c^n_{3e}Qs^n_{3j-1/2}}{M_{O_2}}+\frac{c^n_{5e}Qs^n_{5j-1/2}}{M_{NO}}+\frac{c^n_{2e}Qs^n_{2j-1/2}}{M_N}\right]$$

$$-md^n_5\left(k^4_f\rho\right)^n_{j-1/2}\left(c^n_{5e}Qs^n_{5j-1/2}\right)$$

$$\frac{\left(1-\left(c^n_{2e}Qs^n_{2j-1/2}+c^n_{3e}Qs^n_{3j-1/2}+c^n_{4e}Qs^n_{4j-1/2}+c^n_{5e}Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}+$$

$$md^n_5\left(k^4_b\rho^2\right)^n_{j-1/2}\frac{M_{NO}}{M_NM_O}\left(c^n_{4e}Qs^n_{4j-1/2}\right)\left(c^n_{2e}Qs^n_{2j-1/2}\right)$$

$$\left[\frac{c^n_{4e}Qs^n_{4j-1/2}}{M_O}+\frac{c^n_{3e}Qs^n_{3j-1/2}}{M_{O_2}}+\frac{c^n_{5e}Qs^n_{5j-1/2}}{M_{NO}}+\frac{c^n_{2e}Qs^n_{2j-1/2}}{M_N}\right]+$$

$$md^n_5\left(k^4_b\rho^2\right)^n_{j-1/2}\frac{M_{NO}}{M_NM_O}\left(c^n_{4e}Qs^n_{4j-1/2}\right)\left(c^n_{2e}Qs^n_{2j-1/2}\right)$$

$$\frac{\left(1-\left(c^n_{2e}Qs^n_{2j-1/2}+c^n_{3e}Qs^n_{3j-1/2}+c^n_{4e}Qs^n_{4j-1/2}+c^n_{5e}Qs^n_{5j-1/2}\right)\right)}{M_{N_2}}-$$

$$md^n_5\left(k^5_f\rho\right)^n_{j-1/2}\frac{1}{M_O}\left(c^n_{5e}Qs^n_{5j-1/2}\right)\left(c^n_{4e}Qs^n_{4j-1/2}\right)+$$

$$md^n_5\left(k^5_b\rho\right)^n_{j-1/2}\frac{M_{NO}}{M_NM_{O_2}}\left(c^n_{3e}Qs^n_{3j-1/2}\right)\left(c^n_{2e}Qs^n_{2j-1/2}\right)+$$

$$md^n_5\left(k^6_f\rho\right)^n_{j-1/2}\frac{M_{NO}}{M_{N_2}M_O}c^n_{4e}Qs^n_{4j-1/2}$$

$$\left(1-\left(c^n_{2e}Qs^n_{2j-1/2}+c^n_{3e}Qs^n_{3j-1/2}+c^n_{4e}Qs^n_{4j-1/2}+c^n_{5e}Qs^n_{5j-1/2}\right)\right)-$$

$$md_5^n \left(k_b^6 \rho\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{5e}^n Qs_{5j-1/2}^n\right) \left(c_{2e}^n Qs_{2j-1/2}^n\right) -$$

$$2\xi^{n-1/2} \frac{\left(Qs_{5j-1/2}^n F_{2j-1/2}^n + Qs_{5j-1/2}^n F_{2j-1/2}^{n-1} - Qs_{5j-1/2}^{n-1} F_{2j-1/2}^n\right)}{k_n} -$$

$$2\xi^{n-1/2} \frac{\left(-Qd_{5j-1/2}^n F_{1j-1/2}^n + Qd_{5j-1/2}^n F_{1j-1/2}^{n-1} - Qd_{5j-1/2}^{n-1} F_{1j-1/2}^n\right)}{k_n}$$

