5435-6009-R0000

ONE-DIMENSIONAL TWO-PHASE REACTING GAS NONEQUILIBRIUM PERFORMANCE PROGRAM

INTERIM ANALYSIS REPORT

10 MAY 1966

Prepared by
S.S. Cherry
J.R. Kliegel

Prepared for
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
MANNED SPACECRAFT CENTER
Contract NAS9-4358

TRW SYSTEMS

ONE-DIMENSIONAL TWO-PHASE REACTING GAS NONEQUILIBRIUM PERFORMANCE PROGRAM

INTERIM ANALYSIS REPORT

Prepared [signature]
S. S. Cherry

Prepared [signature]
J. R. Kliegel
Program Manager

Approved [signature]
D. H. Lee, Manager
Chemical Propulsion
Technology Department

Prepared for

National Aeronautics and Space Administration
Manned Spacecraft Center

Under Contract No. NAS9-4358

TRW SYSTEMS
One Space Park, Redondo Beach, California

CONTENTS

NOMENCLATURE

a	Nozzle area, also reaction rate parameter
A	Diabatic heat addition term linking fluid dynamic and relaxation processes
b	Reaction rate parameter
B	Energy exchange term linking fluid dynamic and relaxation processes
c	Species mass fraction
c_F	Thrust coefficient
C	Total particle drag term
$C_{Di}^{(o)}$	Particle drag coefficient
C_P	Heat capacity of gas phase at constant pressure
C*	Characteristic exhaust velocity
D_i	Subsonic particle continuity term
E	Diabatic heat addition term
f	Derivative
f_{pi}	Momentum exchange term
F	Free energy
F_i	Supersonic particle continuity term
g_{pi}	Energy exchange term
h	Enthalpy, also integration increment
H	Total enthalpy
ΔH_F	Heat of formation
ΔH_{pi}	Latent heat at melting
I_{sp}	Specific impulse
k	Variable increment, also reaction rate parameter
K	Equilibrium constant
Kn_i	Particle Knudsen number

m	Reaction rate ratio
m_{pi}	Bulk density
M	Mach number, also third body reaction term
n	Reaction rate parameter, also summation or iteration index
N_P	Pressure expansion coefficient
N_T	Temperature expansion coefficient
$Nu_i^{(o)}$	Particle Nusselt number
P	Pressure
Pr	Gas Prandtl number
r_{pi}	Particle radius
r^*	Nozzle throat radius
R	Gas constant
Re_i	Particle Reynolds number
R^*	Nozzle wall radius of curvature at throat
S	Entropy, also summation term
T	Temperature
T_{pmi}	Melting temperature
V	Velocity
x	Axial distance
y	Dependent variable
α_i	Partial derivative, $\partial f_i / \partial x$
$\beta_{i,j}$	Partial derivative, $\partial f_i / \partial y_j$
γ	Gamma
δ_i	Incremental error
$\delta_{i,j}$	Kronecker delta
ϵ	Area ratio

NOMENCLATURE (Continued)

ρ	Density
ρ_{pi}	Particle density in gas phase
μ	Gas viscosity
θ	Nozzle cone angle

Subscripts:

c	Refers to chamber conditions
i	Refers to ith species or equation
j	Refers to jth reaction or variable
o	Refers to reference conditions
pi	Refers to ith particle size group

Superscripts:

C	Refers to corrected increment
P	Refers to predicted increment
*	Refers to throat conditions
(o)	Refers to no slip condition

BLANK PAGE

1. INTRODUCTION

This report contains a complete engineering description of the second computer program being developed by TRW Systems for NASA (MSC) under Contract NAS9-4358, Development of Six (6) Computer Programs for Analytical Prediction of Delivered Specific Impulse.

The objective of this contract is to develop a family of six computer programs to calculate inviscid, one-dimensional, and axisymmetric non-equilibrium nozzle flow fields. Assuming that equilibrium conditions exist in the combustion chamber, these programs will calculate the non-equilibrium nozzle expansion of propellant exhaust mixtures containing the six elements: carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine, and one metal element, either aluminum, beryllium, boron or lithium. These computer programs will account for the nonequilibrium effects of finite rate chemical reactions between gaseous combustion products and velocity and thermal lags between gaseous and condensed combustion products.

The computer program described in this report calculates the inviscid one-dimensional equilibrium, frozen and nonequilibrium nozzle expansion of propellant exhaust mixtures containing the six elements: carbon, hydrogen, oxygen, nitrogen, fluorine, and chlorine and one metal element, either aluminum, beryllium, boron or lithium. The computer program considers all significant gaseous species present in the exhaust mixtures of propellants containing these elements and all gas phase chemical reactions which can occur between the exhaust products. The computer program is designed for engineering use and is specified and programmed in a straightforward manner to facilitate its use as a development tool. In order to reduce the computation time per case to a minimum, the program utilizes a second order implicit integration method. This integration method has been demonstrated to reduce the computation time per case several orders of magnitude when directly compared with the computation times required utilizing standard explicit integration methods such as fourth order Runge-Kutta or Adams-Moulton methods.

Section 2 contains a derivation of the equations governing the inviscid, one-dimensional flow of a two phase reacting gas mixture in the form in which they are integrated in the computer program.

Section 3 contains a brief discussion of the use of both implicit and explicit integration methods to integrate relaxation equations, and a complete derivation of the second order implicit integration method used in the computer program.

Section 4 contains a detailed engineering description of all the calculations performed in the computer program.

At the completion and delivery of this computer program to NASA (MSC), an updated version of this document describing the engineering analyses, a similar document describing the programming and program logic, and a user's manual describing the use of the program will be delivered to NASA (MSC) to complete the program documentation.

2. CONSERVATION EQUATIONS

The conservation equations governing the inviscid one-dimensional flow of a two phase reacting gas mixture can be simply derived utilizing the following assumptions:

- There are no mass or energy losses from the system
- The gas is inviscid except for its interactions with the condensed particles
- Each component of the gas is a perfect gas
- The internal degrees of freedom (rotational and vibrational) of each component of the gas are in equilibrium
- The volume occupied by the condensed particles is negligible
- The thermal (Brownian) motion of the condensed particles is negligible
- The condensed particles do not interact
- The condensed particle size distribution may be approximated by groups of different size spheres
- The internal temperature of the condensed particles is uniform
- Energy exchange between the gas and the condensed particles occurs only by convection
- The only forces on the condensed particles are viscous drag forces
- There is no mass transfer from the gas to the condensed phase during the nozzle expansion

These assumptions have been previously used in all studies of reacting gas[1] and gas-particle[2] nozzle flows.

The conservation equations are derived here in the form used in the present analysis.

For each component of the gas the continuity equation is

$$\frac{d}{dx}(\rho_i Va) = \omega_i r^* a \qquad (2\text{-}1)$$

where the axial coordinate (x) has been normalized with the throat radius. Summing over all components of the mixture, the overall continuity equation for the gas is obtained

$$\frac{d}{dx}(\rho V a) = 0 \tag{2-2}$$

By use of the above equation, Equation (2-1) can be rewritten as

$$\frac{dc_i}{dx} = \frac{\omega_i r^*}{\rho V} \tag{2-3}$$

For each particle size group the continuity equation is

$$\frac{d}{dx}(\rho_{pi} V_{pi} a) = 0 \tag{2-4}$$

since there is no mass transfer from the gas to the condensed phase. The change in gas and particle momentum at any station in the nozzle is

$$\frac{d}{dx}(\rho V a V)$$

and

$$\frac{d}{dx} \sum_{i=o}^{N} (\rho_{pi} V_{pi} a V_{pi})$$

while the pressure force acting at any nozzle station is $a\frac{dP}{dx}$. Thus the overall momentum equation for the mixture is

$$\frac{d}{dx}(\rho V a V) + \frac{d}{dx}\left(\sum_{i=o}^{N} \rho_{pi} V_{pi} a V_{pi}\right) + a\frac{dP}{dx} = 0 \tag{2-5}$$

which becomes

$$\rho V \frac{dV}{dx} + \sum_{i=o}^{N} \rho_{pi} V_{pi} \frac{dV_{pi}}{dx} + \frac{dP}{dx} = 0 \tag{2-6}$$

through use of the continuity equations.

Similarly, the overall energy equation for the mixture is

$$\rho V\left(\frac{dh}{dx} + \frac{VdV}{dx}\right) + \sum_{i=o}^{N} \rho_{pi} V_{pi}\left(\frac{dh_{pi}}{dx} + V_{pi}\frac{dV_{pi}}{dx}\right) = 0 \qquad (2\text{-}7)$$

where for the gas phase

$$h = \sum_{i=o}^{N} c_i h_i \qquad (2\text{-}8)$$

and

$$h_i = \int_o^T c_{pi} dT + h_{io} \qquad (2\text{-}9)$$

while for each particle group

$$h_{pi} = \int_o^T c_{pi} dT + h_{io} \quad , \quad T < T_{pmi} \qquad (2\text{-}10)$$

and

$$h_{pi} = \int_o^T c_{pi} dT + h_{io} + \Delta H_{pi} \quad , \quad T > T_{pmi} \qquad (2\text{-}11)$$

For each component of the gas, the equation of state is

$$P_i = \rho_i R_i T \qquad (2\text{-}12)$$

Summing over all components of the mixture, the overall equation of state for the gas is obtained

$$P = \rho R T \qquad (2\text{-}13)$$

where

$$R = \sum_{i=1}^{N} c_i R_i \qquad (2\text{-}13a)$$

The particle drag equation is

$$V_{pi}\frac{dV_{pi}}{dx} = \frac{9}{2}\frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2}(V - V_{pi}) \qquad (2\text{-}14)$$

and the particle heat transfer equation is

$$V_{pi} \frac{dh_{pi}}{dx} = - \frac{3\mu g_{pi} r^*}{m_{pi} r_{pi}^2} \frac{C_P}{P_r} (T_{pi} - T) \qquad (2\text{-}15)$$

for each particle group.

Since the expansion through a nozzle can be specified either by the expansion process or by the nozzle geometry, two forms of the above equations are of interest.

If the expansion process is specified and the pressure is known as a function of distance through the nozzle, the above equations become

$$\frac{dc_i}{dx} = \frac{\omega_i r^*}{\rho V} \qquad (2\text{-}16)$$

$$\frac{d\rho_{pi}}{dx} = \left[\frac{1}{\gamma P} \frac{M^2 - 1}{M^2} \frac{dP}{dx} - D_i\right] \rho_{pi} \quad , \quad i = 1, 2, \cdots, 5 \qquad (2\text{-}17)$$

$$\frac{dV}{dx} = - \frac{1}{\rho V} \left[\frac{dP}{dx} + c\right] \qquad (2\text{-}18)$$

$$\frac{d\rho}{dx} = \left[\frac{1}{\gamma P} \frac{dP}{dx} - A\right] \rho \qquad (2\text{-}19)$$

$$\frac{dT}{dx} = \left[\frac{\gamma - 1}{\gamma} \frac{1}{P} \frac{dP}{dx} - B\right] T \qquad (2\text{-}20)$$

while if the nozzle geometry is specified, the above equations become

$$\frac{dc_i}{dx} = \frac{\omega_i r^*}{\rho V} \qquad (2\text{-}21)$$

$$\frac{d\rho_{pi}}{dx} = - \left[\frac{1}{a} \frac{da}{dx} - F_i\right] \quad , \quad i = 1, 2, \cdots, 5 \qquad (2\text{-}22)$$

$$\frac{dV}{dx} = \left[\frac{1}{a} \frac{da}{dx} - E\right] \frac{V}{M^2 - 1} \qquad (2\text{-}23)$$

$$\frac{d\rho}{dx} = - \left\{ \left[\frac{1}{a} \frac{da}{dx} - E \right] \frac{M^2}{M^2 - 1} + A \right\} \rho \tag{2-24}$$

$$\frac{dT}{dx} = - \left\{ \left[\frac{1}{a} \frac{da}{dx} - E \right] \frac{(\gamma - 1)M^2}{M^2 - 1} + B \right\} T \tag{2-25}$$

$$\frac{dP}{dx} = - \left[\frac{1}{a} \frac{da}{dx} - E \right] \frac{\gamma M^2}{M^2 - 1} \; P \tag{2-26}$$

where

$$B = \frac{\gamma - 1}{\gamma} \frac{r^*}{PV} \left\{ \sum_{i=1}^{n} \omega_i h_i - \sum_{i=1}^{5} \rho_{pi} \left[\frac{9}{2} \frac{\mu f_{pi}}{m_{pi} \gamma_{pi}^2} \left(V - V_{pi}\right)^2 + \frac{3\mu g_{pi}}{m_{pi}\gamma_{pi}^2} \frac{C_{Pg}}{P_r} (T_{pi} - T) \right] \right\} \tag{2-27}$$

$$A = \frac{r^*}{PV} \sum_{i=1}^{n} \omega_i R_i T - B \tag{2-27a}$$

$$C = \sum_{i=1}^{5} \rho_{pi} \frac{9}{2} \frac{\mu f_{pi} r^*}{m_{pi}\gamma_{pi}^2} (V - V_{pi}) \tag{2-27b}$$

$$E = A + \frac{C}{\rho V^2} \tag{2-27c}$$

$$F_i = - \frac{f_{i+57}}{V_{pi}} \quad , \quad i = 1, 2, \cdots, 5 \tag{2-27d}$$

$$D_i = E - F_i \quad , \quad i = 1, 2, \cdots, 5 \tag{2-27e}$$

$$M = \frac{V}{\sqrt{\gamma R T}} \tag{2-27f}$$

$$\gamma = \frac{C_p}{C_p - R} \tag{2-27g}$$

and

$$C_p = \sum_{i=1}^{n} c_i C_{pi} \qquad (2\text{-}27h)$$

The first set of equations is completely specified at the sonic point while the second set of equations is singular. Thus, if the expansion through the nozzle is specified by the pressure distribution, the equations governing the expansion can be directly integrated through the sonic point without mathematical difficulty. The expansion from the chamber through the sonic point is specified by the pressure distribution in the present program in order to eliminate numerical difficulties at the sonic point. In the expansion section downstream of the sonic point, however, the area variation is specified and the second set of equations is integrated through the supersonic expansion section.

In specifying the nozzle pressure distribution from the chamber through the sonic point, rather than the known area distribution, a question naturally arises regarding how accurately the calculation represents the flow through a specified nozzle geometry. Experience has shown that by iterating on the inlet pressure distribution, the difference in the expansion and predicted performance caused by utilizing the inlet pressure distribution to specify the inlet expansion process rather than the inlet nozzle geometry is negligible.

Assuming that equilibrium conditions exist in the combustion chamber, the present program has been written to calculate the nonequilibrium nozzle expansion of propellant exhaust mixtures containing the six elements: carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine and one metal element, either aluminum, beryllium, boron or lithium. Gold[3] has established that the species and chemical reactions given in Tables 2-1 through 2-7 need to be considered in calculating the nonequilibrium nozzle expansions of propellant exhaust mixtures containing these elements. Considering these species and chemical reactions, the net species production rates (ω_i) for each species considered by the program are:

For CO_2

$$\omega_1 = -44.011\rho^2 \left[X_1 + X_{13} + X_{14} - X_{18} - X_{21} + X_{50} - X_{111} + X_{165} - X_{166} + X_{203} - X_{245}\right]$$

For H_2O

$$\omega_2 = -18.016\rho^2 \left[X_2 + X_{15} + X_{16} + X_{17} - X_{31} + X_{110} + X_{120} - X_{130} + X_{134} + X_{138} - X_{147} + X_{165} + X_{203} + X_{234} + X_{235} + X_{253} - X_{258} - X_{259} - X_{260} + X_{266}\right]$$

For CO

$$\omega_3 = 28.011\rho^2 \left[X_1 - X_3 + X_{13} + X_{14} - 2X_{18} - X_{19} - X_{20} - X_{21} - X_{22} + X_{50} - X_{51} - X_{64} - X_{76} - X_{111} + X_{114} + X_{165} - X_{166} - X_{167} + X_{172} + X_{203} - X_{204} - X_{236} - X_{245}\right]$$

For Cl_2

$$\omega_4 = -70.914\rho^2 \left[X_4 - X_{23} - X_{24} - X_{68} - X_{72} - X_{75} - X_{78} - X_{136} - X_{188} - X_{192} - X_{193} - X_{196} - X_{276} - X_{280}\right]$$

For F_2

$$\omega_5 = -38.000\rho^2 \left[X_5 - X_{27} - X_{29} - X_{88} - X_{91} - X_{95} - X_{143} - X_{208} - X_{213} - X_{214} - X_{220} - X_{267} - X_{272}\right]$$

For HCl

$$\omega_6 = -36.465\rho^2 \left[X_6 - X_{15} + X_{23} + 2X_{24} + X_{25} - X_{26} - X_{32} + X_{65} - X_{67} - X_{69} + X_{77} - X_{80} + X_{84} + X_{92} + X_{112} + X_{121} - X_{128} - X_{134} + X_{135} - X_{137} + X_{139} + X_{168} - X_{189} + X_{194} - X_{195} - X_{198} + X_{205} + X_{217} - X_{244} + X_{246} + X_{258} - X_{265} + X_{276} - X_{277} - X_{278} - X_{279} - X_{281}\right]$$

For HF

$$\omega_7 = -20.008\rho^2 \left[X_7 + X_{26} + X_{27} + X_{28} + 2X_{29} - X_{30} + X_{31} + X_{57} - X_{84} + X_{85} - X_{89} - X_{92} + X_{93} - X_{97} + X_{113} + X_{122} + X_{169} + X_{183} - X_{205} + X_{206} - X_{209} - X_{215} - X_{217} + X_{218} - X_{222} + X_{237} + X_{247} + X_{254} - X_{266} + X_{267} - X_{268} - X_{270} - X_{273} + X_{277}\right]$$

For H_2

$$\omega_8 = -2.016\rho^2 \left[X_8 - X_{16} - X_{24} - X_{28} - X_{29} + X_{32} + X_{33} + X_{34} - X_{131} + X_{238} + X_{248} + X_{255} + X_{259} - X_{263} + X_{268} + X_{278}\right]$$

For N_2

$$\omega_9 = -28.016\rho^2 \left[X_9 + X_{35} + X_{36} + X_{160} - X_{163}\right]$$

For NO

$$\omega_{10} = -30.008\rho^2 \Big[X_{10} - X_{20} + X_{21} - X_{35} - 2X_{36} + X_{37} + X_{38} + X_{52} + X_{66} + X_{86} - X_{117} + X_{161} + X_{162} + X_{163} + X_{170} + X_{171} - X_{200} - X_{250}\Big]$$

For OH

$$\omega_{11} = 17.008\rho^2 \Big[X_2 - X_{11} + X_{13} + X_{15} + X_{16} + 2X_{17} + X_{19} + X_{25} + X_{30} - X_{31} + X_{33} + 2X_{34} + X_{37} + X_{39} + X_{57} + X_{59} - X_{67} + X_{77} + X_{81} + X_{93} + X_{98} + X_{108} + X_{110} + X_{112} + X_{116} - X_{123} + X_{129} + X_{132} - X_{140} - X_{141} + X_{168} + X_{169} + X_{175} + X_{183} + X_{185} + X_{194} - X_{195} + X_{199} + X_{218} + X_{223} + X_{225} + X_{234} - X_{239} - X_{240} + X_{248} - X_{249} + X_{251} - X_{260} + X_{261} + X_{262} + X_{264} - X_{269} - X_{270} - X_{279}\Big]$$

For O_2

$$\omega_{12} = -32.000\rho^2 \Big[X_{12} - X_{14} - X_{22} + X_{34} + X_{36} - X_{38} + X_{39} - X_{82} - X_{99} - X_{118} - X_{170} - X_{177} - X_{186} - X_{201} + X_{241} - X_{249}\Big]$$

For C

$$\omega_{13} = 12.001\rho^2 \Big[X_3 + X_{18} + X_{19} + X_{20} + X_{22} + X_{51} + X_{64} - X_{114} + X_{167} - X_{172} + X_{204} + X_{236}\Big]$$

For Cl

$$\omega_{14} = 35.457\rho^2 \Big[2X_4 + X_6 - X_{15} - X_{23} + X_{25} - X_{26} - X_{32} + X_{42} + X_{43} + X_{44} + X_{54} - X_{62} + X_{70} - X_{75} - X_{78} - X_{79} - X_{87} - X_{94} + X_{100} + X_{104} - X_{115} - X_{124} - X_{128} - X_{129} - X_{136} - X_{142} + X_{151} + X_{152} + X_{153} - X_{173} - X_{184} - X_{188} + X_{190} - X_{192} - X_{193} - X_{196} - X_{197} - X_{207} - X_{219} + X_{227} - X_{244} + X_{246} - X_{261} - X_{271} - X_{280} + X_{282} + X_{283} + X_{284}\Big]$$