We can recast the equation in the form of:

$$(r_7)_j = (e_4)_j \delta F_{1j} + (e_8)_j \delta F_{1j-1} + (e_{12})_j \delta F_{2j} + (e_{16})_j \delta F_{2j-1} + (e_{41})_j \delta Qs_{2j} + (e_{42})_j \delta Qs_{2j-1} +$$

$$(e_{43})_j \delta Qs_{3j} + (e_{44})_j \delta Qs_{3j-1} + (e_{45})_j \delta Qs_{4j} + (e_{46})_j \delta Qs_{4j-1} + (e_{47})_j \delta Qs_{5j} +$$

$$(e_{48})_j \delta Qs_{5j-1} + (e_{55})_j \delta Qd_{4j} + (e_{56})_j \delta Qd_{4j-1}. \quad \text{(B.81)}$$

The coefficients in (B.81) are defined as:

$$(e_4)_j = \frac{1}{2} Qd_{5j}^n + \frac{\alpha^n}{2} Qd_{5j}^n + \frac{\alpha^n}{2} Qd_{5j-1/2}^{n-1} = \frac{\alpha_1}{2} Qd_{5j}^n + \frac{\alpha^n}{2} Qd_{5j-1/2}^{n-1}, \quad \text{(B.82)}$$

$$(e_8)_j = \frac{1}{2} Qd_{5j-1}^n + \frac{\alpha^n}{2} Qd_{5j-1}^n + \frac{\alpha^n}{2} Qd_{5j-1/2}^{n-1} = \frac{\alpha_1}{2} Qd_{5j-1}^n + \frac{\alpha^n}{2} Qd_{5j-1/2}^{n-1}. \quad \text{(B.83)}$$

$$(e_{12})_j = -\frac{ms_5^n}{2} - \frac{\alpha^n}{2} Qs_{5j}^n + \frac{\alpha^n}{2} Qs_{5j-1/2}^{n-1}, \quad \text{(B.84)}$$

$$(e_{16})_j = -\frac{ms_5^n}{2} - \frac{\alpha^n}{2} Qs_{5j-1}^n + \frac{\alpha^n}{2} Qs_{5j-1/2}^{n-1}, \tag{B.85}$$

$$\begin{aligned}
(e_{41})_j = & -\frac{md_5^n}{2} \left(k_f^4 \rho\right)_{j-1/2}^n \left(c_{5e}^n Q s_{5j}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] + \\
& \frac{md_5^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O} \left(c_{4e}^n Q s_{4j}^n\right) \left(c_{2e}^n\right) \\
& \left[\frac{c_{4e}^n Q s_{4j}^n}{M_O} + \frac{c_{3e}^n Q s_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Q s_{5j}^n}{M_{NO}} + \frac{c_{2e}^n Q s_{2j}^n}{M_N}\right] + \\
& \frac{md_5^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O} \left(c_{4e}^n Q s_{4j}^n\right) \left(c_{2e}^n\right) \\
& \frac{\left(1 - \left(c_{2e}^n Q s_{2j}^n + c_{3e}^n Q s_{3j}^n + c_{4e}^n Q s_{4j}^n + c_{5e}^n Q s_{5j}^n\right)\right)}{M_{N_2}} + \\
& \frac{md_5^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O} \left(c_{4e}^n Q s_{4j}^n\right) \left(c_{2e}^n Q s_{2j}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] + \\
& \frac{md_5^n}{2} \left(k_b^5 \rho\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_{O_2}} \left(c_{3e}^n Q s_{3j}^n\right) \left(c_{2e}^n\right) + \\
& \frac{md_5^n}{2} \left(k_f^6 \rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O} \left(c_{4e}^n Q s_{4j}^n\right) \left(-c_{2e}^n\right) - \\
& \frac{md_5^n}{2} \left(k_b^6 \rho\right)_{j-1/2}^n \frac{1}{M_N} \left(c_{5e}^n Q s_{5j}^n\right) \left(c_{2e}^n\right),
\end{aligned} \tag{B.86}$$

$$\begin{aligned}
(e_{42})_j = & -\frac{md_5^n}{2} \left(k_f^4 \rho\right)_{j-1/2}^n \left(c_{5e}^n Q s_{5j-1}^n\right) \left[\frac{c_{2e}^n}{M_N} - \frac{c_{2e}^n}{M_{N_2}}\right] + \\
& \frac{md_5^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O} \left(c_{4e}^n Q s_{4j-1}^n\right) \left(c_{2e}^n\right) \\
& \left[\frac{c_{4e}^n Q s_{4j-1}^n}{M_O} + \frac{c_{3e}^n Q s_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Q s_{5j-1}^n}{M_{NO}} + \frac{c_{2e}^n Q s_{2j-1}^n}{M_N}\right] + \\
& \frac{md_5^n}{2} \left(k_b^4 \rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O} \left(c_{4e}^n Q s_{4j-1}^n\right) \left(c_{2e}^n\right) \\
& \frac{\left(1 - \left(c_{2e}^n Q s_{2j-1}^n + c_{3e}^n Q s_{3j-1}^n + c_{4e}^n Q s_{4j-1}^n + c_{5e}^n Q s_{5j-1}^n\right)\right)}{M_{N_2}} +
\end{aligned}$$

$$\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{2e}^n}{M_N}-\frac{c_{2e}^n}{M_{N_2}}\right]+$$
$$\frac{md_5^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_{O_2}}\left(c_{3e}^n Qs_{3j-1}^n\right)\left(c_{2e}^n\right)+$$
$$\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{2e}^n\right)-$$
$$\frac{md_5^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n \frac{1}{M_N}\left(c_{5e}^n Qs_{5j-1}^n\right)\left(c_{2e}^n\right), \tag{B.87}$$

$$(e_{43})_j = -\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n Qs_{5j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$\frac{md_5^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_{O_2}}\left(c_{2e}^n Qs_{2j}^n\right)\left(c_{3e}^n\right)+$$
$$\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(-c_{3e}^n\right), \tag{B.88}$$

$$(e_{44})_j = -\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n Qs_{5j-1}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{3e}^n}{M_{O_2}}-\frac{c_{3e}^n}{M_{N_2}}\right]+$$
$$\frac{md_5^n}{2}\left(k_b^5\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_{O_2}}\left(c_{2e}^n Qs_{2j-1}^n\right)\left(c_{3e}^n\right)+$$
$$\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{3e}^n\right), \tag{B.89}$$

$$(e_{45})_j = -\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n Qs_{5j}^n\right)\left[\frac{c_{4e}^n}{M_O}-\frac{c_{4e}^n}{M_{N_2}}\right]+$$
$$\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{2e}^n Qs_{2j}^n\right)\left(c_{4e}^n\right)$$
$$\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O}+\frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}}+\frac{c_{5e}^n Qs_{5j}^n}{M_{NO}}+\frac{c_{2e}^n Qs_{2j}^n}{M_N}\right]+$$

$$
\begin{aligned}
&\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{2e}^n Q s_{2j}^n\right)\left(c_{4e}^n\right) \\
&\frac{\left(1-\left(c_{2e}^n Q s_{2j}^n + c_{3e}^n Q s_{3j}^n + c_{4e}^n Q s_{4j}^n + c_{5e}^n Q s_{5j}^n\right)\right)}{M_{N_2}} + \\
&\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Q s_{4j}^n\right)\left(c_{2e}^n Q s_{2j}^n\right)\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right] - \\
&\frac{md_5^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{5e}^n Q s_{5j}^n\right)\left(c_{4e}^n\right) + \\
&\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n Q s_{4j}^n\right)\left(-c_{4e}^n\right) + \\
&\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n\right)\left(1-\left(c_{2e}^n Q s_{2j}^n + c_{3e}^n Q s_{3j}^n + c_{4e}^n Q s_{4j}^n + c_{5e}^n Q s_{5j}^n\right)\right),
\end{aligned}
\tag{B.90}
$$