For F

$$\omega_{15} = 19.000\rho^2 \Big[\partial X_5 + X_7 + X_{26} - X_{27} + X_{28} + X_{30} + X_{31} + X_{46} + X_{47} + X_{48} + X_{56} - X_{58} + X_{60} + X_{87} - X_{88} - X_{91} + X_{94} - X_{95} - X_{96} + X_{101} + X_{105} + X_{113} + X_{119} + X_{141} + X_{142} - X_{143} + X_{145} + X_{155} + X_{156} + X_{157} + X_{158} - X_{174} + X_{207} - X_{208} + X_{210} - X_{213} - X_{214} + X_{219} - X_{220} - X_{221} + X_{224} + X_{228} + X_{237} + X_{247} + X_{252} + X_{269} + X_{271} - X_{272} + X_{274} + X_{275}\Big]$$

For H

$$\omega_{16} = 1.008\rho^2 \Big[X_2 + X_6 + X_7 + 2X_8 + X_{11} - X_{13} - X_{16} - X_{19} + X_{23} + X_{27} - X_{28} + X_{32} + X_{33} - X_{37} - X_{39} - X_{59} + X_{65} - X_{69} - X_{80} - X_{81} + X_{85} - X_{89} - X_{97} - X_{98} + X_{103} - X_{116} - X_{125} - X_{130} - X_{131} + X_{135} - X_{137} - X_{144} - X_{146} - X_{147} - X_{175} - X_{185} - X_{189} - X_{198} - X_{199} + X_{206} - X_{209} - X_{215} - X_{222} - X_{223} + X_{226} + X_{229} + X_{235} + X_{238} + X_{240} + X_{243} - X_{256} - X_{262} - X_{263} - X_{273} - X_{274} - X_{281} - X_{282}\Big]$$

For N

$$\omega_{17} = 14.008\rho^2 \Big[2X_9 + X_{10} - X_{20} + X_{21} + X_{35} + X_{37} + X_{38} + X_{66} + X_{86} - X_{117} + X_{148} + X_{160} + X_{162} + X_{171} - X_{176} - X_{190} - X_{200} - X_{210} - X_{250}\Big]$$

For O

$$\omega_{18} = 16.000\rho^2 \Big[X_1 + X_3 + X_{10} + X_{11} + 2X_{12} - X_{14} - X_{17} X_{22} - X_{25} - X_{30} - X_{33} - X_{35} - X_{38} + X_{39} + X_{40} + X_{45} + X_{49} + X_{53} + X_{58} - X_{63} - X_{70} - X_{82} + X_{96} - X_{99} + X_{106} + X_{115} - X_{118} - X_{126} - X_{132} - X_{145} + X_{149} + X_{150} + X_{154} + X_{159} + X_{161} + X_{173} + X_{174} + X_{176} - X_{177} + X_{184} - X_{186} + X_{197} - X_{201} + X_{221} - X_{224} + X_{230} + X_{239} + X_{241} - X_{257} - X_{264} - X_{275} - X_{283}\Big]$$

For Al

$$\omega_{19} = 26.97\rho^2 \Big[X_{40} + X_{41} + X_{42} + X_{46} - X_{50} - X_{51} - X_{52} - X_{53} - X_{54}$$
$$- X_{55} + X_{59} + X_{61} + X_{68} + X_{69} + X_{71} + X_{83} + X_{88}$$
$$+ X_{89}\Big]$$

For AlO

$$\omega_{20} = -42.97\rho^2 \Big[X_{40} - X_{41} - X_{44} - X_{48} - X_{50} - X_{51} - X_{52} - X_{53}$$
$$- X_{55} + X_{57} + X_{58} + X_{59} + X_{60} + X_{61} - X_{62}\ 2X_{63}$$
$$- X_{67} - X_{70} - X_{73} - X_{78} - X_{80} - X_{90} - X_{95} - X_{97}\Big]$$

For Al_2O

$$\omega_{21} = -69.94\rho^2 \Big[X_{41} - X_{54} - X_{56} - X_{60} + X_{62} + X_{63} - X_{72}\Big]$$

For AlCl

$$\omega_{22} = -62.427\rho^2 \Big[X_{42} - X_{43} - X_{45} - X_{55} - X_{62} + X_{64} + X_{65} + X_{66}$$
$$+ X_{67} + X_{68} + X_{69} + X_{70} + 2X_{71} + X_{72} + X_{73} + X_{74}$$
$$- X_{75} - X_{76} - X_{81} - X_{82} - X_{84} - X_{87}\Big]$$

For $AlCl_2$

$$\omega_{23} = -97.884\rho^2 \Big[X_{43} - X_{65} - X_{71} - X_{73} + X_{75} - X_{77} - X_{79}\Big]$$

For AlOCl

$$\omega_{24} = -78.427\rho^2 \Big[X_{44} + X_{45} - X_{64} - X_{66} - X_{74} + X_{77} + X_{78} + X_{79}$$
$$+ X_{80} + X_{81} + X_{82} - X_{92} - X_{94}\Big]$$

For AlF

$$\omega_{25} = -45.97\rho^2 \Big[X_{46} - X_{47} - X_{49} - X_{57} - X_{58} - X_{74} + 2X_{83} + X_{84}$$
$$+ X_{85} + X_{86} + X_{87} + X_{88} + X_{89} + X_{90} - X_{91}$$
$$- X_{98} - X_{99}\Big]$$

For AlF_2

$$\omega_{26} = -64.97\rho^2 \left[X_{47} - X_{83} - X_{85} - X_{90} + X_{91} - X_{93} - X_{96}\right]$$

For AlOF

$$\omega_{27} = -61.97\rho^2 \left[X_{48} + X_{49} + X_{56} - X_{61} + X_{74} - X_{86} + X_{90} + X_{92} + X_{93} + X_{94} + X_{95} + X_{96} + X_{97} + X_{98} + X_{99}\right]$$

For B

$$\omega_{28} = 10.820\rho^2 \left[X_{148} + X_{149} + X_{151} + X_{155} - X_{160} - X_{161} - X_{162} + X_{164} + X_{166} + X_{172} + X_{175} + X_{177} + X_{178} + X_{180} + X_{187} + X_{188} + X_{189} + X_{202} + X_{208} + X_{209} + X_{211}\right]$$

For BN

$$\omega_{29} = -24.828\rho^2 \left[X_{148} - X_{160} - X_{161} - X_{163} - X_{170} - X_{176} - X_{190} - X_{210}\right]$$

For BO

$$\omega_{30} = -26.820\rho^2 \left[X_{149} - X_{150} - X_{158} - X_{162} - X_{163} + 2X_{164} + X_{165} + X_{166} + X_{167} + X_{168} + X_{169} + X_{170} + X_{171} + X_{172} + X_{173} + X_{174} + X_{175} + X_{176} + X_{177} + X_{178} + X_{179} + X_{180} + X_{181} + X_{182} - X_{185} - X_{186} - X_{196} - X_{198} - X_{212} - X_{220} - X_{222}\right]$$

For BO_2

$$\omega_{31} = -42.820\rho^2 \left[X_{150} - X_{164} - X_{165} - X_{167} - X_{171} - X_{179} - X_{182} + X_{183} + X_{184} + X_{185} + X_{186} - X_{195} - X_{215} - X_{224}\right]$$

For BCl

$$\omega_{32} = -46.277\rho^2 \Big[X_{151} - X_{152} - X_{154} - X_{168} - X_{173} + X_{178} - X_{179} + 2X_{187} + X_{188} + X_{189} + X_{190} + X_{191} - X_{192} - X_{199} - X_{200} - X_{201} - X_{205} - X_{207}\Big]$$

For BCl_2

$$\omega_{33} = -81.734\rho^2 \Big[X_{152} - X_{153} - X_{187} + X_{192} - X_{193} - X_{194} - X_{197}\Big]$$

For BCl_3

$$\omega_{34} = -117.191\rho^2 \Big[X_{153} + X_{193}\Big]$$

For BOCl

$$\omega_{35} = -62.277\rho^2 \Big[X_{154} - X_{178} + X_{179} - X_{184} - X_{191} + X_{194} + X_{195} + X_{196} + X_{197} + X_{198} + X_{199} + X_{200} + X_{201} - X_{217} - X_{219}\Big]$$

For BF

$$\omega_{36} = -29.820\rho^2 \Big[X_{155} - X_{156} - X_{159} - X_{169} - X_{174} + X_{180} - X_{182} - X_{191} + 2X_{202} + X_{203} + X_{204} + X_{205} + X_{206} + X_{207} + X_{208} + X_{209} + X_{210} + X_{211} + X_{212} - X_{213} - X_{223}\Big]$$

For BF_2

$$\omega_{37} = -48.820\rho^2 \Big[X_{156} - X_{157} - X_{181} - X_{202} - X_{206} + X_{211} - X_{212} + X_{213} - X_{214} - X_{215} - X_{216} - X_{218} - X_{221}\Big]$$

For BF_3

$$\omega_{38} = -67.820\rho^2 \Big[X_{157} + X_{181} - X_{211} + X_{214} + X_{215}\Big]$$

For BOF

$$\omega_{39} = -45.820\rho^2 \left[X_{158} + X_{159} - X_{180} - X_{181} + X_{182} - X_{183} + X_{191} - X_{203} - X_{204} + X_{212} + 2X_{216} + X_{217} + X_{218} + X_{219} + X_{220} + X_{221} + X_{222} + X_{223} + X_{224}\right]$$

For Be

$$\omega_{40} = 9.013\rho^2 \left[X_{102} + X_{104} + X_{105} + X_{106} + X_{107} - X_{109} + X_{111} + X_{114} + X_{116} + X_{117} + X_{118} + X_{125} + X_{127} + X_{130} + X_{133} + X_{136} + X_{137} + X_{143} + X_{144}\right]$$

For BeO

$$\omega_{41} = 25.913\rho^2 \left[X_{103} - X_{106} + X_{107} - X_{110} - X_{111} - X_{112} - X_{113} - X_{114} - X_{115} - X_{116} - X_{117} - X_{118} - X_{119} + X_{123} + X_{124} + 2X_{126} + X_{128} + X_{131} + X_{132} + X_{140} + X_{145}\right]$$

For Be_2O

$$\omega_{42} = -34.026\rho^2 \left[X_{107} - X_{119} + X_{120} + X_{121} + X_{122} + X_{123} + X_{124} + X_{125} + X_{126}\right]$$

For BeOH

$$\omega_{43} = -26.021\rho^2 \left[X_{102} + X_{103} - X_{108} - X_{110} - X_{113} - 2X_{120} - X_{121} - X_{122} - X_{123} - X_{125} + 2X_{127} + X_{128} + X_{129} + X_{130} + X_{131} + X_{132} - X_{134} - X_{138} - X_{141} - X_{147}\right]$$

For BeCl

$$\omega_{44} = 44.470\rho^2 \left[X_{100} - X_{104} + X_{112} + X_{115} + X_{121} + X_{124} + X_{129} - 2X_{133} - X_{134} - X_{135} - X_{136} - X_{137} + X_{139} + X_{142}\right]$$

For $BeCl_2$

$$\omega_{45} = -79.927\rho^2 \left[X_{100} - X_{133} - X_{135}\right]$$

For BeF

$$\omega_{46} = 28.013\rho^2 \left[X_{101} - X_{105} + 2X_{109} - X_{119} + X_{122} - X_{138} - X_{139} - X_{140} - X_{141} - X_{142} - X_{143} - X_{144} - X_{145} + X_{146}\right]$$

For BeF_2

$$\omega_{47} = -47.013\rho^2 \left[X_{101} + X_{109} + X_{146}\right]$$

For BeO_2H_2

$$\omega_{48} = -43.029\rho^2 \left[X_{108} - X_{127} + X_{147}\right]$$

For Li

$$\omega_{49} = 6.940\rho^2 \left[X_{225} + X_{227} + X_{228} + X_{229} + X_{230} + X_{231} - X_{234} - X_{235} - X_{236} - X_{237} - X_{238} - X_{239} - X_{240} - X_{241} - X_{242} - X_{243} + X_{244} + X_{245} + X_{250} + X_{272} + X_{273} + X_{280} + X_{281}\right]$$

For LiH

$$\omega_{50} = -7.948\rho^2 \left[X_{229} - X_{233} - X_{236} - X_{237} - X_{238} - X_{241} + X_{243} - X_{247} - X_{248} - X_{254} - X_{255} - X_{258} - X_{261} - X_{266} - X_{267} - X_{273} - X_{275} - X_{277} - X_{281}\right]$$

For LiO

$$\omega_{51} = 22.940\rho^2 \left[X_{226} - X_{230} + X_{231} + X_{236} + X_{240} + X_{241} + X_{242} - X_{245} - X_{246} - X_{247} - X_{248} - X_{249} - X_{250} - X_{251} - X_{252} + X_{256} + 2X_{257} + X_{260} + X_{263} + X_{264} + X_{270} + X_{275} + X_{279} + X_{283} - X_{284}\right]$$

For Li_2O

$$\omega_{52} = -29.880\rho^2 \left[X_{231} - X_{243} - X_{251} - X_{252} + X_{253} + X_{254} + X_{255} + X_{256} + X_{257} - X_{265} - X_{284}\right]$$

For LiOH

$$\omega_{53} = -23.948\rho^2 \left[X_{225} + X_{226} - X_{235} + X_{242} + X_{243} - X_{246} - X_{247} + X_{251} - 2X_{253} - X_{254} - X_{255} + X_{258} + X_{259} + X_{260} + X_{261} + X_{262} + X_{263} + X_{263} + X_{264} + X_{265} - X_{266} - X_{269}\right]$$

For LiF

$$\omega_{54} = -25.940\rho^2 \left[X_{228} - 2X_{232} + X_{252} - X_{254} + X_{266} + X_{267} + X_{268} + X_{269} + X_{270} + X_{271} + X_{272} + X_{273} + X_{274} + X_{275} - X_{277}\right]$$

For LiCl

$$\omega_{55} = -42.397\rho^2 \left[X_{227} - 2X_{233} - X_{258} - X_{261} + X_{265} - X_{271} + X_{276} + X_{277} + X_{278} + X_{279} + X_{280} + X_{281} + X_{282} + X_{283} + X_{284}\right]$$

For Li_2F_2

$$\omega_{56} = -51.880\rho^2 \left[X_{232}\right]$$

For Li_2Cl_2

$$\omega_{57} = -84.794\rho^2 \left[X_{233}\right]$$

where the net production rate for each reaction (X_j) considered by the program is given in Section 4.2.1.

Table 2-1. Gaseous Chemical Species Considered in the Program

Species Number	Chemical Species	Species Number	Chemical Species	Species Number	Chemical Species
1	CO_2	20	AlO	39	BOF
2	H_2O	21	Al_2O	40	Be
3	CO	22	AlCl	41	BeO
4	Cl_2	23	$AlCl_2$	42	Be_2O
5	F_2	24	AlOCl	43	BeOH
6	HCl	25	AlF	44	BeCl
7	HF	26	AlF_2	45	$BeCl_2$
8	H_2	27	AlOF	46	BeF
9	N_2	28	B	47	BeF_2
10	NO	29	BN	48	BeO_2H_2
11	OH	30	BO	49	Li
12	O_2	31	BO_2	50	LiH
13	C	32	BCl	51	LiO
14	Cl	33	BCl_2	52	Li_2O
15	F	34	BCl_3	53	LiOH
16	H	35	BOCl	54	LiF
17	N	36	BF	55	LiCl
18	O	37	BF_2	56	Li_2F_2
19	Al	38	BF_3	57	Li_2Cl_2

Table 2-2. Condensed Chemical Species Considered in the Program

Aluminum Specie	Beryllium Specie	Boron Specie	Other Specie
$Al_2O_3(c)$	BeO(c)	B(c)	C(c)
		BN(c)	

Table 2-3. Chemical Reactions Considered in the Program Involving C, H, O, Cl, F and N Species Only

Reaction Number	Chemical Reaction	Reaction Number	Chemical Reaction
1	$CO_2 + M \rightleftarrows CO + O + M$	21	$CO + NO \rightleftarrows CO_2 + N$
2	$H_2O + M \rightleftarrows OH + H + M$	22	$CO + O \rightleftarrows O_2 + C$
3	$CO + M \rightleftarrows C + O + M$	23	$HCl + Cl \rightleftarrows Cl_2 + H$
4	$Cl_2 + M \rightleftarrows 2Cl + M$	24	$2HCl \rightleftarrows Cl_2 + H_2$
5	$F_2 + M \rightleftarrows 2F + M$	25	$HCl + O \rightleftarrows OH + Cl$
6	$HCl + M \rightleftarrows H + Cl + M$	26	$HF + Cl \rightleftarrows HCl + F$
7	$HF + M \rightleftarrows H + F + M$	27	$HF + F \rightleftarrows F_2 + H$
8	$H_2 + M \rightleftarrows 2H + M$	28	$HF + H \rightleftarrows H_2 + F$
9	$N_2 + M \rightleftarrows 2N + M$	29	$2HF \rightleftarrows F_2 + H_2$
10	$NO + M \rightleftarrows N + O + M$	30	$HF + O \rightleftarrows OH + F$
11	$OH + M \rightleftarrows O + H + M$	31	$HF + OH \rightleftarrows H_2O + F$
12	$O_2 + M \rightleftarrows 2O + M$	32	$H_2 + Cl \rightleftarrows HCl + H$
13	$CO_2 + H \rightleftarrows CO + OH$	33	$H_2 + O \rightleftarrows OH + H$
14	$CO_2 + O \rightleftarrows CO + O_2$	34	$H_2 + O_2 \rightleftarrows 2OH$
15	$H_2O + Cl \rightleftarrows HCl + OH$	35	$N_2 + O \rightleftarrows NO + N$
16	$H_2O + H \rightleftarrows H_2 + OH$	36	$N_2 + O_2 \rightleftarrows 2NO$
17	$H_2O + O \rightleftarrows 2OH$	37	$NO + H \rightleftarrows OH + N$
18	$2CO \rightleftarrows CO_2 + C$	38	$NO + O \rightleftarrows O_2 + N$
19	$CO + H \rightleftarrows OH + C$	39	$O_2 + H \rightleftarrows OH + O$
20	$CO + N \rightleftarrows NO + C$		

Table 2-4. Chemical Reactions Considered in the Program Involving Gaseous Aluminum Species