$$
\begin{aligned}
\left(e_{46}\right)_j = &-\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n \left(c_{5e}^n Q s_{5j-1}^n\right)\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right] + \\
&\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{2e}^n Q s_{2j-1}^n\right)\left(c_{4e}^n\right) \\
&\left[\frac{c_{4e}^n Q s_{4j-1}^n}{M_O} + \frac{c_{3e}^n Q s_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Q s_{5j-1}^n}{M_{NO}} + \frac{c_{2e}^n Q s_{2j-1}^n}{M_N}\right] + \\
&\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{2e}^n Q s_{2j-1}^n\right)\left(c_{4e}^n\right) \\
&\frac{\left(1-\left(c_{2e}^n Q s_{2j-1}^n + c_{3e}^n Q s_{3j-1}^n + c_{4e}^n Q s_{4j-1}^n + c_{5e}^n Q s_{5j-1}^n\right)\right)}{M_{N_2}} + \\
&\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n \frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Q s_{4j-1}^n\right)\left(c_{2e}^n Q s_{2j-1}^n\right)\left[\frac{c_{4e}^n}{M_O} - \frac{c_{4e}^n}{M_{N_2}}\right] - \\
&\frac{md_5^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n \frac{1}{M_O}\left(c_{5e}^n Q s_{5j-1}^n\right)\left(c_{4e}^n\right) + \\
&\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n Q s_{4j-1}^n\right)\left(-c_{4e}^n\right) + \\
&\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n \frac{M_{NO}}{M_{N_2} M_O}\left(c_{4e}^n\right)\left(1-\left(c_{2e}^n Q s_{2j-1}^n + c_{3e}^n Q s_{3j-1}^n + c_{4e}^n Q s_{4j-1}^n + c_{5e}^n Q s_{5j-1}^n\right)\right),
\end{aligned}
\tag{B.91}
$$

$$
\begin{gathered}
\left(e_{47}\right)_j = -\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n\right) \\
\left[\frac{c_{4e}^n Qs_{4j}^n}{M_O} + \frac{c_{3e}^n Qs_{3j}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j}^n}{M_N}\right] + \\
-\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n\right) \\
\frac{\left(1-\left(c_{2e}^n Qs_{2j}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j}^n + c_{5e}^n Qs_{5j}^n\right)\right)}{M_{N_2}} - \\
\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n Qs_{5j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}} - \frac{c_{5e}^n}{M_{N_2}}\right] + \\
\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{2e}^n Qs_{2j}^n\right)\left[\frac{c_{5e}^n}{M_{NO}} - \frac{c_{5e}^n}{M_{N_2}}\right] - \\
\frac{md_5^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(c_{5e}^n\right) + \\
\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_{NO}}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j}^n\right)\left(-c_{5e}^n\right) - \\
\frac{md_5^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n Qs_{2j}^n\right)\left(c_{5e}^n\right) - \\
\frac{\alpha^n}{2}F_{2j}^n - \frac{\alpha^n}{2}F_{2j-1/2}^{n-1},
\end{gathered} \tag{B.92}
$$

$$
\begin{gathered}
\left(e_{48}\right)_j = -\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n\right) \\
\left[\frac{c_{4e}^n Qs_{4j-1}^n}{M_O} + \frac{c_{3e}^n Qs_{3j-1}^n}{M_{O_2}} + \frac{c_{5e}^n Qs_{5j-1}^n}{M_{NO}} + \frac{c_{2e}^n Qs_{2j-1}^n}{M_N}\right] + \\
-\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n\right) \\
\frac{\left(1-\left(c_{2e}^n Qs_{2j-1}^n + c_{3e}^n Qs_{3j}^n + c_{4e}^n Qs_{4j-1}^n + c_{5e}^n Qs_{5j-1}^n\right)\right)}{M_{N_2}} - \\
\frac{md_5^n}{2}\left(k_f^4\rho\right)_{j-1/2}^n\left(c_{5e}^n Qs_{5j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}} - \frac{c_{5e}^n}{M_{N_2}}\right] +
\end{gathered}
$$