Reaction Number	Chemical Reaction	Reaction Number	Chemical Reaction
40	$AlO + M \rightleftharpoons Al + O + M$	70	$AlCl + O \rightleftharpoons AlO + Cl$
41	$Al_2O + M \rightleftharpoons Al + AlO + M$	71	$2AlCl \rightleftharpoons Al + AlCl_2$
42	$AlCl + M \rightleftharpoons Al + Cl + M$	72	$AlCl + AlOCl \rightleftharpoons Al_2O + Cl_2$
43	$AlCl_2 + M \rightleftharpoons AlCl + Cl + M$	73	$AlCl + AlOCl \rightleftharpoons AlO + AlCl_2$
44	$AlOCl + M \rightleftharpoons AlO + Cl + M$	74	$AlCl + AlOF \rightleftharpoons AlF + AlOCl$
45	$AlOCl + M \rightleftharpoons AlCl + O + M$	75	$AlCl_2 + Cl \rightleftharpoons AlCl + Cl_2$
46	$AlF + M \rightleftharpoons Al + F + M$	76	$AlOCl + CO \rightleftharpoons AlCl + CO_2$
47	$AlF_2 + M \rightleftharpoons AlF + F + M$	77	$AlOCl + HCl \rightleftharpoons AlCl_2 + OH$
48	$AlOF + M \rightleftharpoons AlO + F + M$	78	$AlOCl + Cl \rightleftharpoons AlO + Cl_2$
49	$AlOF + M \rightleftharpoons AlF + O + M$	79	$AlOCl + Cl \rightleftharpoons AlCl_2 + O$
50	$Al + CO_2 \rightleftharpoons AlO + CO$	80	$AlOCl + H \rightleftharpoons AlO + HCl$
51	$Al + CO \rightleftharpoons AlO + C$	81	$AlOCl + H \rightleftharpoons AlCl + OH$
52	$Al + NO \rightleftharpoons AlO + N$	82	$AlOCl + O \rightleftharpoons AlCl + O_2$
53	$Al + O_2 \rightleftharpoons AlO + O$	83	$2AlF \rightleftharpoons Al + AlF_2$
54	$Al + AlOCl \rightleftharpoons Al_2O + Cl$	84	$AlF + HCl \rightleftharpoons AlCl + HF$
55	$Al + AlOCl \rightleftharpoons AlO + AlCl$	85	$AlF + HF \rightleftharpoons AlF_2 + H$
56	$Al + AlOF \rightleftharpoons Al_2O + F$	86	$AlF + NO \rightleftharpoons AlOF + N$
57	$AlO + HF \rightleftharpoons AlF + OH$	87	$AlF + Cl \rightleftharpoons AlCl + F$
58	$AlO + F \rightleftharpoons AlF + O$	88	$AlF + F \rightleftharpoons Al + F_2$
59	$AlO + H \rightleftharpoons Al + OH$	89	$AlF + H \rightleftharpoons Al + HF$
60	$AlO + AlF \rightleftharpoons Al_2O + F$	90	$AlF + AlOF \rightleftharpoons AlO + AlF_2$
61	$AlO + AlF \rightleftharpoons Al + AlOF$	91	$AlF_2 + F \rightleftharpoons AlF + F_2$
62	$Al_2O + Cl \rightleftharpoons AlO + AlCl$	92	$AlOF + HCl \rightleftharpoons AlOCl + HF$
63	$Al_2O + O \rightleftharpoons 2AlO$	93	$AlOF + HF \rightleftharpoons AlF_2 + OH$
64	$AlCl + CO \rightleftharpoons AlOCl + C$	94	$AlOF + Cl \rightleftharpoons AlOCl + F$
65	$AlCl + HCl \rightleftharpoons AlCl_2 + H$	95	$AlOF + F \rightleftharpoons AlO + F_2$
66	$AlCl + NO \rightleftharpoons AlOCl + N$	96	$AlOF + O \rightleftharpoons AlF_2 + O$
67	$AlCl + OH \rightleftharpoons AlO + HCl$	97	$AlOF + H \rightleftharpoons AlO + HF$
68	$AlCl + Cl \rightleftharpoons Al + Cl_2$	98	$AlOF + H \rightleftharpoons AlF + OH$
69	$AlCl + H \rightleftharpoons Al + HCl$	99	$AlOF + O \rightleftharpoons AlF + O_2$

Table 2-5. Chemical Reactions Considered in the Program Involving Beryllium Species

Reaction Number	Chemical Reaction	Reaction Number	Chemical Reaction
100	$CeCl_2 + M \rightleftharpoons BeCl + Cl + M$	124	$Be_2O + Cl \rightleftharpoons BeO + BeCl$
101	$BeF_2 + M \rightleftharpoons BeF + F + M$	125	$Be_2O + H \rightleftharpoons Be + BeOH$
102	$BeOH + M \rightleftharpoons Be + OH + M$	126	$Be_2O + O \rightleftharpoons 2BeO$
103	$BeOH + M \rightleftharpoons BeO + H + M$	127	$2BeOH \rightleftharpoons Be + BeO_2H_2$
104	$BeCl + M \rightleftharpoons Be + Cl + M$	128	$BeOH + Cl \rightleftharpoons BeO + HCl$
105	$BeF + M \rightleftharpoons Be + F + M$	129	$BeOH + Cl \rightleftharpoons BeCl + OH$
106	$BeO + M \rightleftharpoons Be + O + M$	130	$BeOH + H \rightleftharpoons Be + H_2O$
107	$Be_2O + M \rightleftharpoons Be + BeO + M$	131	$BeOH + H \rightleftharpoons BeO + H_2$
108	$BeO_2H + M \rightleftharpoons BeOH + OH + M$	132	$BeOH + O \rightleftharpoons BeO + OH$
109	$Be + BeF_2 \rightleftharpoons 2BeF$	133	$2BeCl \rightleftharpoons BeCl + Be$
110	$BeO + H_2O \rightleftharpoons BeOH + OH$	134	$BeCl + H_2O \rightleftharpoons BeOH + HCl$
111	$BeO + CO \rightleftharpoons Be + CO_2$	135	$BeCl + HCl \rightleftharpoons BeCl_2 + H$
112	$BeO + HCl \rightleftharpoons BeCl + OH$	136	$BeCl + Cl \rightleftharpoons Be + Cl_2$
113	$BeO + HF \rightleftharpoons BeOH + F$	137	$BeCl + H \rightleftharpoons Be + HCl$
114	$BeO + C \rightleftharpoons Be + CO$	138	$BeF + H_2O \rightleftharpoons BeOH + HF$
115	$BeO + Cl \rightleftharpoons BeCl + O$	139	$BeF + HCl \rightleftharpoons BeCl + HF$
116	$BeO + H \rightleftharpoons Be + OH$	140	$BeF + OH \rightleftharpoons BeO + HF$
117	$BeO + N \rightleftharpoons Be + NO$	141	$BeF + OH \rightleftharpoons BeOH + F$
118	$BeO + O \rightleftharpoons Be + O_2$	142	$BeF + Cl \rightleftharpoons BeCl + F$
119	$BeO + BeF \rightleftharpoons Be_2O + F$	143	$BeF + F \rightleftharpoons Be + F_2$
120	$Be_2O + H_2O \rightleftharpoons 2BeOH$	144	$BeF + H \rightleftharpoons Be + HF$
121	$Be_2O + HCl \rightleftharpoons BeCl + BeOH$	145	$BeF + O \rightleftharpoons BeO + F$
122	$Be_2O + HF \rightleftharpoons BeF + BeOH$	146	$BeF_2 + H \rightleftharpoons BeF + HF$
123	$Be_2O + OH \rightleftharpoons BeO + BeOH$	147	$BeO_2H_2 + H \rightleftharpoons BeOH + H_2O$

Table 2-6. Chemical Reactions Considered in the Program Involving Boron Species

Reaction Number	Chemical Reaction	Reaction Number	Chemical Reaction
148	$BN + M \rightleftharpoons B + N + M$	172	$BO + C \rightleftharpoons B + CO$
149	$BO + M \rightleftharpoons B + O + M$	173	$BO + Cl \rightleftharpoons BCl + O$
150	$BO_2 + M \rightleftharpoons BO + O + M$	174	$BO + F \rightleftharpoons BF + O$
151	$BCl + M \rightleftharpoons B + Cl + M$	175	$BO + H \rightleftharpoons B + OH$
152	$BCl_2 + M \rightleftharpoons BCl + Cl + M$	176	$BO + N \rightleftharpoons BN + O$
153	$BCl_3 + M \rightleftharpoons BCl_2 + X1 + M$	177	$BO + O \rightleftharpoons B + O_2$
154	$BOCl + M \rightleftharpoons BCl + O + M$	178	$BO + BCl \rightleftharpoons B + BOCl$
155	$BF + M \rightleftharpoons B + F + M$	179	$BO + BOCl \rightleftharpoons BO_2 + BCl$
156	$BF_2 + M \rightleftharpoons BF + F + M$	180	$BO + BF \rightleftharpoons B + BOF$
157	$BF_3 + M \rightleftharpoons BF_2 + F + M$	181	$BO + BF_3 \rightleftharpoons BF_2 + BOF$
158	$BOF + M \rightleftharpoons BO + F + M$	182	$BO + BOF \rightleftharpoons BF + BO_2$
159	$BOF + M \rightleftharpoons BF + O + M$	183	$BO_2 + HF \rightleftharpoons BOF + OH$
160	$B + N_2 \rightleftharpoons BN + N$	184	$BO_2 + Cl \rightleftharpoons BOCl + O$
161	$B + NO \rightleftharpoons BN + O$	185	$BO_2 + H \rightleftharpoons BO + OH$
162	$B + NO \rightleftharpoons BO + N$	186	$BO_2 + O \rightleftharpoons BO + O_2$
163	$BN + NO \rightleftharpoons BO + N_2$	187	$2BCl \rightleftharpoons B + BCl_2$
164	$2BO \rightleftharpoons B + BO_2$	188	$BCl + Cl \rightleftharpoons B + Cl_2$
165	$BO + CO_2 \rightleftharpoons BO_2 + CO$	189	$BCl + H \rightleftharpoons B + HCl$
166	$BO + CO \rightleftharpoons B + CO_2$	190	$BCl + N \rightleftharpoons BN + Cl$
167	$BO + CO \rightleftharpoons BO_2 + C$	191	$BCl + BOF \rightleftharpoons BOCl + BF$
168	$BO + HCl \rightleftharpoons BCl + OH$	192	$BCl_2 + Cl \rightleftharpoons BCl + Cl_2$
169	$BO + HF \rightleftharpoons BF + OH$	193	$BCl_3 + Cl \rightleftharpoons BCl_2 + Cl_2$
170	$BO + NO \rightleftharpoons BN + O_2$	194	$BOCl + HCl \rightleftharpoons BCl_2 + OH$
171	$BO + NO \rightleftharpoons BO_2 + N$	195	$BOCl + OH \rightleftharpoons BO_2 + HCl$

Table 2-6. Chemical Reactions Considered in the Program Involving Boron Species (Continued)

Reaction Number	Chemical Reaction	Reaction Number	Chemical Reaction
196	$BOCl + Cl \rightleftharpoons BO + Cl_2$	211	$BF + BF_2 \rightleftharpoons B + BF_3$
197	$BOCl + Cl \rightleftharpoons BCl_2 + O$	212	$BF + BOF \rightleftharpoons BO + BF_2$
198	$BOCl + H \rightleftharpoons BO + HCl$	213	$BF_2 + F \rightleftharpoons BF + F_2$
199	$BOCl + H \rightleftharpoons BCl + OH$	214	$BF_3 + F \rightleftharpoons BF_2 + F_2$
200	$BOCl + N \rightleftharpoons BCl + NO$	215	$BF_3 + H \rightleftharpoons BF_2 + HF$
201	$BOCl + O \rightleftharpoons BCl + O_2$	216	$2BOF \rightleftharpoons BO_2 + BF_2$
202	$2BF \rightleftharpoons B + BF_2$	217	$BOF + HCl \rightleftharpoons BOCl + HF$
203	$BF + CO_2 \rightleftharpoons BOF + CO$	218	$BOF + HF \rightleftharpoons BF_2 + OH$
204	$BF + CO \rightleftharpoons BOF + C$	219	$BOF + Cl \rightleftharpoons BOCl + F$
205	$BF + HCl \rightleftharpoons BCl + HF$	220	$BOF + F \rightleftharpoons BO + F_2$
206	$BF + HF \rightleftharpoons BF_2 + H$	221	$BOF + F \rightleftharpoons BF_2 + O$
207	$BF + Cl \rightleftharpoons BCl + F$	222	$BOF + H \rightleftharpoons BO + HF$
208	$BF + F \rightleftharpoons B + F_2$	223	$BOF + H \rightleftharpoons BF + OH$
209	$BF + H \rightleftharpoons B + HF$	224	$BOF + O \rightleftharpoons BO_2 + F$
210	$BF + N \rightleftharpoons BN + F$		

Table 2-7. Chemical Reactions Considered in the Program Involving Lithium Species

Reaction Number	Chemical Reaction	Reaction Number	Chemical Reaction
225	$LiOH + M \rightleftharpoons Li + OH + M$	255	$Li_2O + H_2 \rightleftharpoons LiH + LiOH$
226	$LiOH + M \rightleftharpoons LiO + H + M$	256	$Li_2O + H \rightleftharpoons LiH + LiO$
227	$LiCl + M \rightleftharpoons Li + Cl + M$	257	$Li_2O + O \rightleftharpoons 2LiO$
228	$LiF + M \rightleftharpoons Li + F + M$	258	$LiOH + HCl \rightleftharpoons LiCl + H_2O$
229	$LiH + M \rightleftharpoons Li + H + M$	259	$LiOH + H_2 \rightleftharpoons LiH + H_2O$
230	$LiO + M \rightleftharpoons Li + O + M$	260	$LiOH + OH \rightleftharpoons LiO + H_2O$
231	$Li_2O + M \rightleftharpoons Li + LiO + M$	261	$LiOH + Cl \rightleftharpoons LiCl + OH$
232	$Li_2F_2 + M \rightleftharpoons 2LiF + M$	262	$LiOH + H \rightleftharpoons LiH + OH$
233	$Li_2Cl_2 + M \rightleftharpoons 2LiCl + M$	263	$LiOH + H \rightleftharpoons LiO + H_2$
234	$Li + H_2O \rightleftharpoons Li H + OH$	264	$LiOH + O \rightleftharpoons LiO + OH$
235	$Li + H_2O \rightleftharpoons LiOH + H$	265	$LiOH + LiCl \rightleftharpoons Li_2O + HCl$
236	$Li + CO \rightleftharpoons LiO + C$	266	$LiF + H_2O \rightleftharpoons LiOH + HF$
237	$Li + HF \rightleftharpoons LiH + F$	267	$LiF + HF \rightleftharpoons LiH + F_2$
238	$Li + H_2 \rightleftharpoons Li H + H$	268	$LiF + H_2 \rightleftharpoons LiH + HF$
239	$Li + OH \rightleftharpoons LiH + O$	269	$LiF + OH \rightleftharpoons LiOH + F$
240	$Li + OH \rightleftharpoons LiO + H$	270	$LiF + OH \rightleftharpoons LiO + HF$
241	$Li + O_2 \rightleftharpoons LiO + O$	271	$LiF + Cl \rightleftharpoons LiCl + F$
242	$Li + LiOH \rightleftharpoons LiH + LiO$	272	$LiF + F \rightleftharpoons Li + F_2$
243	$Li + LiOH \rightleftharpoons Li_2O + H$	273	$LiF + H \rightleftharpoons Li + HF$
244	$LiH + Cl \rightleftharpoons Li + HCl$	274	$LiF + H \rightleftharpoons LiH + F$
245	$LiO + CO \rightleftharpoons Li + CO_2$	275	$LiF + O \rightleftharpoons LiO + F$
246	$LiO + HCl \rightleftharpoons LiOH + Cl$	276	$LiCl + HCl \rightleftharpoons LiH + Cl_2$
247	$LiO + HF \rightleftharpoons LiOH + F$	277	$LiCl + HF \rightleftharpoons LiF + HCl$
248	$LiO + H_2 \rightleftharpoons LiH + OH$	278	$LiCl + H_2 \rightleftharpoons LiH + HCl$
249	$LiO + OH \rightleftharpoons LiH + O_2$	279	$LiCl + OH \rightleftharpoons LiO + HCl$
250	$LiO + N \rightleftharpoons Li + NO$	280	$LiCl + Cl \rightleftharpoons Li + Cl_2$
251	$LiO + LiOH \rightleftharpoons Li_2O + OH$	281	$LiCl + H \rightleftharpoons Li + HCl$
252	$LiO + LiF \rightleftharpoons Li_2O + F$	282	$LiCl + H \rightleftharpoons LiH + Cl$
253	$Li_2O + H_2O \rightleftharpoons 2LiOH$	283	$LiCl + O \rightleftharpoons LiO + Cl$
254	$Li_2O + HF \rightleftharpoons LiOH + LiF$	284	$LiCl + LiO \rightleftharpoons Li_2O + Cl$

The dissociation-recombination reactions have a distinct reaction rate associated with each third body. Benson and Fueno[4] have shown that the temperature dependence of recombination rates is approximately T^{-1} independent of the third body. Thus the rates associated with each third body can be considered by calculating the third body term (M_j) as

$$M_j = \sum_{i=1}^{57} m_{j,i} c_i \qquad (2\text{-}28)$$

where $m_{j,i}$ is the ratio of the recombination rate associated with the ith species (third body) and the recombination rate (k_j) associated with the reference species (third body) in the calculation.

The above equations are all of the form

$$\frac{dy_i}{dx} = f_i(x, y, \cdots, y_n) \quad , \quad i = 1, 2, \cdots, n \qquad (2\text{-}29)$$

The numerical method used in the program to integrate these equations is described in detail in Section 3. All calculations performed in the program are described in Section 4.

BLANK PAGE

3. NUMERICAL INTEGRATION METHOD

It has been shown by Tyson[5] that in the numerical integration of relaxation equations in near equilibrium flow regions (such as the chamber and nozzle inlet in rocket engines), explicit integration methods are unstable unless the integration step size is of the order of the characteristic relaxation distance of the relaxation equations. Since the characteristic relaxation distance is orders of magnitude smaller than the characteristic physical dimensions of the system of interest (such as the nozzle throat diameter and length) in near equilibrium flow regions, the use of explicit methods to integrate relaxation equations in these regions results in excessively long computation times. Implicit integration methods were shown to be inherently stable in integrating relaxation equations in all flow situations (whether near equilibrium or frozen) and can thus be used to integrate with step sizes of the order of the physical dimensions of the system of interest throughout the integration reducing the computation time per case several orders of magnitude. Since it has been demonstrated that there are significant advantages in using implicit rather than explicit integration methods for integrating relaxation equations, a second order implicit integration method has been chosen for use in TRW/NASA One-Dimensional Nonequilibrium Performance Programs.

3.1 STABILITY CONSIDERATIONS

The numerical considerations leading to the above conclusions can be illustrated by considering the simple relaxation equation

$$\frac{dy}{dx} = - \frac{y - y_e}{\tau} \tag{3-1}$$

which represents the relaxation toward equilibrium of chemical reactions, gas particle lags, etc. In this equation, y_e is the equilibrium condition and τ is the characteristic relaxation distance of the equation. In the equilibrium limit, τ is very small compared to the physical dimensions of the system of interest while in the frozen limit, τ, is very large compared to the physical dimensions of the system of interest. The mathematical behavior of solutions to the above equation can be found by considering the simple case where τ is constant and

$$y_e = y_{eo} + a(x - x_o) \tag{3-2}$$

which is equivalent to terminating the Taylor series for y_e after the first term. The exact solution of Equation (3-1) for this case can be shown to be

$$y(x_o + h) = y(x_o) + \left[y_{eo} - y(x_o) - a\tau\right]\left[1 - e^{-h/\tau}\right] + ah \tag{3-3}$$

where $y(x_o)$ is the initial value of y and h is the integration step.

It is seen that the solution consists of two parts, a term which varies slowly with x and a term which exponentially decays with a relaxation length of τ, the characteristic relaxation length of Equation (3-1). Thus after a few relaxation lengths

$$y(x) \simeq y_{eo} + ah \quad , \quad h >> \tau \tag{3-4}$$

which is independent of $y(x_o)$ the initial condition. Since explicit integration methods construct the solution of Equation (3-1) as a Taylor series about the initial condition $y(x_o)$, the above example indicates that explicit integration methods should be limited to step sizes of the order of a few relaxation lengths.

That this is indeed the case can be shown by explicitly integrating Equation (3-1) using Euler's method. The explicit finite difference form of Equation (3-1) is then

$$\frac{y(x_o + h) - y(x_o)}{h} = -\frac{y(x_o) - y_{eo}}{\tau} \tag{3-5}$$

which yields the truncated Taylor series

$$y(x_o + h) = y(x_o)\left(1 - \frac{h}{\tau}\right) + y_{eo}\frac{h}{\tau} \tag{3-6}$$

when solved for $y(x_o + h)$. After n integration steps, it is found that

$$y(x_o + nh) = y(x_o)\left[1 - \frac{h}{\tau}\right]^n + \sum_{i=1}^{n}\left[y_{eo} + (i - 1)\,ah\right]\left[1 - \frac{h}{\tau}\right]^{-n-i}\frac{h}{\tau} \tag{3-7}$$

Examination of this equation shows that the dependence on the initial condition $y(x_o)$ will decay only if $1 - h/\tau < 1$, otherwise $y(x_o + nh)$ will oscillate with rapidly increasing amplitude. Hence the calculation will be stable only if $h/\tau < 2$. Similar results are obtained for other explicit integration methods. (The stable step size for Runge-Kutta integrations is $h/\tau < 5.6$.) Thus the stable step size for explicit integration of relaxation equations is of the order of the relaxation distance which explains the large computation times associated with explicit integration of relaxation equations in near equilibrium flow regions. As shown below, the use of implicit integration methods allows the integration of relaxation equations on a step size which is independent of the relaxation length.