$$\frac{md_5^n}{2}\left(k_b^4\rho^2\right)_{j-1/2}^n\frac{M_{NO}}{M_N M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{2e}^n Qs_{2j-1}^n\right)\left[\frac{c_{5e}^n}{M_{NO}}-\frac{c_{5e}^n}{M_{N_2}}\right]-$$
$$\frac{md_5^n}{2}\left(k_f^5\rho\right)_{j-1/2}^n\frac{1}{M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(c_{5e}^n\right)+$$
$$\frac{md_5^n}{2}\left(k_f^6\rho\right)_{j-1/2}^n\frac{M_{NO}}{M_{N_2}M_O}\left(c_{4e}^n Qs_{4j-1}^n\right)\left(-c_{5e}^n\right)-$$
$$\frac{md_5^n}{2}\left(k_b^6\rho\right)_{j-1/2}^n\frac{1}{M_N}\left(c_{2e}^n Qs_{2j-1}^n\right)\left(c_{5e}^n\right)-$$
$$\frac{\alpha^n}{2}F_{2j-1}^n-\frac{\alpha^n}{2}F_{2j-1/2}^{n-1}, \qquad \text{(B.93)}$$

$$(e_{55})_j=\frac{\left(\frac{C}{Sm_5}\right)_j^n}{h_j}+\frac{1}{2}F_{1j}^n+\frac{\alpha^n}{2}F_{1j}^n-\frac{\alpha^n}{2}F_{1j-1/2}^{n-1}, \qquad \text{(B.94)}$$

$$(e_{56})_j=\frac{\left(\frac{C}{Sm_5}\right)_{j-1}^n}{h_j}+\frac{1}{2}F_{1j-1}^n+\frac{\alpha^n}{2}F_{1j-1}^n-\frac{\alpha^n}{2}F_{1j-1/2}^{n-1}. \qquad \text{(B.95)}$$

Eighth Equation

$$(r_8)_{j-1} = \delta F_{2j}^n - \delta F_{2j-1}^n - \frac{h_j}{2}\left(\delta F_{3j}^n + \delta F_{3j-1}^n\right), \tag{B.96}$$

where $(r_8)_{j-1} \equiv F_{2j-1}^n - F_{2j}^n + h_j F_{3j-1}^n$.

Nineth Equation

$$(r_9)_{j-1} = \delta G_{1j}^n - \delta G_{1j-1}^n - \frac{h_j}{2}\left(\delta G_{2j}^n + \delta G_{2j-1}^n\right), \tag{B.97}$$

where $(r_9)_{j-1} \equiv G_{1j-1}^n - G_{1j}^n + h_j G_{2j-1}^n$.

Tenth Equation

$$(r_{10})_{j-1} = \delta Qs_{2j}^n - \delta Qs_{2j-1}^n - \frac{h_j}{2}\left(\delta Qd_{2j}^n + \delta Qd_{2j-1}^n\right), \tag{B.98}$$

where $(r_{10})_{j-1} \equiv Qs_{2j-1}^n - Qs_{2j}^n + h_j Qd_{2j-1}^n$.

Eleventh Equation

$$(r_{11})_{j-1} = \delta Qs^n_{3j} - \delta Qs^n_{3j-1} - \frac{h_j}{2}\left(\delta Qd^n_{3j} + \delta Qd^n_{3j-1}\right), \tag{B.99}$$

where $(r_{11})_{j-1} \equiv Qs^n_{3j-1} - Qs^n_{3j} + h_j Qd^n_{3j-1}$.

Twelveth Equation

$$(r_{12})_{j-1} = \delta Qs^n_{4j} - \delta Qs^n_{4j-1} - \frac{h_j}{2}\left(\delta Qd^n_{4j} + \delta Qd^n_{4j-1}\right), \tag{B.100}$$

where $(r_{12})_{j-1} \equiv Qs^n_{4j-1} - Qs^n_{4j} + h_j Qd^n_{4j-1}$.