Implicitly integrating Equation (3-1) using Euler's method, the finite difference form of Equation (3-1) is

$$\frac{y(x_o + h) - y(x_o)}{h} = -\frac{y(x_o + h) - y_{eo} - ah}{\tau} \tag{3-8}$$

which yields

$$y(x_o + h) = \frac{y(x_o) + (y_{eo} + ah)\frac{h}{\tau}}{1 + \frac{h}{\tau}} \tag{3-9}$$

when solved for $y(x_o + h)$. After n integration steps it is found that

$$y(x_o + nh) = \frac{y(x_o)}{\left[1 + \frac{h}{\tau}\right]^n} + \sum_{i=1}^{n} \frac{y_{eo} + iah}{\left[1 + \frac{h}{\tau}\right]^{n+1-i}} \frac{h}{\tau} \tag{3-10}$$

Examination of this equation shows that the dependence on the initial condition $y(x_o)$ always decays, regardless of the step size. Hence the implicit calculation will always be stable. As an extreme example, consider one integration step, $h = x - x_o$. From Equation (3-9), it is seen that

$$y(x) \simeq y_{eo} + ah \quad , \quad h >> \tau \tag{3-11}$$

when the step size is large compared to the relaxation length and

$$y(x) = y(x_o)\left(1 - \frac{h}{\tau}\right) + y_{eo}\frac{h}{\tau} + \cdots, \quad h_o << \tau \qquad (3\text{-}12)$$

when the step size is small compared to the relaxation length.

It is seen that in the equilibrium limit (τ small, h/τ large) the exact solution and the implicit integration of the relaxation equation go to the same limit which is independent of the relaxation distance and depends only on the rate of change of the equilibrium condition. In the frozen case (τ large and h/τ small) the implicit and explicit methods are essentially the same (terminated Taylor series). Thus, implicit numerical integration methods can be used to integrate relaxation equations using step sizes of the order of the physical dimensions of the system interest in all flow situations whether near equilibrium or near frozen. For a complete discussion of the numerical integration of relaxation equations, the reader is referred to Reference 5.

In choosing a numerical integration method, the primary items of concern are the stability, accuracy and simplicity of the method. As shown by Tyson(5) and discussed above, implicit methods are to be preferred for numerically integrating relaxation equations due to their inherent stability. Having chosen the basic integration method for stability reasons, the order of the integration method is determined by accuracy and simplicity considerations. In general, the higher the order of the integration method, the more complex the method becomes requiring more information in the form of past values or past derivatives of the function being integrated. Second order methods (accurate to h^2 with error of order h^3) have the advantage of simplicity and flexibility since they require only one past value of the function while retaining sufficient accuracy to allow the use of reasonably economical step sizes. Since it is also desired to use this numerical integration method in characteristic mesh calculations which are inherently limited to second order accuracy, a second order implicit numerical integration method was chosen for use in the TRW/NASA One-Dimensional Nonequilibrium Performance Programs. A complete derivation of the numerical integration method used in these programs is given in the following section.

3.2 DERIVATION OF NUMERICAL INTEGRATION METHOD

Consider the coupled set of first order simultaneous differential equations.

$$\frac{dy_i}{dx} = f_i(x, y_1, \cdots, y_N) \quad , \quad i = 1, 2, \cdots, N \tag{3-13}$$

It will be assumed that the equations are not singular and that a solution exists which may be developed as a Taylor series about the forward point

$$k_{i,n+1} = \left.\frac{dy_i}{dx}\right|_{x_n+h} h - \left.\frac{d^2y_i}{dx^2}\right|_{x_n+h} \frac{h^2}{2} + \left.\frac{d^3y_i}{dx^3}\right|_{x_n+h} \frac{h^3}{6} - \left.\frac{d^4y_i}{dx^4}\right|_{x_n+h} \frac{h^4}{24} + \cdots \tag{3-14}$$

where $k_{i,n+1}$ is the increment in y_i and h is sufficiently small. For equal integration steps

$$k_{i,n+1} + k_{i,n} = 2\left.\frac{dy_i}{dx}\right|_{x_n+h} h - 4\left.\frac{d^2y_i}{dx^2}\right|_{x_n+h} \frac{h^2}{2} + 8\left.\frac{d^3y_i}{dx^3}\right|_{x_n+h} \frac{h^3}{6}$$

$$16\left.\frac{d^4y_i}{dx^4}\right|_{x_n+h} \frac{h^4}{24} + \cdots \tag{3-15}$$

Solving these equations for the derivative at the forward point, it is found that

$$\left.\frac{dy_i}{dx}\right|_{x_n+h} = \frac{3k_{i,n+1} - k_{i,n}}{2h} + \left.\frac{d^3y_i}{dx^3}\right|_{x_n+h} \frac{h^2}{3} - \cdots \tag{3-16}$$

Expanding the function $f_i(x, y, \cdots, y_N)$ as a Taylor's series about the back point (x_n), it is found that

$$\left.\frac{dy_i}{dx}\right|_{x_n+h} + f_{i,n} + \alpha_{i,n} h + \sum_{j=1}^{N} \beta_{i,j,n} k_{j,n+1} + \left.\frac{d^3y}{dx^3}\right|_{x_n} \frac{h^2}{2} + \cdots \tag{3-17}$$

where

$$f_i = f_i(x, y, \cdots, y_N) \tag{3-18a}$$

$$\alpha_i = \frac{\partial f_i}{\partial x} \tag{3-18b}$$

$$\beta_{i,j} = \frac{\partial f_i}{\partial y_j} \tag{3-18c}$$

and the subscript n refers to the functions f_i, α_i and $\beta_{i,j}$ evaluated at the point x_n. Since

$$\left.\frac{d^3y}{dx^3}\right|_{x_n} = \left.\frac{d^3y}{dx^3}\right|_{x_n+h} - \left.\frac{d^4y}{dx^4}\right|_{x_n+h} h + \cdots \tag{3-19a}$$

and

$$\left.\frac{d^4y}{dx^4}\right|_{x_n} = \left.\frac{d^4y}{dx^4}\right|_{x_n+h} \cdots, \tag{3-19b}$$

Equation (3-17) can be rewritten as

$$\left.\frac{dy_i}{dx}\right|_{x_n+h} = f_{i,n} + \alpha_{i,n}h + \sum_{j=1}^{N} \beta_{i,j,n}k_{j,n+1} + \left.\frac{d^3y_i}{dx^3}\right|_{x_n+h} \frac{h^2}{2} \cdots \tag{3-20}$$

Equating the two expressions for the derivative at the forward point [Equations (3-16) and (3-20)], it is found that

$$\frac{3k_{i,n+1} - k_{i,n}}{2h} = f_{i,n} + \alpha_{i,n}h + \sum_{j=1}^{N} \beta_{i,j,n} k_{j,n+1} + \left.\frac{d^3y_i}{dx^3}\right|_{x_n+h} \frac{h^2}{6} + \cdots \tag{3-21}$$

or

$$k_{i,n+1} = \frac{1}{3}\left[k_{i,n} + 2\left(f_{i,n} + \beta_{i,n}h + \sum_{j=1}^{N} \beta_{i,j,n}k_{j,n+1}\right)h\right] + \left.\frac{d^3y_i}{dx^3}\right|_{x_n+h} \frac{h^3}{9} + \cdots$$

(3-22)

Neglecting the third order derivative term and solving the set of N linear nonhomogeneous algebraic equations

$$\left(1 - \frac{2}{3}\beta_{i,i,n}h\right)k_{i,n+1} - \sum_{j=1}^{N}(1 - \delta_{i,j})\beta_{i,j,n}k_{j,n+1} = \frac{1}{3}\left[k_{i,n} + 2(f_{i,n} + \alpha_{i,n}h)h\right]$$

(3-23)

where $\delta_{i,j}$ is the Kronecker delta thus yields a second order implicit solution of the above set of coupled first order simultaneous differential equations.

For unequal step sizes, it can be similarly shown that solving the set of N linear nonhomogeneous algebraic equations

$$\left(1 - \frac{h_{n+1} + h_n}{2h_{n+1} + h_n}\beta_{i,i,n}h_{n+1}\right)k_{i,n+1} - \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n}\sum_{j=1}^{N}(1 - \delta_{i,j})\beta_{i,j,n}k_{j,n+1}$$

$$= \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n}\left[k_{i,n} + (f_{i,n} + \alpha_{i,n}h_{n+1})\frac{h_n}{h_{n+1}}(h_{n+1} + h_n)\right] \tag{3-24}$$

yields a second order implicit solution of the above set of coupled first order simultaneous differential equations.

Similarly, if the integration begins at an equilibrium point

$$\left(\left.\frac{dy_i}{dx}\right|_{x_o} = 0\right)$$

solving the set of N linear nonhomogeneous algebraic equations

$$\left(1 - \frac{1}{2}\beta_{i,i,o}h\right)k_{i,1} - \frac{1}{2}\sum_{j=1}^{N}(1 - \delta_{i,j})\beta_{i,j,o}k_{j,1} = \frac{1}{2}\alpha_{i,o}h \tag{3-25}$$

yields a second order implicit solution of the above set of coupled first order simultaneous differential equations.

In Equation (3-21), the third derivative term was neglected which resulted in an integration error of

$$k_i - k_i^{(c)} = \left.\frac{d^3y}{dx^3}\right|_{x_n+h} \frac{h^3}{3} + \cdots \tag{3-26}$$

where $k_i^{(c)}$ is the correct (true) value of the increment k_i. Thus the ratio of the neglected third derivative term to the first derivation terms in Equation (3-21) can be used to determine the allowable integration step size. Since

$$\left.\frac{d^3y}{dx^3}\right|_{x_n+h} = \frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{h^3} + \frac{3}{2}\left.\frac{d^4y}{dx^4}\right|_{x_n+h} h + \cdots \tag{3-27}$$

the absolute value of the ratio of the neglected term to the remaining terms in Equation (3-21) is

$$\frac{1}{3}\left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}}\right|$$

Since this ratio varies as the step size squared, doubting or halving the step size will change this ratio by a factor of four. Thus in order to maintain this ratio within prescribed limits without doubting or halving each step, the prescribed limits must differ by at least a factor of four. Thus in the present program, the integration step size is calculated from

$$h_{n+2} = 2h_{n+1}, \quad \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}}\right| < \frac{\delta}{10} \tag{3-28}$$

$$h_{n+2} = \frac{1}{2}h_{n+1}, \quad \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}}\right| > \delta \tag{3-29}$$

$$h_{n+2} = h_{n+1}, \quad \frac{\delta}{10} \leq \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}}\right| \leq \delta \tag{3-30}$$

where δ is the maximum allowable ratio of the neglected term to the remaining terms in Equation (3-21).

4. PROGRAM SUBROUTINES

The program internally calculates in engineering units (lbm, ft, sec, ^{O}R) where the poundal has been chosen as the unit of force in order to eliminate conversion constants in the calculations.

The engineering nomenclature used in deriving the conservation equations (described in Section 2) and the integration method (described in Section 3) has been retained in specifying the program subroutines so that all calculations performed in the program can be readily related to the equations being solved. The program has been organized into seven subroutines to separate logically independent calculations in order to facilitate programming and program checkout. The logical and calculational functions are summarized below:

- The Input Subroutine (described in Section 4.1) processes the input data, converts the data to the proper units, stores the converted data and calculates those quantities required during the nozzle integrations.
- The Derivative Evaluation Subroutine (described in Section 4.2) calculates the derivatives and partial derivatives of the chemical relaxation equations and the fluid dynamic equations which are used in the Integration Subroutine.
- The Integration Subroutine (described in Section 4.3) integrates the chemical relaxation equations and the fluid dynamic equations using the second order implicit integration method derived in Section 3.
- The Species Thermal Function Subroutine (described in Section 4.4) calculates the required species thermal functions from the input thermodynamic data.
- The Equilibrium Function Subroutine (described in Section 4.5) calculates the required equilibrium function for the dissociation-recombination reactions.
- The Gas Thermal Function Subroutine (described in Section 4.6) calculates the required gas mixture thermal properties.
- The Output Subroutine (described in Section 4.7) processes the output data, converts the data to the proper units and calculates the required output quantities.

A detailed description of the calculations performed in these subroutines is given in the following sections.

4.1 INPUT SUBROUTINE

This subroutine processes the input data, converts the data to the proper units, stores the converted data and calculates those quantities required during the nozzle integration. There, calculations are performed in the following order:

- The species gas constants are calculated
- The species thermal functions are input, converted from chemists' units to the units in which the program computes, and stored.
- The temperature derivatives of the species thermal functions are calculated and stored
- The heat of reaction for each of the recombination reactions is calculated
- The reaction rates are input, converted from chemists' units to the units in which the program computes, and stored
- The case data are input and those quantities required during the nozzle integration are calculated

The calculations performed by this subroutine are described in the following sections.

4.1.1 Species Gas Constant Calculations

The species gas constants are calculated from the following relationships:

R_1 = 1129.74	R_{15} = 2616.89	R_{29} = 2002.62	R_{43} = 1910.80
R_2 = 2759.82	R_{16} = 49326.4	R_{30} = 1853.88	R_{44} = 1118.08
R_3 = 1775.05	R_{17} = 3549.47	R_{31} = 1161.16	R_{45} = 622.08
R_4 = 701.15	R_{18} = 3107.56	R_{32} = 1074.42	R_{46} = 1774.93
R_5 = 1308.45	R_{19} = 1842.88	R_{33} = 608.33	R_{47} = 1057.60
R_6 = 1363.53	R_{20} = 1156.84	R_{34} = 424.27	R_{48} = 1155.52
R_7 = 2485.06	R_{21} = 710.71	R_{35} = 798.38	R_{49} = 7164.41
R_8 = 24663.2	R_{22} = 796.34	R_{36} = 1667.37	R_{50} = 6255.79
R_9 = 1774.74	R_{23} = 507.91	R_{37} = 1018.46	R_{51} = 2167.44
R_{10} = 1656.92	R_{24} = 633.90	R_{38} = 733.13	R_{52} = 1664.02
R_{11} = 2923.39	R_{25} = 1081.36	R_{39} = 1085.14	R_{53} = 2076.21
R_{12} = 1553.78	R_{26} = 765.17	R_{40} = 5516.59	R_{54} = 1916.77
R_{13} = 4139.62	R_{27} = 802.21	R_{41} = 1987.81	R_{55} = 1172.75
R_{14} = 1402.29	R_{28} = 4595.29	R_{42} = 1461.27	R_{56} = 958.38
			R_{57} = 586.38

4.1.2 Species Thermal Functions Input and Conversion

The species thermal functions tabulated at 100°K temperature increments between 100°K and 5000°K in the JANAF thermochemical tables are input and converted to a set of tables in the required units which include the enthalpy of formation. Using the JANAF nomenclature, the converted tables are calculated from

$$F_i = \frac{1}{1.98726}\left[-\frac{F^o - H^o_{298}}{T} + \frac{1000\left(H^o - H^o_{298}\right)_o}{T}\right]_i \quad , \quad i = 1, 2, \cdots, 57$$

$$h_i = 905.770 R_i \left[H^o - H^o_{298} - \left(H^o - H^o_{298}\right)_o + \Delta H^o_F\right]_i \quad , \quad i = 1, 2, \cdots, 57$$

$$C_{pi} = \frac{R_i}{1.98726} \left. C^o_p \right|_i \quad , \quad i = 1, 2, \cdots, 57$$

and stored as functions of temperature at 180°R temperature increments between 180°R and 9000°R.

4.1.3 Species Thermal Function Temperature Derivative Calculation

At each temperature between 180°R and 9000°R, the species thermal function temperature derivatives are calculated from

$$\left.\frac{dC_{pi}}{dT}\right|_{180} = \frac{1}{360}\left[4C_{pi}\Big|_{360} - 3C_{pi}\Big|_{180} - C_{pi}\Big|_{540}\right]$$

$$\left.\frac{d^2C_p}{dT^2}\right|_{180} = \frac{1}{64800}\left[C_{pi}\Big|_{540} - 2C_{pi}\Big|_{360} + C_{pi}\Big|_{180}\right]$$

$$\left.\frac{dC_{pi}}{dT}\right|_{T} = \frac{1}{360}\left[C_{pi}\Big|_{T+180} - C_{pi}\Big|_{T-180}\right] \quad , \quad 360 \leq T \leq 8820$$

$$\left.\frac{d^2C_{pi}}{dT^2}\right|_{T} = \frac{1}{64800}\left[C_{pi}\Big|_{T+180} - 2C_{pi}\Big|_{T} + C_{pi}\Big|_{T-180}\right] \quad , \quad 360 \leq T \leq 8820$$

$$\left.\frac{dC_{pi}}{dT}\right|_{9000} = \frac{1}{360}\left[3C_{pi}\Big|_{9000} - 4C_{pi}\Big|_{8820} + C_{pi}\Big|_{8640}\right]$$

$$\left.\frac{d^2C_{pi}}{dT^2}\right|_{9000} = \frac{1}{64800}\left[C_{pi}\Big|_{9000} - 2C_{pi}\Big|_{8820} + C_{pi}\Big|_{8640}\right]$$

$$\left.\frac{dh_i}{dT}\right|_T = C_{pi}\Big|_T$$

$$\left.\frac{d^2h_i}{dT^2}\right|_T = \left.\frac{dC_{pi}}{dT}\right|_T$$

$$\left.\frac{dF_i}{dT}\right|_T = \left.\frac{F_i - h_i}{T}\right|_T$$

$$\left.\frac{d^2F_i}{dT^2}\right|_T = -\left.\frac{C_{pi}}{T}\right|_T$$

and stored with the species thermal functions.

4.1.4 Heat of Reaction Calculation

The heat of reaction for each of the recombination reactions is calculated from the following relationship:

$$\Delta H_1 = 905.770\left[\Delta H^o_{F,3} + \Delta H^o_{F,18} - \Delta H^o_{F,1}\right]$$

$$\Delta H_2 = 905.770\left[\Delta H^o_{F,11} + \Delta H^o_{F,16} - \Delta H^o_{F,2}\right]$$

$$\Delta H_3 = 905.770\left[\Delta H^o_{F,13} + \Delta H^o_{F,18} - \Delta H^o_{F,3}\right]$$

$$\Delta H_4 = 905.770\left[2\Delta H^o_{F,14} - \Delta H^o_{F,4}\right]$$

$$\Delta H_5 = 905.770\left[2\Delta H^o_{F,15} - \Delta H^o_{F,5}\right]$$

$$\Delta H_6 = 905.770 \left[\Delta H^o_{F,14} + \Delta H^o_{F,15} - \Delta H^o_{F,6}\right]$$

$$\Delta H_7 = 905.770 \left[\Delta H^o_{F,15} + \Delta H^o_{F,16} - \Delta H^o_{F,7}\right]$$

$$\Delta H_8 = 905.770 \left[2\Delta H^o_{F,16} - \Delta H^o_{F,8}\right]$$

$$\Delta H_9 = 905.770 \left[2\Delta H^o_{F,17} - \Delta H^o_{F,9}\right]$$

$$\Delta H_{10} = 905.770 \left[\Delta H^o_{F,17} + \Delta H^o_{F,18} - \Delta H^o_{F,10}\right]$$

$$\Delta H_{11} = 905.770 \left[\Delta H^o_{F,16} + \Delta H^o_{F,18} - \Delta H^o_{F,11}\right]$$

$$\Delta H_{12} = 905.770 \left[2\Delta H^o_{F,18} - \Delta H^o_{F,12}\right]$$

$$\Delta H_{40} = 905.770 \left[\Delta H^o_{F,18} + \Delta H^o_{F,19} - \Delta H^o_{F,20}\right]$$

$$\Delta H_{41} = 905.770 \left[\Delta H^o_{F,19} + \Delta H^o_{F,20} - \Delta H^o_{F,21}\right]$$

$$\Delta H_{42} = 905.770 \left[\Delta H^o_{F,14} + \Delta H^o_{F,19} - \Delta H^o_{F,22}\right]$$

$$\Delta H_{43} = 905.770 \left[\Delta H^o_{F,14} + \Delta H^o_{F,22} - \Delta H^o_{F,23}\right]$$

$$\Delta H_{44} = 905.770 \left[\Delta H^o_{F,14} + \Delta H^o_{F,20} - \Delta H^o_{F,24}\right]$$

$$\Delta H_{45} = 905.770 \left[\Delta H^o_{F,18} + \Delta H^o_{F,22} - \Delta H^o_{F,24}\right]$$

$$\Delta H_{46} = 905.770 \left[\Delta H^o_{F,15} + \Delta H^o_{F,19} - \Delta H^o_{F,25}\right]$$

$$\Delta H_{47} = 905.770 \left[\Delta H^o_{F,15} + \Delta H^o_{F,25} - \Delta H^o_{F,26}\right]$$

$$\Delta H_{48} = 905.770 \left[\Delta H^o_{F,15} + \Delta H^o_{F,20} - \Delta H^o_{F,27}\right]$$

$$\Delta H_{49} = 905.770 \left[\Delta H^o_{F,18} + \Delta H^o_{F,25} - \Delta H^o_{F,27}\right]$$

$$\Delta H_{100} = 905.770 \left[\Delta H^o_{F,14} + \Delta H^o_{F,44} - \Delta H^o_{F,45}\right]$$

$$\Delta H_{101} = 905.770 \left[\Delta H^{o}_{F,15} + \Delta H^{o}_{F,46} - \Delta H^{o}_{F,47}\right]$$

$$\Delta H_{102} = 905.770 \left[\Delta H^{o}_{F,11} + \Delta H^{o}_{F,40} - \Delta H^{o}_{F,43}\right]$$

$$\Delta H_{103} = 905.770 \left[\Delta H^{o}_{F,16} + \Delta H^{o}_{F,41} - \Delta H^{o}_{F,43}\right]$$

$$\Delta H_{104} = 905.770 \left[\Delta H^{o}_{F,14} + \Delta H^{o}_{F,40} - \Delta H^{o}_{F,44}\right]$$

$$\Delta H_{105} = 905.770 \left[\Delta H^{o}_{F,15} + \Delta H^{o}_{F,40} - \Delta H^{o}_{F,46}\right]$$

$$\Delta H_{106} = 905.770 \left[\Delta H^{o}_{F,18} + \Delta H^{o}_{F,40} - \Delta H^{o}_{F,41}\right]$$

$$\Delta H_{107} = 905.770 \left[\Delta H^{o}_{F,40} + \Delta H^{o}_{F,41} - \Delta H^{o}_{F,42}\right]$$

$$\Delta H_{108} = 905.770 \left[\Delta H^{o}_{F,11} + \Delta H^{o}_{F,43} - \Delta H^{o}_{F,48}\right]$$

$$\Delta H_{148} = 905.770 \left[\Delta H^{o}_{F,17} + \Delta H^{o}_{F,28} - \Delta H^{o}_{F,29}\right]$$

$$\Delta H_{149} = 905.770 \left[\Delta H^{o}_{F,18} + \Delta H^{o}_{F,28} - \Delta H^{o}_{F,30}\right]$$

$$\Delta H_{150} = 905.770 \left[\Delta H^{o}_{F,18} + \Delta H^{o}_{F,30} - \Delta H^{o}_{F,31}\right]$$

$$\Delta H_{151} = 905.770 \left[\Delta H^{o}_{F,14} + \Delta H^{o}_{F,28} - \Delta H^{o}_{F,32}\right]$$

$$\Delta H_{152} = 905.770 \left[\Delta H^{o}_{F,14} + \Delta H^{o}_{F,32} - \Delta H^{o}_{F,33}\right]$$

$$\Delta H_{153} = 905.770 \left[\Delta H^{o}_{F,14} + \Delta H^{o}_{F,33} - \Delta H^{o}_{F,34}\right]$$

$$\Delta H_{154} = 905.770 \left[\Delta H^{o}_{F,18} + \Delta H^{o}_{F,32} - \Delta H^{o}_{F,35}\right]$$

$$\Delta H_{155} = 905.770 \left[\Delta H^{o}_{F,15} + \Delta H^{o}_{F,28} - \Delta H^{o}_{F,36}\right]$$

$$\Delta H_{156} = 905.770 \left[\Delta H^{o}_{F,15} + \Delta H^{o}_{F,36} - \Delta H^{o}_{F,37}\right]$$

$$\Delta H_{157} = 905.770 \left[\Delta H^{o}_{F,15} + \Delta H^{o}_{F,37} - \Delta H^{o}_{F,38}\right]$$

$$\Delta H_{158} = 905.770 \left[\Delta H^o_{F,15} + \Delta H^o_{F,30} - \Delta H^o_{F,39}\right]$$

$$\Delta H_{159} = 905.770 \left[\Delta H^o_{F,18} + \Delta H^o_{F,36} - \Delta H^o_{F,39}\right]$$

$$\Delta H_{225} = 905.770 \left[\Delta H^o_{F,11} + \Delta H^o_{F,49} - \Delta H^o_{F,53}\right]$$

$$\Delta H_{226} = 905.770 \left[\Delta H^o_{F,16} + \Delta H^o_{F,51} - \Delta H^o_{F,53}\right]$$

$$\Delta H_{227} = 905.770 \left[\Delta H^o_{F,14} + \Delta H^o_{F,49} - \Delta H^o_{F,55}\right]$$

$$\Delta H_{228} = 905.770 \left[\Delta H^o_{F,15} + \Delta H^o_{F,49} - \Delta H^o_{F,54}\right]$$

$$\Delta H_{229} = 905.770 \left[\Delta H^o_{F,16} + \Delta H^o_{F,49} - \Delta H^o_{F,50}\right]$$

$$\Delta H_{230} = 905.770 \left[\Delta H^o_{F,18} + \Delta H^o_{F,49} - \Delta H^o_{F,51}\right]$$

$$\Delta H_{231} = 905.770 \left[\Delta H^o_{F,49} + \Delta H^o_{F,51} - \Delta H^o_{F,52}\right]$$

$$\Delta H_{232} = 905.770 \left[2\Delta H^o_{F,54} - \Delta H^o_{F,56}\right]$$

$$\Delta H_{233} = 905.770 \left[2\Delta H^o_{F,55} - \Delta H^o_{F,57}\right]$$

4.1.5 Reaction Rate Input and Conversion

The reaction rate parameters a_j, n_j and b_j are input and converted to the required units. (Since the reaction rate parameter n_j is a dimensionless temperature exponent, it does not require conversion.) The converted reaction rate parameters are calculated from the following relationships:

$$b_j = 905.770\, b'_j \quad , \quad j = 1, 2, \cdots, 57$$

$$a_1 = 0.11515 \cdot 10^{-10} (1.8)^{n_1}\, a'_1$$

$$a_2 = 0.30101 \cdot 10^{-9} (1.8)^{n_2}\, a'_2$$

$$a_3 = 0.36853 \cdot 10^{-10} (1.8)^{n_3}\, a'_3$$

$$a_4 = 0.41048 \cdot 10^{-11} (1.8)^{n_4}\, a'_4$$

$$a_5 = 0.14295 \cdot 10^{-10} (1.8)^{n_5}\, a'_5$$

$$a_6 = 0.14043 \cdot 10^{-9} (1.8)^{n_6}\, a'_6$$

$$a_7 = 0.26945 \cdot 10^{-9} (1.8)^{n_7}\, a'_7$$

$$a_8 = 0.50793 \cdot 10^{-8}(1.8)^{n_8}\, a'_8$$

$$a_9 = 0.26299 \cdot 10^{-10}(1.8)^{n_9}\, a'_9$$

$$a_{10} = 0.23025 \cdot 10^{-10}(1.8)^{n_{10}}\, a'_{10}$$

$$a_{11} = 0.31997 \cdot 10^{-9}(1.8)^{n_{11}}\, a'_{11}$$

$$a_{12} = 0.20158 \cdot 10^{-10}(1.8)^{n_{12}}\, a'_{12}$$

$$a_{13} = 0.33623 \cdot 10^{-4}(1.8)^{n_{13}}\, a'_{13}$$

$$a_{14} = 0.17871 \cdot 10^{-4}(1.8)^{n_{14}}\, a'_{14}$$

$$a_{15} = 0.25828 \cdot 10^{-4}(1.8)^{n_{15}}\, a'_{15}$$

$$a_{16} = 0.46717 \cdot 10^{-3}(1.8)^{n_{16}}\, a'_{16}$$

$$a_{17} = 0.55375 \cdot 10^{-4}(1.8)^{n_{17}}\, a'_{17}$$

$$a_{18} = 0.30302 \cdot 10^{-4}(1.8)^{n_{18}}\, a'_{18}$$

$$a_{19} = 0.78412 \cdot 10^{-4}(1.8)^{n_{19}}\, a'_{19}$$

$$a_{20} = 0.44443 \cdot 10^{-4}(1.8)^{n_{20}}\, a'_{20}$$

$$a_{21} = 0.25982 \cdot 10^{-4}(1.8)^{n_{21}}\, a'_{21}$$

$$a_{22} = 0.41676 \cdot 10^{-4}(1.8)^{n_{22}}\, a'_{22}$$

$$a_{23} = 0.22409 \cdot 10^{-3}(1.8)^{n_{23}}\, a'_{23}$$

$$a_{24} = 0.11205 \cdot 10^{-3}(1.8)^{n_{24}}\, a'_{24}$$

$$a_{25} = 0.26562 \cdot 10^{-4}(1.8)^{n_{25}}\, a'_{25}$$

$$a_{26} = 0.23120 \cdot 10^{-4}(1.8)^{n_{26}}\, a'_{26}$$

$$a_{27} = 0.41819 \cdot 10^{-3}(1.8)^{n_{27}}\, a'_{27}$$

$$a_{28} = 0.41819 \cdot 10^{-3}(1.8)^{n_{28}}\, a'_{28}$$

$$a_{29} = 0.20909 \cdot 10^{-3}(1.8)^{n_{29}}\, a'_{29}$$

$$a_{30} = 0.49569 \cdot 10^{-4}(1.8)^{n_{30}}\, a'_{30}$$

$$a_{31} = 0.46796 \cdot 10^{-4}(1.8)^{n_{31}}\, a'_{31}$$

$$a_{32} = 0.43579 \cdot 10^{-3}(1.8)^{n_{32}}\, a'_{32}$$

$$a_{33} = 0.93434 \cdot 10^{-3}(1.8)^{n_{33}}\, a'_{33}$$

$$a_{34} = 0.55375 \cdot 10^{-4}(1.8)^{n_{34}}\, a'_{34}$$

$$a_{35} = 0.38107 \cdot 10^{-4}(1.8)^{n_{35}}\, a'_{35}$$

$$a_{36} = 0.17789 \cdot 10^{-4}(1.8)^{n_{36}}\, a'_{36}$$

$$a_{37} = 0.67234 \cdot 10^{-4}(1.8)^{n_{37}}\, a'_{37}$$

$$a_{38} = 0.35735 \cdot 10^{-4}(1.8)^{n_{38}}\, a'_{38}$$

$$a_{39} = 0.58863 \cdot 10^{-4}(1.8)^{n_{39}}\, a'_{39}$$

$$a_{40} = 0.11955 \cdot 10^{-10}(1.8)^{n_{40}}\, a'_{40}$$

$$a_{41} = 0.44503 \cdot 10^{-11}(1.8)^{n_{41}}\, a'_{41}$$

$$a_{42} = 0.53945 \cdot 10^{-10}(1.8)^{n_{42}}\, a'_{42}$$

$$a_{43} = 0.23310 \cdot 10^{-11}(1.8)^{n_{43}}\, a'_{43}$$

$a_{44} = 0.33882 \cdot 10^{-11}(1.8)^{n_{44}} a'_{44}$

$a_{45} = 0.51657 \cdot 10^{-10}(1.8)^{n_{45}} a'_{45}$

$a_{46} = 0.10067 \cdot 10^{-10}(1.8)^{n_{46}} a'_{46}$

$a_{47} = 0.59070 \cdot 10^{-10}(1.8)^{n_{47}} a'_{47}$

$a_{48} = 0.63194 \cdot 10^{-10}(1.8)^{n_{48}} a'_{48}$

$a_{49} = 0.70146 \cdot 10^{-10}(1.8)^{n_{49}} a'_{49}$

$a_{50} = 0.13305 \cdot 10^{-4}(1.8)^{n_{50}} a'_{50}$

$a_{51} = 0.31029 \cdot 10^{-4}(1.8)^{n_{51}} a'_{51}$

$a_{52} = 0.26606 \cdot 10^{-4}(1.8)^{n_{52}} a'_{52}$

$a_{53} = 0.23293 \cdot 10^{-4}(1.8)^{n_{53}} a'_{53}$

$a_{54} = 0.64575 \cdot 10^{-5}(1.8)^{n_{54}} a'_{54}$

$a_{55} = 0.59690 \cdot 10^{-5}(1.8)^{n_{55}} a'_{55}$

$a_{56} = 0.12051 \cdot 10^{-4}(1.8)^{n_{56}} a'_{56}$

$a_{57} = 0.20483 \cdot 10^{-4}(1.8)^{n_{57}} a'_{57}$

$a_{58} = 0.21773 \cdot 10^{-4}(1.8)^{n_{58}} a'_{58}$

$a_{59} = 0.34908 \cdot 10^{-4}(1.8)^{n_{59}} a'_{59}$

$a_{60} = 0.12051 \cdot 10^{-4}(1.8)^{n_{60}} a'_{60}$

$a_{61} = 0.95791 \cdot 10^{-5}(1.8)^{n_{61}} a'_{61}$

$a_{62} = 0.59690 \cdot 10^{-5}(1.8)^{n_{62}} a'_{62}$

$a_{63} = 0.96713 \cdot 10^{-5}(1.8)^{n_{63}} a'_{63}$

$a_{64} = 0.17003 \cdot 10^{-4}(1.8)^{n_{64}} a'_{64}$

$a_{65} = 0.16233 \cdot 10^{-3}(1.8)^{n_{65}} a'_{65}$

$a_{66} = 0.14508 \cdot 10^{-4}(1.8)^{n_{66}} a'_{66}$

$a_{67} = 0.10221 \cdot 10^{-4}(1.8)^{n_{67}} a'_{67}$

$a_{68} = 0.83690 \cdot 10^{-5}(1.8)^{n_{68}} a'_{68}$

$a_{69} = 0.16282 \cdot 10^{-4}(1.8)^{n_{69}} a'_{69}$

$a_{70} = 0.10511 \cdot 10^{-4}(1.8)^{n_{70}} a'_{70}$

$a_{71} = 0.60648 \cdot 10^{-5}(1.8)^{n_{71}} a'_{71}$

$a_{72} = 0.32287 \cdot 10^{-5}(1.8)^{n_{72}} a'_{72}$

$a_{73} = 0.38070 \cdot 10^{-5}(1.8)^{n_{73}} a'_{73}$

$a_{74} = 0.44415 \cdot 10^{-5}(1.8)^{n_{74}} a'_{74}$

$a_{75} = 0.36178 \cdot 10^{-5}(1.8)^{n_{75}} a'_{75}$

$a_{76} = 0.58292 \cdot 10^{-5}(1.8)^{n_{76}} a'_{76}$

$a_{77} = 0.96211 \cdot 10^{-5}(1.8)^{n_{77}} a'_{77}$

$a_{78} = 0.52556 \cdot 10^{-5}(1.8)^{n_{78}} a'_{78}$

$a_{79} = 0.10227 \cdot 10^{-4}(1.8)^{n_{79}} a'_{79}$

$$a_{80} = 0.10221 \cdot 10^{-4}(1.8)^{n_{80}}\, a'_{80}$$

$$a_{81} = 0.15084 \cdot 10^{-4}(1.8)^{n_{81}}\, a'_{81}$$

$$a_{82} = 0.80172 \cdot 10^{-5}(1.8)^{n_{82}}\, a'_{82}$$

$$a_{83} = 0.91368 \cdot 10^{-5}(1.8)^{n_{83}}\, a'_{83}$$

$$a_{84} = 0.12823 \cdot 10^{-4}(1.8)^{n_{84}}\, a'_{84}$$

$$a_{85} = 0.24455 \cdot 10^{-3}(1.8)^{n_{85}}\, a'_{85}$$

$$a_{86} = 0.18450 \cdot 10^{-4}(1.8)^{n_{86}}\, a'_{86}$$

$$a_{87} = 0.13503 \cdot 10^{-4}(1.8)^{n_{87}}\, a'_{87}$$

$$a_{88} = 0.15624 \cdot 10^{-4}(1.8)^{n_{88}}\, a'_{88}$$

$$a_{89} = 0.29673 \cdot 10^{-4}(1.8)^{n_{89}}\, a'_{89}$$

$$a_{90} = 0.57355 \cdot 10^{-5}(1.8)^{n_{90}}\, a'_{90}$$

$$a_{91} = 0.91678 \cdot 10^{-5}(1.8)^{n_{91}}\, a'_{91}$$

$$a_{92} = 0.10207 \cdot 10^{-4}(1.8)^{n_{92}}\, a'_{92}$$

$$a_{93} = 0.14493 \cdot 10^{-4}(1.8)^{n_{93}}\, a'_{93}$$

$$a_{94} = 0.10748 \cdot 10^{-4}(1.8)^{n_{94}}\, a'_{94}$$

$$a_{95} = 0.98076 \cdot 10^{-5}(1.8)^{n_{95}}\, a'_{95}$$

$$a_{96} = 0.15407 \cdot 10^{-4}(1.8)^{n_{96}}\, a'_{96}$$

$$a_{97} = 0.18627 \cdot 10^{-4}(1.8)^{n_{97}}\, a'_{97}$$

$$a_{98} = 0.20483 \cdot 10^{-4}(1.8)^{n_{98}}\, a'_{98}$$

$$a_{99} = 0.10887 \cdot 10^{-4}(1.8)^{n_{99}}\, a'_{99}$$

$$a_{100} = 0.32728 \cdot 10^{-11}(1.8)^{n_{100}}\, a'_{100}$$

$$a_{101} = 0.96958 \cdot 10^{-10}(1.8)^{n_{101}}\, a'_{101}$$

$$a_{102} = 0.33665 \cdot 10^{-11}(1.8)^{n_{102}}\, a'_{102}$$

$$a_{103} = 0.20468 \cdot 10^{-9}(1.8)^{n_{103}}\, a'_{103}$$

$$a_{104} = 0.16149 \cdot 10^{-10}(1.8)^{n_{104}}\, a'_{104}$$

$$a_{105} = 0.30135 \cdot 10^{-10}(1.8)^{n_{105}}\, a'_{105}$$

$$a_{106} = 0.35786 \cdot 10^{-10}(1.8)^{n_{106}}\, a'_{106}$$

$$a_{107} = 0.22891 \cdot 10^{-10}(1.8)^{n_{107}}\, a'_{107}$$

$$a_{108} = 0.11660 \cdot 10^{-10}(1.8)^{n_{108}}\, a'_{108}$$

$$a_{109} = 0.20412 \cdot 10^{-4}(1.8)^{n_{109}}\, a'_{109}$$

$$a_{110} = 0.36195 \cdot 10^{-4}(1.8)^{n_{110}}\, a'_{110}$$

$$a_{111} = 0.40382 \cdot 10^{-4}(1.8)^{n_{111}}\, a'_{111}$$

$$a_{112} = 0.21179 \cdot 10^{-4}(1.8)^{n_{112}}\, a'_{112}$$

$$a_{113} = 0.32399 \cdot 10^{-4}(1.8)^{n_{113}}\, a'_{113}$$

$$a_{114} = 0.63448 \cdot 10^{-4}(1.8)^{n_{114}}\, a'_{114}$$

$$a_{115} = 0.22513 \cdot 10^{-4}(1.8)^{n_{115}}\, a'_{115}$$

$$a_{116} = 0.10449 \cdot 10^{-3}(1.8)^{n_{116}} a'_{116}$$

$$a_{117} = 0.59226 \cdot 10^{-4}(1.8)^{n_{117}} a'_{117}$$

$$a_{118} = 0.55538 \cdot 10^{-4}(1.8)^{n_{118}} a'_{118}$$

$$a_{119} = 0.24777 \cdot 10^{-4}(1.8)^{n_{119}} a'_{119}$$

$$a_{120} = 0.23658 \cdot 10^{-4}(1.8)^{n_{120}} a'_{120}$$

$$a_{121} = 0.13843 \cdot 10^{-4}(1.8)^{n_{121}} a'_{121}$$

$$a_{122} = 0.21975 \cdot 10^{-4}(1.8)^{n_{122}} a'_{122}$$

$$a_{123} = 0.24611 \cdot 10^{-4}(1.8)^{n_{123}} a'_{123}$$

$$a_{124} = 0.14401 \cdot 10^{-4}(1.8)^{n_{124}} a'_{124}$$

$$a_{125} = 0.68300 \cdot 10^{-4}(1.8)^{n_{125}} a'_{125}$$

$$a_{126} = 0.25602 \cdot 10^{-4}(1.8)^{n_{126}} a'_{126}$$

$$a_{127} = 0.41304 \cdot 10^{-4}(1.8)^{n_{127}} a'_{127}$$

$$a_{128} = 0.17562 \cdot 10^{-4}(1.8)^{n_{128}} a'_{128}$$

$$a_{129} = 0.21179 \cdot 10^{-4}(1.8)^{n_{129}} a'_{129}$$

$$a_{130} = 0.98648 \cdot 10^{-4}(1.8)^{n_{130}} a'_{130}$$

$$a_{131} = 0.31766 \cdot 10^{-3}(1.8)^{n_{131}} a'_{131}$$

$$a_{132} = 0.37653 \cdot 10^{-4}(1.8)^{n_{132}} a'_{132}$$

$$a_{133} = 0.22236 \cdot 10^{-4}(1.8)^{n_{133}} a'_{133}$$

$$a_{134} = 0.16882 \cdot 10^{-4}(1.8)^{n_{134}} a'_{134}$$

$$a_{135} = 0.19883 \cdot 10^{-3}(1.8)^{n_{135}} a'_{135}$$

$$a_{136} = 0.25062 \cdot 10^{-4}(1.8)^{n_{136}} a'_{136}$$

$$a_{137} = 0.48738 \cdot 10^{-4}(1.8)^{n_{137}} a'_{137}$$

$$a_{138} = 0.30768 \cdot 10^{-4}(1.8)^{n_{138}} a'_{138}$$

$$a_{139} = 0.18003 \cdot 10^{-4}(1.8)^{n_{139}} a'_{139}$$

$$a_{140} = 0.32008 \cdot 10^{-4}(1.8)^{n_{140}} a'_{140}$$

$$a_{141} = 0.32399 \cdot 10^{-4}(1.8)^{n_{141}} a'_{141}$$

$$a_{142} = 0.18958 \cdot 10^{-4}(1.8)^{n_{142}} a'_{142}$$

$$a_{143} = 0.46770 \cdot 10^{-4}(1.8)^{n_{143}} a'_{143}$$

$$a_{144} = 0.88826 \cdot 10^{-4}(1.8)^{n_{144}} a'_{144}$$

$$a_{145} = 0.33705 \cdot 10^{-4}(1.8)^{n_{145}} a'_{145}$$

$$a_{146} = 0.28579 \cdot 10^{-4}(1.8)^{n_{146}} a'_{146}$$

$$a_{147} = 0.34169 \cdot 10^{-4}(1.8)^{n_{147}} a'_{147}$$

$$a_{148} = 0.34038 \cdot 10^{-10}(1.8)^{n_{148}} a'_{148}$$

$$a_{149} = 0.29809 \cdot 10^{-10}(1.8)^{n_{149}} a'_{149}$$

$$a_{150} = 0.12026 \cdot 10^{-10}(1.8)^{n_{150}} a'_{150}$$

$$a_{151} = 0.13459 \cdot 10^{-10}(1.8)^{n_{151}} a'_{151}$$

$a_{152} = 0.31450 \cdot 10^{-11}(1.8)^{n_{152}} a'_{152}$

$a_{153} = 0.17807 \cdot 10^{-11}(1.8)^{n_{153}} a'_{153}$

$a_{154} = 0.69696 \cdot 10^{-10}(1.8)^{n_{154}} a'_{154}$

$a_{155} = 0.25102 \cdot 10^{-10}(1.8)^{n_{155}} a'_{155}$

$a_{156} = 0.91082 \cdot 10^{-11}(1.8)^{n_{156}} a'_{156}$

$a_{157} = 0.55634 \cdot 10^{-10}(1.8)^{n_{157}} a'_{157}$

$a_{158} = 0.10127 \cdot 10^{-10}(1.8)^{n_{158}} a'_{158}$

$a_{159} = 0.10816 \cdot 10^{-10}(1.8)^{n_{159}} a'_{159}$

$a_{160} = 0.46057 \cdot 10^{-4}(1.8)^{n_{160}} a'_{160}$

$a_{161} = 0.40324 \cdot 10^{-4}(1.8)^{n_{161}} a'_{161}$

$a_{162} = 0.42637 \cdot 10^{-4}(1.8)^{n_{162}} a'_{162}$

$a_{163} = 0.21318 \cdot 10^{-4}(1.8)^{n_{163}} a'_{163}$

$a_{164} = 0.34574 \cdot 10^{-4}(1.8)^{n_{164}} a'_{164}$

$a_{165} = 0.13355 \cdot 10^{-4}(1.8)^{n_{165}} a'_{165}$

$a_{166} = 0.33637 \cdot 10^{-4}(1.8)^{n_{166}} a'_{166}$

$a_{167} = 0.31145 \cdot 10^{-4}(1.8)^{n_{167}} a'_{167}$

$a_{168} = 0.20351 \cdot 10^{-4}(1.8)^{n_{168}} a'_{168}$

$a_{169} = 0.31583 \cdot 10^{-4}(1.8)^{n_{169}} a'_{169}$

$a_{170} = 0.20161 \cdot 10^{-4}(1.8)^{n_{170}} a'_{170}$

$a_{171} = 0.26705 \cdot 10^{-4}(1.8)^{n_{171}} a'_{171}$

$a_{172} = 0.52851 \cdot 10^{-4}(1.8)^{n_{172}} a'_{172}$

$a_{173} = 0.21634 \cdot 10^{-4}(1.8)^{n_{173}} a'_{173}$

$a_{174} = 0.33572 \cdot 10^{-4}(1.8)^{n_{174}} a'_{174}$

$a_{175} = 0.87043 \cdot 10^{-4}(1.8)^{n_{175}} a'_{175}$

$a_{176} = 0.40324 \cdot 10^{-4}(1.8)^{n_{176}} a'_{176}$

$a_{177} = 0.46263 \cdot 10^{-4}(1.8)^{n_{177}} a'_{177}$

$a_{178} = 0.23772 \cdot 10^{-4}(1.8)^{n_{178}} a'_{178}$

$a_{179} = 0.80836 \cdot 10^{-5}(1.8)^{n_{179}} a'_{179}$

$a_{180} = 0.32309 \cdot 10^{-4}(1.8)^{n_{180}} a'_{180}$

$a_{181} = 0.71609 \cdot 10^{-5}(1.8)^{n_{181}} a'_{181}$

$a_{182} = 0.12545 \cdot 10^{-4}(1.8)^{n_{182}} a'_{182}$

$a_{183} = 0.20555 \cdot 10^{-4}(1.8)^{n_{183}} a'_{183}$

$a_{184} = 0.16075 \cdot 10^{-4}(1.8)^{n_{184}} a'_{184}$

$a_{185} = 0.35116 \cdot 10^{-4}(1.8)^{n_{185}} a'_{185}$

$a_{186} = 0.18664 \cdot 10^{-4}(1.8)^{n_{186}} a'_{186}$

$a_{187} = 0.18113 \cdot 10^{-4}(1.8)^{n_{187}} a'_{187}$

$$a_{188} = 0.20877 \cdot 10^{-4}(1.8)^{n_{188}} a'_{188}$$
$$a_{189} = 0.40598 \cdot 10^{-4}(1.8)^{n_{189}} a'_{189}$$
$$a_{190} = 0.18196 \cdot 10^{-4}(1.8)^{n_{190}} a'_{190}$$
$$a_{191} = 0.86254 \cdot 10^{-5}(1.8)^{n_{191}} a'_{191}$$
$$a_{192} = 0.48811 \cdot 10^{-5}(1.8)^{n_{192}} a'_{192}$$
$$a_{193} = 0.27637 \cdot 10^{-5}(1.8)^{n_{193}} a'_{193}$$
$$a_{194} = 0.11523 \cdot 10^{-4}(1.8)^{n_{194}} a'_{194}$$
$$a_{195} = 0.10259 \cdot 10^{-4}(1.8)^{n_{195}} a'_{195}$$
$$a_{196} = 0.84222 \cdot 10^{-5}(1.8)^{n_{196}} a'_{196}$$
$$a_{197} = 0.12249 \cdot 10^{-4}(1.8)^{n_{197}} a'_{197}$$
$$a_{198} = 0.16379 \cdot 10^{-4}(1.8)^{n_{198}} a'_{198}$$
$$a_{199} = 0.20351 \cdot 10^{-4}(1.8)^{n_{199}} a'_{199}$$
$$a_{200} = 0.11535 \cdot 10^{-4}(1.8)^{n_{200}} a'_{200}$$
$$a_{201} = 0.51993 \cdot 10^{-5}(1.8)^{n_{201}} a'_{201}$$
$$a_{202} = 0.30324 \cdot 10^{-4}(1.8)^{n_{202}} a'_{202}$$
$$a_{203} = 0.12481 \cdot 10^{-4}(1.8)^{n_{203}} a'_{203}$$
$$a_{204} = 0.29106 \cdot 10^{-4}(1.8)^{n_{204}} a'_{204}$$
$$a_{205} = 0.17300 \cdot 10^{-4}(1.8)^{n_{205}} a'_{205}$$
$$a_{206} = 0.32550 \cdot 10^{-3}(1.8)^{n_{206}} a'_{206}$$
$$a_{207} = 0.18218 \cdot 10^{-4}(1.8)^{n_{207}} a'_{207}$$
$$a_{208} = 0.38959 \cdot 10^{-4}(1.8)^{n_{208}} a'_{208}$$
$$a_{209} = 0.73992 \cdot 10^{-4}(1.8)^{n_{209}} a'_{209}$$
$$a_{210} = 0.33956 \cdot 10^{-4}(1.8)^{n_{210}} a'_{210}$$
$$a_{211} = 0.21829 \cdot 10^{-4}(1.8)^{n_{211}} a'_{211}$$
$$a_{212} = 0.12239 \cdot 10^{-4}(1.8)^{n_{212}} a'_{212}$$
$$a_{213} = 0.14136 \cdot 10^{-4}(1.8)^{n_{213}} a'_{213}$$
$$a_{214} = 0.86345 \cdot 10^{-5}(1.8)^{n_{214}} a'_{214}$$
$$a_{215} = 0.16399 \cdot 10^{-4}(1.8)^{n_{215}} a'_{215}$$
$$a_{216} = 0.76625 \cdot 10^{-5}(1.8)^{n_{216}} a'_{216}$$
$$a_{217} = 0.12856 \cdot 10^{-4}(1.8)^{n_{217}} a'_{217}$$
$$a_{218} = 0.19292 \cdot 10^{-4}(1.8)^{n_{218}} a'_{218}$$
$$a_{219} = 0.13537 \cdot 10^{-4}(1.8)^{n_{219}} a'_{219}$$
$$a_{220} = 0.15718 \cdot 10^{-4}(1.8)^{n_{220}} a'_{220}$$
$$a_{221} = 0.20506 \cdot 10^{-4}(1.8)^{n_{221}} a'_{221}$$
$$a_{222} = 0.29850 \cdot 10^{-4}(1.8)^{n_{222}} a'_{222}$$
$$a_{223} = 0.31583 \cdot 10^{-4}(1.8)^{n_{223}} a'_{223}$$

$a_{224} = 0.19689 \cdot 10^{-4}(1.8)^{n_{224}} a'_{224}$

$a_{225} = 0.43720 \cdot 10^{-10}(1.8)^{n_{225}} a'_{225}$

$a_{226} = 0.22317 \cdot 10^{-9}(1.8)^{n_{226}} a'_{226}$

$a_{227} = 0.20971 \cdot 10^{-10}(1.8)^{n_{227}} a'_{227}$

$a_{228} = 0.39136 \cdot 10^{-10}(1.8)^{n_{228}} a'_{228}$

$a_{229} = 0.73769 \cdot 10^{-9}(1.8)^{n_{229}} a'_{229}$

$a_{230} = 0.46475 \cdot 10^{-10}(1.8)^{n_{230}} a'_{230}$

$a_{231} = 0.32415 \cdot 10^{-10}(1.8)^{n_{231}} a'_{231}$

$a_{232} = 0.76692 \cdot 10^{-10}(1.8)^{n_{232}} a'_{232}$

$a_{233} = 0.28758 \cdot 10^{-11}(1.8)^{n_{233}} a'_{233}$

$a_{234} = 0.11850 \cdot 10^{-5}(1.8)^{n_{234}} a'_{234}$

$a_{235} = 0.66358 \cdot 10^{-3}(1.8)^{n_{235}} a'_{235}$

$a_{236} = 0.58136 \cdot 10^{-4}(1.8)^{n_{236}} a'_{236}$

$a_{237} = 0.10607 \cdot 10^{-3}(1.8)^{n_{237}} a'_{237}$

$a_{238} = 0.19993 \cdot 10^{-2}(1.8)^{n_{238}} a'_{238}$

$a_{239} = 0.12596 \cdot 10^{-3}(1.8)^{n_{239}} a'_{239}$

$a_{240} = 0.69272 \cdot 10^{-3}(1.8)^{n_{240}} a'_{240}$

$a_{241} = 0.43642 \cdot 10^{-4}(1.8)^{n_{241}} a'_{241}$

$a_{242} = 0.87854 \cdot 10^{-4}(1.8)^{n_{242}} a'_{242}$

$a_{243} = 0.53183 \cdot 10^{-3}(1.8)^{n_{243}} a'_{243}$

$a_{244} = 0.63299 \cdot 10^{-4}(1.8)^{n_{244}} a'_{244}$

$a_{245} = 0.52445 \cdot 10^{-4}(1.8)^{n_{245}} a'_{245}$

$a_{246} = 0.18864 \cdot 10^{-4}(1.8)^{n_{246}} a'_{246}$

$a_{247} = 0.35204 \cdot 10^{-4}(1.8)^{n_{247}} a'_{247}$

$a_{248} = 0.11849 \cdot 10^{-4}(1.8)^{n_{248}} a'_{248}$

$a_{249} = 0.62981 \cdot 10^{-4}(1.8)^{n_{249}} a'_{249}$

$a_{250} = 0.76920 \cdot 10^{-4}(1.8)^{n_{250}} a'_{250}$

$a_{251} = 0.31520 \cdot 10^{-4}(1.8)^{n_{251}} a'_{251}$

$a_{252} = 0.28216 \cdot 10^{-4}(1.8)^{n_{252}} a'_{252}$

$a_{253} = 0.27931 \cdot 10^{-4}(1.8)^{n_{253}} a'_{253}$

$a_{254} = 0.25785 \cdot 10^{-4}(1.8)^{n_{254}} a'_{254}$

$a_{255} = 0.84158 \cdot 10^{-4}(1.8)^{n_{255}} a'_{255}$

$a_{256} = 0.78992 \cdot 10^{-4}(1.8)^{n_{256}} a'_{256}$

$a_{257} = 0.30439 \cdot 10^{-4}(1.8)^{n_{257}} a'_{257}$

$a_{258} = 0.20972 \cdot 10^{-4}(1.8)^{n_{258}} a'_{258}$

$a_{259} = 0.11187 \cdot 10^{-4}(1.8)^{n_{259}} a'_{259}$

$$a_{260} = 0.38729 \cdot 10^{-4}(1.8)^{n_{260}} a'_{260}$$

$$a_{261} = 0.22214 \cdot 10^{-4}(1.8)^{n_{261}} a'_{261}$$

$$a_{262} = 0.11849 \cdot 10^{-3}(1.8)^{n_{262}} a'_{262}$$

$$a_{263} = 0.34637 \cdot 10^{-3}(1.8)^{n_{263}} a'_{263}$$

$$a_{264} = 0.41056 \cdot 10^{-4}(1.8)^{n_{264}} a'_{264}$$

$$a_{265} = 0.14701 \cdot 10^{-4}(1.8)^{n_{265}} a'_{265}$$

$$a_{266} = 0.33431 \cdot 10^{-4}(1.8)^{n_{266}} a'_{266}$$

$$a_{267} = 0.53037 \cdot 10^{-4}(1.8)^{n_{267}} a'_{267}$$

$$a_{268} = 0.10073 \cdot 10^{-4}(1.8)^{n_{268}} a'_{268}$$

$$a_{269} = 0.35205 \cdot 10^{-4}(1.8)^{n_{269}} a'_{269}$$

$$a_{270} = 0.34900 \cdot 10^{-4}(1.8)^{n_{270}} a'_{270}$$

$$a_{271} = 0.19885 \cdot 10^{-4}(1.8)^{n_{271}} a'_{271}$$

$$a_{272} = 0.60740 \cdot 10^{-4}(1.8)^{n_{272}} a'_{272}$$

$$a_{273} = 0.11537 \cdot 10^{-3}(1.8)^{n_{273}} a'_{273}$$

$$a_{274} = 0.10607 \cdot 10^{-3}(1.8)^{n_{274}} a'_{274}$$

$$a_{275} = 0.36752 \cdot 10^{-4}(1.8)^{n_{275}} a'_{275}$$

$$a_{276} = 0.25423 \cdot 10^{-4}(1.8)^{n_{276}} a'_{276}$$

$$a_{277} = 0.16935 \cdot 10^{-4}(1.8)^{n_{277}} a'_{277}$$

$$a_{278} = 0.55270 \cdot 10^{-4}(1.8)^{n_{278}} a'_{278}$$

$$a_{279} = 0.19149 \cdot 10^{-4}(1.8)^{n_{279}} a'_{279}$$

$$a_{280} = 0.32549 \cdot 10^{-4}(1.8)^{n_{280}} a'_{280}$$

$$a_{281} = 0.63299 \cdot 10^{-4}(1.8)^{n_{281}} a'_{281}$$

$$a_{282} = 0.56841 \cdot 10^{-4}(1.8)^{n_{282}} a'_{282}$$

$$a_{283} = 0.19694 \cdot 10^{-4}(1.8)^{n_{283}} a'_{283}$$

$$a_{284} = 0.15119 \cdot 10^{-4}(1.8)^{n_{284}} a'_{284}$$

The reaction rate parameters $m_{i,j}$ are input and converted to the required units. The converted reaction rate parameters are calculated from the following relationships:

$$m_{i,1} = \frac{m'_{i,1}}{44.011}$$

$$m_{i,2} = \frac{m'_{i,2}}{18.016}$$

$$m_{i,3} = \frac{m'_{i,3}}{28.011}$$

$$m_{i,4} = \frac{m'_{i,4}}{70.914}$$

$$m_{i,5} = \frac{m'_{i,5}}{38.0}$$

$$m_{i,6} = \frac{m'_{i,6}}{36.465}$$

$$m_{i,7} = \frac{m'_{i,7}}{20.008}$$

$$m_{i,8} = \frac{m'_{i,8}}{2.016}$$

$$m_{i,9} = \frac{m'_{i,9}}{28.016}$$

$$m_{i,10} = \frac{m'_{i,10}}{30.008}$$

$$m_{i,11} = \frac{m'_{i,11}}{17.008}$$

$$m_{i,12} = \frac{m'_{i,12}}{32.000}$$

$$m_{i,13} = \frac{m'_{i,13}}{12.011}$$

$$m_{i,14} = \frac{m'_{i,14}}{35.457}$$

$$m_{i,15} = \frac{m'_{i,15}}{19.000}$$

$$m_{i,16} = \frac{m'_{i,16}}{1.008}$$

$$m_{i,17} = \frac{m'_{i,17}}{14.008}$$

$$m_{i,18} = \frac{m'_{i,18}}{16.000}$$

$$m_{i,19} = \frac{m'_{i,19}}{26.980}$$

$$m_{i,20} = \frac{m'_{i,20}}{42.980}$$

$$m_{i,21} = \frac{m'_{i,21}}{69.960}$$

$$m_{i,22} = \frac{m'_{i,22}}{62.437}$$

$$m_{i,23} = \frac{m'_{i,23}}{97.894}$$

$$m_{i,24} = \frac{m'_{i,24}}{78.437}$$

$$m_{i,25} = \frac{m'_{i,25}}{45.980}$$

$$m_{i,26} = \frac{m'_{i,26}}{64.980}$$

$$m_{i,27} = \frac{m'_{i,27}}{61.980}$$

$$m_{i,28} = \frac{m'_{i,28}}{10.820}$$

$$m_{i,29} = \frac{m'_{i,29}}{24.828}$$

$$m_{i,30} = \frac{m'_{i,30}}{26.820}$$

$$m_{i,31} = \frac{m'_{i,31}}{42.820}$$

$$m_{i,32} = \frac{m'_{i,32}}{46.277}$$

$$m_{i,33} = \frac{m'_{i,33}}{81.734}$$

$$m_{i,34} = \frac{m'_{i,34}}{117.191}$$

$$m_{i,35} = \frac{m'_{i,35}}{62.277}$$

$$m_{i,36} = \frac{m'_{i,36}}{29.820}$$

$$m_{i,37} = \frac{m'_{i,37}}{48.820}$$

$$m_{i,38} = \frac{m'_{i,38}}{67.820}$$

$$m_{i,39} = \frac{m'_{i,39}}{45.820}$$

$$m_{i,40} = \frac{m'_{i,40}}{9.013}$$

$$m_{i,41} = \frac{m'_{i,41}}{25.013}$$

$$m_{i,42} = \frac{m'_{i,42}}{34.026}$$

$$m_{i,43} = \frac{m'_{i,43}}{26.021}$$

$$m_{i,44} = \frac{m'_{i,44}}{44.470}$$

$$m_{i,45} = \frac{m'_{i,45}}{79.927}$$

$$m_{i,46} = \frac{m'_{i,46}}{28.013}$$

$$m_{i,47} = \frac{m'_{i,47}}{47.013}$$

$$m_{i,48} = \frac{m'_{i,48}}{43.029}$$

$$m_{i,49} = \frac{m'_{i,49}}{6.940}$$

$$m_{i,50} = \frac{m'_{i,50}}{7.948}$$

$$m_{i,51} = \frac{m'_{i,51}}{22.940}$$

$$m_{i,52} = \frac{m'_{i,52}}{29.880}$$

$$m_{i,53} = \frac{m'_{i,53}}{23.948}$$

$$m_{i,54} = \frac{m'_{i,54}}{25.940}$$

$$m_{i,55} = \frac{m'_{i,55}}{42.397}$$

$$m_{i,56} = \frac{m'_{i,56}}{51.880}$$

$$m_{i,57} = \frac{m'_{i,57}}{84.794}$$

The index, i, indicates the dissociation-recombination reaction equation number and has the values:

$i = 1, 2, \cdots, 12, 40, 41, \cdots, 49, 100, 101, \cdots, 108, 148, 149, \cdots, 159, 225, 226, \cdots, 233.$

4.1.6 Case Data Input and Conversion

The case data are input and the chamber pressure, the initial pressure and the nozzle throat radius are converted to the required units. The converted quantities are calculated from

$$P_c = 4633.056\ P'_c$$

$$P = 4633.056\ P'$$

$$P^* = 4633.056\ P^{*\prime}$$

$$r^* = \frac{r^{*\prime}}{12}$$

If the initial species concentrations are input as mole fractions, the required mass fractions are calculated

$$c_i = \frac{1}{R_i}\ \frac{c'_{i,m}}{\bar{c}}\ , \qquad i = 1, 2, \cdots, 57$$

where

$$\bar{c} = \sum_{i=1}^{57} \frac{c'_{i,m}}{R_i}$$

The case data are output to supply a permanent case record with the nozzle integration results.