Thirteenth Equation

$(r_{13})_{j-1} = \delta Qs^n_{5j} - \delta Qs^n_{5j-1} - \frac{h_j}{2}\left(\delta Qd^n_{5j} + \delta Qd^n_{5j-1}\right)$,

where $(r_{13})_{j-1} \equiv Qs^n_{5j-1} - Qs^n_{5j} + h_j Qd^n_{5j-1}$.

Appendix C: Block Elimination Method

The linear system has a block tridiagonal structure and can be expressed in matrix-vector form:

$$A\overline{\delta} = \overline{r}. \tag{C.1}$$

The energy equation is solved separately after the momentum equation and the equations for species conservation are solved in this work. Solving momentum and mass conservation equation using enthalpy from previous iteration provides us the mass fractions of species and velocity profile of the flow. The eleven dimensional vectors, $\overline{r}$ and $\overline{\delta}$, for each value of j with the coefficient matrix A and the compound vectors are given:

$$\overline{\delta_j} = \begin{pmatrix} \delta F_1 \\ \delta F_2 \\ \delta F_3 \\ \delta Qs_2 \\ \delta Qs_3 \\ \delta Qs_4 \\ \delta Qs_5 \\ \delta Qd_2 \\ \delta Qd_3 \\ \delta Qd_4 \\ \delta Qd_5 \end{pmatrix} ; \overline{r_j} = \begin{pmatrix} (r_1)_j \\ (r_2)_j \\ (r_4)_j \\ (r_5)_j \\ (r_6)_j \\ (r_7)_j \\ (r_8)_j \\ (r_{10})_j \\ (r_{11})_j \\ (r_{12})_j \\ (r_{13})_j \end{pmatrix}, \tag{C.2}$$

$$A = \begin{pmatrix} A_0 & C_0 & & & & \\ B_1 & A_1 & C_1 & & & \\ & \cdot & \cdot & \cdot & \cdot & \\ & & B_j & A_j & C_j & \\ & & & B_{J-1} & A_{J-1} & C_{J-1} \\ & & & & B_J & A_J \end{pmatrix}, \tag{C.3}$$

and the 11x11 matrices are given by;

$$A_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\gamma_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\gamma_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\gamma_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\gamma_3 \\ 0 & -1 & -\frac{h_1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_1}{2} \end{pmatrix}, \qquad \text{(C.4)}$$

$$A_j = \begin{pmatrix} 1 & -\frac{h_j}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (s_3)_j & (s_5)_j & (s_1)_j & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (e_1)_j & (e_9)_j & 0 & (e_{17})_j & (e_{19})_j & (e_{21})_j & (e_{23})_j & (e_{49})_j & 0 & 0 & 0 \\ (e_2)_j & (e_{10})_j & 0 & (e_{25})_j & (e_{27})_j & (e_{29})_j & (e_{31})_j & 0 & (e_{51})_j & 0 & 0 \\ (e_3)_j & (e_{11})_j & 0 & (e_{33})_j & (e_{35})_j & (e_{37})_j & (e_{39})_j & 0 & 0 & (e_{53})_j & 0 \\ (e_4)_j & (e_{12})_j & 0 & (e_{41})_j & (e_{43})_j & (e_{45})_j & (e_{47})_j & 0 & 0 & 0 & (e_{55})_j \\ 0 & -1 & -\frac{h_{j+1}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} \end{pmatrix},$$