4.2 DERIVATIVE EVALUATION SUBROUTINE

Given the flow properties at a point, this subroutine calculates the derivatives (f_i) and partial derivatives (α_i and $\beta_{i,j}$) of the chemical relaxations equations and the fluid dynamic equations. These calculations are performed in the following order:

- The species free energy, enthalpy, heat capacity and the heat capacity temperature derivative are calculated using the Species Thermal Function Subroutine (described in Section 4. 4).
- The dissociation-recombination reaction equilibrium constants and their temperature derivatives are calculated using the Equilibrium Function Subroutine (described in Section 4. 5).
- The mixture gas constant, heat capacity, gamma and the partial derivatives of gamma are calculated using the Gas Thermal Function Subroutine (described in Section 4.   ).
- The contribution of the individual reactions to the net species production rate (X_j) and its partial derivatives are calculated.
- The derivatives (f_i) and partial derivatives (α_i and $\beta_{i,j}$) of the chemical relaxation equations are calculated.
- In the subsonic and transonic nozzle inlet and throat, the pressure and its derivatives are calculated from the pressure table by quadratic interpolation.
- In the supersonic nozzle expansion cone, the nozzle area and Mach number and their derivatives are calculated.
- The diabatic heat addition terms coupling the chemical relaxation equations and the fluid dynamic equations are calculated.
- The derivatives (f_i) and partial derivatives (α_i and $\beta_{i,j}$) of the fluid dynamic equations are calculated.

A detailed description of these calculations is given in the following sections.

4. 2. 1 Calculation of X_j and Its Partial Derivatives

For the reactions of interest, X_j and its derivatives are calculated from the following relationships:

Reaction 1, $CO_2 + M \rightleftharpoons CO + O + M$

$$k_1 = a_1 T^{-n_1} e^{-b_1/T}$$

$$M_1 = \sum_{i=1}^{57} m_{1,i} c_i$$

$$X_1 = \left[K_1 c_1 - \rho c_3 c_{18}\right] M_1 k_1$$

$$\frac{\partial X_1}{\partial c_j} = \frac{X_1}{M_1} m_{1,j} + \delta_{1,j} K_1 M_1 k_1 - \delta_{3,j} \rho c_{18} M_1 k_1$$

$$- \delta_{18,j} \rho c_3 M_1 k_1 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_1}{\partial \rho} = -c_3 c_{18} M_1 k_1$$

$$\frac{\partial X_1}{\partial T} = c_1 M_1 k_1 \frac{dK_1}{dT} - \left[n_1 - \frac{b_1}{T}\right] \frac{X_1}{T}$$

Reaction 2, $H_2O + M \rightleftharpoons OH + H + M$

$$k_2 = a_2 T^{-n_2} e^{-b_2/T}$$

$$M_2 = \sum_{i=1}^{57} m_{2,i} c_i$$

$$X_2 = \left[K_2 c_2 - \rho c_{11} c_{16}\right] M_2 k_2$$

$$\frac{\partial X_2}{\partial c_j} = \frac{X_2}{M_2} m_{2,j} + \delta_{2,j} K_2 M_2 k_2 - \delta_{11,j} \rho c_{16} M_2 k_2$$

$$- \delta_{16,j} \rho c_{11} M_2 k_2 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_2}{\partial \rho} = -c_{11} c_{16} M_2 k_2$$

$$\frac{\partial X_2}{\partial T} = c_2 M_2 k_2 \frac{dK_2}{dT} - \left[n_2 - \frac{b_2}{T}\right] \frac{X_2}{T}$$

Reaction 3, $CO + M \rightleftharpoons C + O + M$

$$k_3 = a_3 T^{-n_3} e^{-b_3/T}$$

$$M_3 = \sum_{i=1}^{57} m_{3,i} c_i$$

$$X_3 = \left[K_3 c_3 - \rho c_{13} c_{18}\right] M_3 k_3$$

$$\frac{\partial X_3}{\partial c_j} = \frac{X_3}{M_3} m_{3,j} + \delta_{3,j} K_3 M_3 k_3 - \delta_{13,j} \rho c_{18} M_3 k_3$$

$$-\delta_{18,j} \rho c_{13} M_3 k_3 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_3}{\partial \rho} = -c_{13} c_{18} M_3 k_3$$

$$\frac{\partial X_3}{\partial T} = c_3 M_3 k_3 \frac{dK_3}{dT} - \left[n_3 - \frac{b_3}{T}\right] \frac{X_3}{T}$$

Reaction 4, $Cl_2 + M \rightleftharpoons 2Cl + M$

$$k_4 = a_4 T^{-n_4} e^{-b_4/T}$$

$$M_4 = \sum_{i=1}^{57} m_{4,i} c_i$$

$$X_4 = \left[K_4 c_4 - \rho c_{14}^2\right] M_4 k_4$$

$$\frac{\partial X_4}{\partial c_j} = \frac{X_4}{M_4} m_{4,j} + \delta_{4,j} K_4 M_4 k_4 - 2\delta_{14,j} \rho c_{14} M_4 k_4 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_4}{\partial \rho} = -c_{14}^2 M_4 k_4$$

$$\frac{\partial X_4}{\partial T} = c_4 M_4 k_4 \frac{dK_4}{dT} - \left[n_4 - \frac{b_4}{T}\right] \frac{X_4}{T}$$

Reaction 5, $F_2 + M \rightleftharpoons 2F + M$

$$k_5 = a_5 T^{-n_5} e^{-b_5/T}$$

$$M_5 = \sum_{i=1}^{57} m_{5,i} c_i$$

$$X_5 = \left[K_5 c_5 - \rho c_{15}^2\right] M_5 k_5$$

$$\frac{\partial X_5}{\partial c_j} = \frac{X_5}{M_5} m_{5,j} + \delta_{5,j} K_5 M_5 k_5 - 2\delta_{15,j} \rho c_{15} M_5 k_5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_5}{\partial \rho} = -c_{15}^2 M_5 k_5$$

$$\frac{\partial X_5}{\partial T} = c_5 M_5 k_5 \frac{dK_5}{dT} - \left[n_5 - \frac{b_5}{T}\right] \frac{X_5}{T}$$

Reaction 6, $HCl + M \rightleftharpoons H + Cl + M$

$$k_6 = a_6 T^{-n_6} e^{-b_6/T}$$

$$M_6 = \sum_{i=1}^{57} m_{6,i} c_i$$

$$X_6 = \left[K_6 c_6 - \rho c_{14} c_{16}\right] M_6 k_6$$

$$\frac{\partial X_6}{\partial c_j} = \frac{X_6}{M_6} m_{6,j} + \delta_{6,j} K_6 M_6 k_6 - \delta_{14,j} \rho c_{16} M_6 k_6$$

$$- \delta_{16,j} \rho c_{14} M_6 k_6 \quad , \quad j = 1, 2, \ldots, 57$$

$$\frac{\partial X_6}{\partial \rho} = -c_{14}c_{16}M_6k_6$$

$$\frac{\partial X_6}{\partial T} = c_6M_6k_6\frac{dK_6}{dT} - \left[n_6 - \frac{b_6}{T}\right]\frac{X_6}{T}$$

Reaction 7, $HF + M \rightleftharpoons H + F + M$

$$k_7 = a_7T^{-n_7}e^{-b_7/T}$$

$$M_7 = \sum_{i=1}^{57} m_{7,i}c_i$$

$$X_7 = \left[K_7c_7 - \rho c_{15}c_{16}\right]M_7k_7$$

$$\frac{\partial X_7}{\partial c_j} = \frac{X_7}{M_7}m_{7,j} + \delta_{7,j}K_7M_7k_7 - \delta_{15,j}\rho c_{16}M_7k_7 - \delta_{16,j}\rho c_{15}M_7k_7, \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_7}{\partial \rho} = -c_{15}c_{16}M_7k_7$$

$$\frac{\partial X_7}{\partial T} = c_7M_7k_7\frac{dK_7}{dT} - \left[n_7 - \frac{b_7}{T}\right]\frac{X_7}{T}$$

Reaction 8, $H_2 + M \rightleftharpoons 2H + M$

$$k_8 = a_8T^{-n_8}e^{-b_8/T}$$

$$M_8 = \sum_{i=1}^{57} m_{8,i}c_i$$

$$X_8 = \left[K_8c_8 - \rho c_{16}^2\right]M_8k_8$$

$$\frac{\partial X_8}{\partial c_j} = \frac{X_8}{M_8}m_{8,j} + \delta_{8,j}K_8M_8k_8 - 2\delta_{16,j}\rho c_{16}M_8k_8, \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_8}{\partial \rho} = -c_{16}^2 M_8 k_8$$

$$\frac{\partial X_8}{\partial T} = c_8 M_8 k_8 \frac{dK_8}{dT} - \left[n_8 - \frac{b_8}{T}\right] \frac{X_8}{T}$$

Reaction 9, $N_2 + M \rightleftharpoons 2N + M$

$$k_9 = a_9 T^{-n_9} e^{-b_9/T}$$

$$M_9 = \sum_{i=1}^{57} m_{9,i} c_i$$

$$X_9 = \left[K_9 c_9 - \rho c_{17}^2\right] M_9 k_9$$

$$\frac{\partial X_9}{\partial c_j} = \frac{X_9}{M_9} m_{9,j} + \delta_{9,j} K_9 M_9 k_9 - 2\delta_{17,j} \rho c_{17} M_9 k_9 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_9}{\partial \rho} = -c_{17}^2 M_9 k_9$$

$$\frac{\partial X_9}{\partial T} = c_9 M_9 k_9 \frac{dK_9}{dT} - \left[n_9 - \frac{b_9}{T}\right] \frac{X_9}{T}$$

Reaction 10, $NO + M \rightleftharpoons N + O + M$

$$k_{10} = a_{10} T^{-n_{10}} e^{-b_{10}/T}$$

$$M_{10} = \sum_{i=1}^{57} m_{10,i} c_i$$

$$X_{10} = \left[K_{10} c_{10} - \rho c_{17} c_{18}\right] M_{10} k_{10}$$

$$\frac{\partial X_{10}}{\partial c_j} = \frac{X_{10}}{M_{10}} m_{10,j} + \delta_{10,j} K_{10} M_{10} k_{10} - \delta_{17,j} \rho c_{18} M_{10} k_{10}$$

$$- \delta_{18,j} \rho c_{17} M_{10} k_{10} \quad , \quad j = 1, 2, \ldots, 57$$

$$\frac{\partial X_{10}}{\partial \rho} = -c_{17}c_{18}M_{10}k_{10}$$

$$\frac{\partial X_{10}}{\partial T} = c_{10}M_{10}k_{10}\frac{dK_{10}}{dT} - \left[n_{10} - \frac{b_{10}}{T}\right]\frac{X_{10}}{T}$$

Reaction 11, $OH + M \rightleftharpoons O + H + M$

$$k_{11} = a_{11}T^{-n_{11}}e^{-b_{11}/T}$$

$$M_{11} = \sum_{i=1}^{57} m_{11,i}c_i$$

$$X_{11} = \left[K_{11}c_{11} - \rho c_{16}c_{18}\right]M_{11}k_{11}$$

$$\frac{\partial X_{11}}{\partial c_j} = \frac{X_{11}}{M_{11}}m_{11,j} + \delta_{11,j}K_{11}M_{11}k_{11} - \delta_{16,j}\rho c_{18}M_{11}k_{11}$$

$$- \delta_{18,j}\rho c_{16}M_{11}k_{11} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{11}}{\partial \rho} = -c_{16}c_{18}M_{11}k_{11}$$

$$\frac{\partial X_{11}}{\partial T} = c_{11}M_{11}k_{11}\frac{dK_{11}}{dT} - \left[n_{11} - \frac{b_{11}}{T}\right]\frac{X_{11}}{T}$$

Reaction 12, $O_2 + M \rightleftharpoons 2O + M$

$$k_{12} = a_{12}T^{-n_{12}}e^{-b_{12}/T}$$

$$M_{12} = \sum_{i=1}^{57} m_{12,i}c_i$$

$$X_{12} = \left[K_{12}c_{12} - \rho c_{18}^2\right]M_{12}k_{12}$$

$$\frac{\partial X_{12}}{\partial c_j} = \frac{X_{12}}{M_{12}} m_{12,j} + \delta_{12,j} K_{12} M_{12} k_{12} - 2\delta_{18,j} \rho c_{18} M_{12} k_{12} ,$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{12}}{\partial \rho} = -c_{18}^2 M_{12} k_{12}$$

$$\frac{\partial X_{12}}{\partial T} = c_{12} M_{12} k_{12} \frac{dK_{12}}{dT} - \left[n_{12} - \frac{b_{12}}{T}\right] \frac{X_{12}}{T}$$

Reaction 13, $CO_2 + H \rightleftarrows CO + OH$

$$K_{13} = \frac{K_1}{K_{11}}$$

$$k_{13} = a_{13} T^{-n_{13}} e^{-b_{13}/T}$$

$$X_{13} = \left[K_{13}' c_1 c_{16} - c_3 c_{11}\right] k_{13}$$

$$\frac{\partial X_{13}}{\partial c_j} = \left[\delta_{1,j} K_{13} c_{16} - \delta_{3,j} c_{11} - \delta_{11,j} c_3 + \delta_{16,j} K_{13} c_1\right] k_{13}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{13}}{\partial T} = \left[\frac{1}{K_1}\frac{dK_1}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{13} c_1 c_{16} k_{13} - \left[n_{13} - \frac{b_{13}}{T}\right] \frac{X_{13}}{T}$$

Reaction 14, $CO_2 + O \rightleftharpoons CO + O_2$

$$K_{14} = \frac{K_1}{K_{12}}$$

$$k_{14} = a_{14} T^{-n_{14}} e^{-b_{14}/T}$$

$$X_{14} = \left[K_{14} c_1 c_{18} - c_3 c_{12}\right] k_{14}$$

$$\frac{\partial X_{14}}{\partial c_j} = \left[\delta_{1,j} K_{14} c_{18} - \delta_{3,j} c_{12} - \delta_{12,j} c_3 + \delta_{18,j} K_{14} c_1\right] k_{14}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{14}}{\partial T} = \left[\frac{1}{K_1}\frac{dK_1}{dT} - \frac{1}{K_{12}}\frac{dK_{12}}{dT}\right] K_{14} c_1 c_{18} k_{14} - \left[n_{14} - \frac{b_{14}}{T}\right]\frac{X_{14}}{T}$$

Reaction 15, $H_2O + Cl \rightleftharpoons HCl + OH$

$$K_{15} = \frac{K_2}{K_6}$$

$$k_{15} = a_{15} T^{-n_{15}} e^{-b_{15}/T}$$

$$X_{15} = \left[K_{15} c_2 c_{14} - c_6 c_{11}\right] k_{15}$$

$$\frac{\partial X_{15}}{\partial c_j} = \left[\delta_{2,j} K_{15} c_{14} - \delta_{6,j} c_{11} - \delta_{11,j} c_6 + \delta_{14,j} K_{15} c_2\right] k_{15}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{15}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_6}\frac{dK_6}{dT}\right] K_{15} c_2 c_{14} k_{15} - \left[n_{15} - \frac{b_{15}}{T}\right]\frac{X_{15}}{T}$$

Reaction 16, $H_2O + H \rightleftharpoons H_2 + OH$

$$K_{16} = \frac{K_2}{K_8}$$

$$k_{16} = a_{16} T^{-n_{16}} e^{-b_{16}/T}$$

$$X_{16} = \left[K_{16} c_2 c_{16} - c_8 c_{11}\right] k_{16}$$

$$\frac{\partial X_{16}}{\partial c_j} = \left[\delta_{2,j} K_{16} c_{16} - \delta_{8,j} c_{11} - \delta_{11,j} c_8 + \delta_{16,j} K_{16} c_2\right] k_{16}$$

$$j = 1, 2, \cdots, 57 .$$

$$\frac{\partial X_{16}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_8}\frac{dK_8}{dT}\right] K_{16} c_2 c_{16} k_{16} - \left[n_{16} - \frac{b_{16}}{T}\right]\frac{X_{16}}{T}$$

Reaction 17, $H_2O + O \rightleftharpoons 2OH$

$$K_{17} = \frac{K_2}{K_{11}}$$

$$k_{17} = a_{17} T^{-n_{17}} e^{-b_{17}/T}$$

$$X_{17} = \left[K_{17} c_2 c_{18} - c_{11}^2\right] k_{17}$$

$$\frac{\partial X_{17}}{\partial c_j} = \left[\delta_{2,j} K_{17} c_{18} - 2\delta_{11,j} c_{11} + \delta_{18,j} K_{17} c_2\right] k_{17}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{17}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{17} c_2 c_{18} k_{17} - \left[n_{17} - \frac{b_{17}}{T}\right]\frac{X_{17}}{T}$$

Reaction 18, $2CO \rightleftharpoons CO_2 + C$

$$K_{18} = \frac{K_3}{K_1}$$

$$k_{19} = a_{18} T^{-n_{18}} e^{-b_{18}/T}$$

$$X_{18} = \left[K_{18} c_3^{\,2} - c_1 c_{13}\right] k_{18}$$

$$\frac{\partial X_{18}}{\delta c_j} = \left[-\delta_{1,j} c_{13} + 2\delta_{3,j} K_{18} c_3 - \delta_{13,j} c_1\right] k_{18}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{18}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_1}\frac{dK_1}{dT}\right] K_{18} c_3^{\,2} k_{18} - \left[n_{18} - \frac{b_{18}}{T}\right]\frac{X_{18}}{T}$$