$$(1 \leq j \leq J-1) \qquad \text{(C.5)}$$

$$A_J = \begin{pmatrix} 1 & -\frac{h_J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (s_3)_J & (s_5)_J & (s_1)_J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (e_1)_J & (e_9)_J & 0 & (e_{17})_J & (e_{19})_J & (e_{21})_J & (e_{23})_J & (e_{49})_J & 0 & 0 & 0 \\ (e_2)_J & (e_{10})_J & 0 & (e_{25})_J & (e_{27})_J & (e_{29})_J & (e_{31})_J & 0 & (e_{51})_J & 0 & 0 \\ (e_3)_J & (e_{11})_J & 0 & (e_{33})_J & (e_{35})_J & (e_{37})_J & (e_{39})_J & 0 & 0 & (e_{53})_J & 0 \\ (e_4)_J & (e_{12})_J & 0 & (e_{41})_J & (e_{43})_J & (e_{45})_J & (e_{47})_J & 0 & 0 & 0 & (e_{55})_J \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{C.6}$$

$$B_j = \begin{pmatrix} -1 & -\frac{h_j}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (s_4)_j & (s_6)_j & (s_2)_j & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (e_5)_j & (e_{13})_j & 0 & (e_{18})_j & (e_{20})_j & (e_{22})_j & (e_{24})_j & (e_{50})_j & 0 & 0 & 0 \\ (e_6)_j & (e_{14})_j & 0 & (e_{26})_j & (e_{28})_j & (e_{30})_j & (e_{32})_j & 0 & (e_{52})_j & 0 & 0 \\ (e_7)_j & (e_{15})_j & 0 & (e_{34})_j & (e_{36})_j & (e_{38})_j & (e_{40})_j & 0 & 0 & (e_{54})_j & 0 \\ (e_8)_j & (e_{16})_j & 0 & (e_{42})_j & (e_{44})_j & (e_{46})_j & (e_{48})_j & 0 & 0 & 0 & (e_{56})_j \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (1 \le j \le J) \tag{C.7}$$

$$C_j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -\frac{h_{j+1}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{h_{j+1}}{2} \end{pmatrix} . \quad (C.8)$$

$$(0 \leq j \leq J-1)$$

Using the boundary conditions, the vectors $\overline{r_0}$, $\overline{r_j}$ are defined by;

$$\overline{r_0} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ (r_8)_0 \\ (r_{10})_0 \\ (r_{11})_0 \\ (r_{12})_0 \\ (r_{13})_0 \end{pmatrix} ; \overline{r_J} = \begin{pmatrix} (r_1)_J \\ (r_2)_J \\ (r_4)_J \\ (r_5)_J \\ (r_6)_J \\ (r_7)_J \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} . \quad (C.9)$$

After solving the momentum and mass fraction equations, we solve the energy equation assuming the mass fraction and velocity profiles are known. The energy equation is recast as an algebraic system of two equations written similarly (C.1). The matrices and vectors are defined as follows:

$$A_0 = \begin{pmatrix} \gamma_0 & \gamma_1 \\ -1 & -\frac{h_1}{2} \end{pmatrix} , \quad (C.10)$$

$$A_j = \begin{pmatrix} (\beta_7)_j & (\beta_1)_j \\ -1 & -\frac{h_{j+1}}{2} \end{pmatrix} (1 \leq j \leq J-1), \tag{C.11}$$

$$A_J = \begin{pmatrix} (\beta_7)_J & (\beta_1)_J \\ -1 & 0 \end{pmatrix}, \tag{C.12}$$

$$B_j = \begin{pmatrix} (\beta_8)_j & (\beta_2)_j \\ 0 & 0 \end{pmatrix} (1 \leq j \leq J), \tag{C.13}$$

$$C_j = \begin{pmatrix} 0 & 0 \\ 1 & -\frac{h_{j+1}}{2} \end{pmatrix} (0 \leq j \leq J-1). \tag{C.14}$$

Using the boundary conditions, the vectors $\overline{r_0}$, $\overline{r_J}$ are defined by:

$$\overline{r_0} = \begin{pmatrix} 0 \\ (r_9)_0 \end{pmatrix}; \overline{r_J} = \begin{pmatrix} (r_3)_J \\ 0 \end{pmatrix}. \tag{C.15}$$

The procedure of the iteration is repeated until the criteria for small change of the solution is satisfied. The criteria depends on the boundary conditions on the wall.