Reaction 19, $CO + H \rightleftharpoons OH + C$

$$K_{19} = \frac{K_3}{K_{11}}$$

$$k_{19} = a_{19} T^{-n_{19}} e^{-b_{19}/T}$$

$$X_{19} = \left[K_{19} c_3 c_{16} - c_{11} c_{13}\right] k_{19}$$

$$\frac{\partial X_{19}}{\partial c_j} = \left[\delta_{3,j} K_{19} c_{16} - \delta_{11,j} c_{13} - \delta_{13,j} c_{11} + \delta_{16,j} K_{19} c_3\right] k_{19}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{19}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{19} c_3 c_{16} k_{19} - \left[n_{19} - \frac{b_{19}}{T}\right]\frac{X_{19}}{T}$$

Reaction 20, $CO + N \rightleftharpoons NO + C$

$$K_{20} = \frac{K_3}{K_{10}}$$

$$k_{20} = a_{20} T^{-n_{20}} e^{-b_{20}/T}$$

$$X_{20} = \left[K_{20} c_3 c_{17} - c_{10} c_{13}\right] k_{20}$$

$$\frac{\partial X_{20}}{\partial c_j} = \left[\delta_{3,j} K_{20} c_{17} - \delta_{10,j} c_{13} - \delta_{13,j} c_{10} + \delta_{17,j} K_{20} c_3\right] k_{20}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{20}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_{10}}\frac{dK_{10}}{dT}\right] K_{20} c_3 c_{17} k_{20} - \left[n_{20} - \frac{b_{20}}{T}\right] \frac{X_{20}}{T}$$

Reaction 21, $CO + NO \rightleftharpoons CO_2 + N$

$$K_{21} = \frac{K_{10}}{K_1}$$

$$k_{21} = a_{21} T^{-n_{21}} e^{-b_{21}/T}$$

$$X_{21} = \left[K_{21} c_3 c_{10} - c_1 c_{17}\right] k_{21}$$

$$\frac{\partial X_{21}}{\partial c_j} = \left[-\delta_{1,j} c_{17} + \delta_{3,j} K_{21} c_{10} + \delta_{10,j} K_{21} c_3 - \delta_{17,j} c_1\right] k_{21}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{21}}{\partial T} = \left[\frac{1}{K_{10}}\frac{dK_{10}}{dT} - \frac{1}{K_1}\frac{dK_1}{dT}\right] K_{21} c_3 c_{10} k_{21} - \left[n_{21} - \frac{b_{21}}{T}\right] \frac{X_{21}}{T}$$

Reaction 22, $CO + O \rightleftharpoons O_2 + C$

$$K_{22} = \frac{K_3}{K_{12}}$$

$$k_{22} = a_{22} T^{-n_{22}} e^{-b_{22}/T}$$

$$X_{22} = \left[K_{22} c_3 c_{18} - c_{12} c_{13}\right] k_{22}$$

$$\frac{\partial X_{22}}{\partial c_j} = \left[\delta_{3,j} K_{22} c_{18} - \delta_{12,j} c_{13} - \delta_{13,j} c_{12} + \delta_{18,j} c_3\right] k_{22}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{22}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_{12}}\frac{dK_{12}}{dT}\right] K_{22} c_3 c_{18} k_{22} - \left[n_{22} - \frac{b_{22}}{T}\right]\frac{X_{22}}{T}$$

Reaction 23, $HCl + Cl \rightleftharpoons Cl_2 + H$

$$K_{23} = \frac{K_6}{K_4}$$

$$k_{23} = a_{23} T^{-n_{23}} e^{-b_{23}/T}$$

$$X_{23} = \left[K_{23} c_6 c_{14} - c_4 c_{16}\right] k_{23}$$

$$\frac{\partial X_{23}}{\partial c_j} = \left[-\delta_{4,j} c_{16} + \delta_{6,j} K_{23} c_{14} + \delta_{14,j} K_{23} c_6 - \delta_{16,j} c_4\right] k_{23}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{23}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_4}\frac{dK_4}{dT}\right] K_{23} c_6 c_{14} k_{23} - \left[n_{23} - \frac{b_{23}}{T}\right]\frac{X_{23}}{T}$$

Reaction 24, $2HCl \rightleftharpoons Cl_2 + H_2$

$$K_{24} = \frac{K_6^2}{K_4 K_8}$$

$$k_{24} = a_{24} T^{-n_{24}} e^{-b_{24}/T}$$

$$X_{24} = \left[K_{24} c_6^2 - c_4 c_8\right] k_{24}$$

$$\frac{\partial X_{24}}{\partial c_j} = \left[-\delta_{4,j} c_8 + 2\delta_{6,j} K_{24} c_6 - \delta_{8,j} c_4\right] k_{24}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{24}}{\partial T} = \left[\frac{2}{K_6}\frac{dK_6}{dT} - \frac{1}{K_4}\frac{dK_4}{dT} - \frac{1}{K_8}\frac{dK_8}{dT}\right] K_{24} c_6^2 k_{24} - \left[n_{24} - \frac{b_{24}}{T}\right]\frac{X_{24}}{T}$$

Reaction 25, $HCl + O \rightleftharpoons OH + Cl$

$$K_{25} = \frac{K_6}{K_{11}}$$

$$k_{25} = a_{25} T^{-n_{25}} e^{-b_{25}/T}$$

$$X_{25} = \left[K_{25} c_6 c_{18} - c_{11} c_{14}\right] k_{25}$$

$$\frac{\partial X_{25}}{\partial c_j} = \left[\delta_{6,j} K_{25} c_{18} - \delta_{11,j} c_{14} - \delta_{14,j} c_{11} + \delta_{18,j} K_{25} c_6\right] k_{25}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{25}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{25} c_6 c_{18} k_{25} - \left[n_{25} - \frac{b_{25}}{T}\right]\frac{X_{25}}{T}$$

Reaction 26, $HF + Cl \rightleftharpoons HCl + F$

$$K_{26} = \frac{K_7}{K_6}$$

$$k_{26} = a_{26}T^{-n_{26}} e^{-b_{26}/T}$$

$$X_{26} = \left[K_{26}c_7c_{14} - c_6c_{15}\right]k_{26}$$

$$\frac{\partial X_{26}}{\partial c_j} = \left[-\delta_{6,j}c_{15} + \delta_{7,j}K_{26}c_{14} + \delta_{14,j}K_{26}c_7 - \delta_{15,j}c_6\right]k_{26}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{26}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_6}\frac{dK_6}{dT}\right]K_{26}c_7c_{14}k_{26} - \left[n_{26} - \frac{b_{26}}{T}\right]\frac{X_{26}}{T}$$

Reaction 27, $HF + F \rightleftharpoons F_2 + H$

$$K_{27} = \frac{K_7}{K_5}$$

$$k_{27} = a_{27}T^{-n_{27}} e^{-b_{27}/T}$$

$$X_{27} = \left[K_{27}c_7c_{15} - c_5c_{16}\right]k_{27}$$

$$\frac{\partial X_{27}}{\partial c_j} = \left[-\delta_{5,j}c_{16} + \delta_{7,j}K_{27}c_{15} + \delta_{15,j}K_{27}c_7 - \delta_{16,j}c_5\right]k_{27}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{27}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_5}\frac{dK_5}{dT}\right]K_{27}c_7c_{15}k_{27} - \left[n_{27} - \frac{b_{27}}{T}\right]\frac{X_{27}}{T}$$

Reaction 28, $HF + H \rightleftharpoons H_2 + F$

$$K_{28} = \frac{K_7}{K_8}$$

$$k_{28} = a_{28} T^{-n_{28}} e^{-b_{28}/T}$$

$$X_{28} = \left[K_{28} c_7 c_{16} - c_8 c_{15}\right] k_{28}$$

$$\frac{\partial X_{28}}{\partial c_j} = \left[\delta_{7,j} K_{28} c_{16} - \delta_{8,j} c_{15} - \delta_{15,j} c_8 + \delta_{16,j} K_{28} c_7\right] k_{28}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{28}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_8}\frac{dK_8}{dT}\right] K_{28} c_7 c_{16} k_{28} - \left[n_{28} - \frac{b_{28}}{T}\right] \frac{X_{28}}{T}$$

Reaction 29, $2HF \rightleftharpoons F_2 + H_2$

$$K_{29} = \frac{K_7^2}{K_5 K_8}$$

$$k_{29} = a_{29} T^{-n_{29}} e^{-b_{29}/T}$$

$$X_{29} = \left[K_{29} c_7^2 - c_5 c_8\right] k_{29}$$

$$\frac{\partial X_{29}}{\partial c_j} = \left[-\delta_{5,j} c_8 + 2\delta_{7,j} K_{29} c_7 - \delta_{8,j} c_5\right] k_{29}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{29}}{\partial T} = \left[\frac{2}{K_7}\frac{dK_7}{dT} - \frac{1}{K_5}\frac{dK_5}{dT} - \frac{1}{K_8}\frac{dK_8}{dT}\right] K_{29} c_7^2 k_{29} - \left[n_{29} - \frac{b_{29}}{T}\right] \frac{X_{29}}{T}$$

Reaction 30, $HF + O \rightleftharpoons OH + F$

$$K_{30} = \frac{K_7}{K_{11}}$$

$$k_{30} = a_{30} T^{-n_{30}} e^{-b_{30}/T}$$

$$X_{30} = \left[K_{30} c_7 c_{18} - c_{11} c_{15}\right] k_{30}$$

$$\frac{\partial X_{30}}{\partial c_j} = \left[\delta_{7,j} K_{30} c_{18} - \delta_{11,j} c_{15} - \delta_{15,j} c_{11} + \delta_{18,j} K_{30} c_7\right] k_{30}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{30}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{30} c_7 c_{18} k_{30} - \left[n_{30} - \frac{b_{30}}{T}\right]\frac{X_{30}}{T}$$

Reaction 31, $HF + OH \rightleftharpoons H_2O + F$

$$K_{31} = \frac{K_7}{K_2}$$

$$k_{31} = a_{31} T^{-n_{31}} e^{-b_{31}/T}$$

$$X_{31} = \left[K_{31} c_7 c_{11} - c_2 c_{15}\right] k_{31}$$

$$\frac{\partial X_{31}}{\partial c_j} = \left[-\delta_{2,j} c_{15} + \delta_{7,j} K_{31} c_{11} + \delta_{11,j} K_{31} c_7 - \delta_{15,j} c_2\right] k_{31}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{31}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_2}\frac{dK_2}{dT}\right] K_{31} c_7 c_{11} k_{31} - \left[n_{31} - \frac{b_{31}}{T}\right]\frac{X_{31}}{T}$$

Reaction 32, $H_2 + Cl \rightleftharpoons HCl + H$

$$K_{32} = \frac{K_8}{K_6}$$

$$k_{32} = a_{32} T^{-n_{32}} e^{-b_{32}/T}$$

$$X_{32} = \left[K_{32} c_8 c_{14} - c_6 c_{16}\right] k_{32}$$

$$\frac{\partial X_{32}}{\partial c_j} = \left[-\delta_{6,j} c_{16} + \delta_{8,j} K_{32} c_{14} + \delta_{14,j} K_{32} c_8 - \delta_{16,j} c_6\right] k_{32}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{32}}{\partial T} = \left[\frac{1}{K_8}\frac{dK_8}{dT} - \frac{1}{K_6}\frac{dK_6}{dT}\right] K_{32} c_8 c_{14} k_{32} - \left[n_{32} - \frac{b_{32}}{T}\right] \frac{X_{32}}{T}$$

Reaction 33, $H_2 + O \rightleftharpoons OH + H$

$$K_{33} = \frac{K_8}{K_{11}}$$

$$k_{33} = a_{33} T^{-n_{33}} e^{-b_{33}/T}$$

$$X_{33} = \left[K_{33} c_8 c_{18} - c_{11} c_{16}\right] k_{33}$$

$$\frac{\partial X_{33}}{\partial c_j} = \left[\delta_{8,j} K_{33} c_{18} - \delta_{11,j} c_{16} - \delta_{16,j} c_{11} - \delta_{18,j} K_{33} c_8\right] k_{33}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{32}}{\partial T} = \left[\frac{1}{K_8}\frac{dK_8}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{33} c_8 c_{18} k_{33} - \left[n_{33} - \frac{b_{33}}{T}\right] \frac{X_{33}}{T}$$

Reaction 34, $H_2 + O_2 \rightleftharpoons 2OH$

$$K_{34} = \frac{K_8 K_{12}}{K_{11}^2}$$

$$k_{34} = a_{34} T^{-n_{34}} e^{-b_{34}/T}$$

$$X_{34} = \left[K_{34} c_8 c_{12} - c_{11}^2\right] k_{34}$$

$$\frac{\partial X_{34}}{\partial c_j} = \left[\delta_{8,j} K_{34} c_{12} - 2\delta_{11,j} c_{11} + \delta_{12,j} K_{38} c_8\right] k_{34}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{34}}{\partial T} = \left[\frac{1}{K_8}\frac{dK_8}{dT} + \frac{1}{K_{12}}\frac{dK_{12}}{dT} - \frac{2}{K_{11}}\frac{dK_{11}}{dT}\right] K_{34} c_8 c_{12} k_{34} - \left[n_{34} - \frac{b_{34}}{T}\right]\frac{X_{34}}{T}$$

Reaction 35, $N_2 + O \rightleftharpoons NO + N$

$$K_{35} = \frac{K_9}{K_{10}}$$

$$k_{35} = a_{35} T^{-n_{35}} e^{-b_{35}/T}$$

$$X_{35} = \left[K_{35} c_9 c_{18} - c_{10} c_{17}\right] k_{35}$$

$$\frac{\partial X_{35}}{\partial c_j} = \left[\delta_{9,j} K_{35} c_{18} - \delta_{10,j} c_{17} - \delta_{17,j} c_{10} + \delta_{18,j} K_{35} c_9\right] k_{35}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{35}}{\partial T} = \left[\frac{1}{K_9}\frac{dK_9}{dT} - \frac{1}{K_{10}}\frac{dK_{10}}{dT}\right] K_{35} c_9 c_{18} k_{35} - \left[n_{35} - \frac{b_{35}}{T}\right]\frac{X_{35}}{T}$$

Reaction 36, $N_2 + O_2 \rightleftharpoons 2NO$

$$K_{36} = \frac{K_9 K_{12}}{K_{10}^2}$$

$$k_{36} = a_{36} T^{-n_{36}} e^{-b_{36}/T}$$

$$X_{36} = \left[K_{36} c_9 c_{12} - c_{10}^2\right] k_{36}$$

$$\frac{\partial X_{36}}{\partial c_j} = \left[\delta_{9,j} K_{36} c_{12} - 2\delta_{10,j} c_{10} + \delta_{12,j} K_{36} c_9\right] k_{36}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{36}}{\partial T} = \left[\frac{1}{K_9}\frac{dK_9}{dT} + \frac{1}{K_{12}}\frac{dK_{12}}{dT} - \frac{2}{K_{10}}\frac{dK_{10}}{dT}\right] K_{36} c_9 c_{12} k_{36} - \left[n_{36} - \frac{b_{36}}{T}\right]\frac{X_{36}}{T}$$

Reaction 37, $NO + H \rightleftharpoons OH + N$

$$K_{37} = \frac{K_{10}}{K_{11}}$$

$$k_{37} = a_{37} T^{-n_{37}} e^{-b_{37}/T}$$

$$X_{37} = \left[K_{37} c_{10} c_{16} - c_{11} c_{17}\right] k_{37}$$

$$\frac{\partial X_{37}}{\partial c_j} = \left[\delta_{10,j} K_{37} c_{16} - \delta_{11,j} c_{17} + \delta_{16,j} K_{37} c_{10} - \delta_{17,j} c_{11}\right] k_{37}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{37}}{\partial T} = \left[\frac{1}{K_{10}}\frac{dK_{10}}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{37} c_{10} c_{16} k_{37} - \left[n_{37} - \frac{b_{37}}{T}\right]\frac{X_{37}}{T}$$

Reaction 38, $NO + O \rightleftharpoons O_2 + N$

$$K_{38} = \frac{K_{10}}{K_{12}}$$

$$k_{38} = a_{38}T^{-n_{38}} e^{-b_{38}/T}$$

$$X_{38} = \left[K_{38}c_{10}c_{18} - c_{12}c_{17}\right]k_{38}$$

$$\frac{\partial X_{38}}{\partial c_j} = \left[\delta_{10,j}K_{38}c_{18} - \delta_{12,j}c_{17} - \delta_{17,j}c_{12} + \delta_{18,j}K_{38}c_{10}\right] k_{38}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{38}}{\partial T} = \left[\frac{1}{K_{10}}\frac{dK_{10}}{dT} - \frac{1}{K_{12}}\frac{dK_{12}}{dT}\right]K_{38}c_{10}c_{18}k_{38} - \left[n_{38} - \frac{b_{38}}{T}\right]\frac{X_{38}}{T}$$

Reaction 39, $O_2 + H \rightleftharpoons OH + O$

$$K_{39} = \frac{K_{12}}{K_{11}}$$

$$k_{39} = a_{39}T^{-n_{39}} e^{-b_{39}/T}$$

$$X_{39} = \left[K_{39}c_{12}c_{16} - c_{11}c_{18}\right]k_{39}$$

$$\frac{\partial X_{39}}{\partial c_j} = \left[-\delta_{11,j}c_{18} + \delta_{12,j}K_{39}c_{16} + \delta_{16,j}K_{39}c_{12} - \delta_{18,j}c_{11}\right] k_{39}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{39}}{\partial T} = \left[\frac{1}{K_{12}}\frac{dK_{12}}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right]K_{39}c_{12}c_{16}k_{39} - \left[n_{39} - \frac{b_{39}}{T}\right]\frac{X_{39}}{T}$$

Reaction 40, $AlO + M \rightleftharpoons Al + O + M$

$$k_{40} = a_{40} T^{-n_{40}} e^{-b_{40}/T}$$

$$M_{40} = \sum_{i=1}^{57} m_{40,i} c_i$$

$$X_{40} = \left[K_{40} c_{20} - \rho c_{19} c_{18}\right] M_{40} k_{40}$$

$$\frac{\partial X_{40}}{\partial c_j} = \frac{X_{40}}{M_{40}} m_{40,j} + \delta_{20,j} K_{40} M_{40} k_{40} - \delta_{19,j} \rho c_{18} M_{40} k_{40}$$

$$- \delta_{18,j} \rho c_{19} M_{40} k_{40} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{40}}{\partial \rho} = -c_{19} c_{18} M_{40} k_{40}$$

$$\frac{\partial X_{40}}{\partial T} = c_{20} M_{40} k_{40} \frac{dK_{40}}{dT} - \left[n_{40} - \frac{b_{40}}{T}\right] \frac{X_{40}}{T}$$

Reaction 41, $Al_2O + M \rightleftharpoons Al + AlO + M$

$$k_{41} = a_{41} T^{-n_{41}} e^{-b_{41}/T}$$

$$M_{41} = \sum_{i=1}^{57} m_{41,i} c_i$$

$$X_{41} = \left[K_{41} c_{21} - \rho c_{19} c_{20}\right] M_{41} k_{41}$$

$$\frac{\partial X_{41}}{\partial c_j} = \frac{X_{41}}{M_{41}} m_{41,j} + \delta_{21,j} K_{41} M_{41} k_{41} - \delta_{19,j} \rho c_{20} M_{41} k_{41}$$

$$-\delta_{20,j} \rho c_{19} M_{41} k_{41} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{41}}{\partial \rho} = -c_{19} c_{20} M_{41} k_{41}$$

$$\frac{\partial X_{41}}{\partial T} = c_{21} M_{41} k_{41} \frac{dK_{41}}{dT} - \left[n_{41} - \frac{b_{41}}{T}\right] \frac{X_{41}}{T}$$

Reaction 42, $AlCl + M \rightleftharpoons Al + Cl + M$

$$k_{42} = a_{42} T^{-n_{42}} e^{-b_{42}/T}$$

$$M_{42} = \sum_{i=1}^{57} m_{42,i} c_i$$

$$X_{42} = \left[K_{42} c_{22} - \rho c_{19} c_4\right] M_{42} k_{42}$$

$$\frac{\partial X_{42}}{\partial c_j} = \frac{X_{42}}{M_{42}} m_{42,j} + \delta_{22,j} K_{42} M_{42} k_{42} - \delta_{19,j} \rho c_4 M_{42} k_{42}$$

$$- \delta_{4,j} \rho c_{19} M_{42} k_{42} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{42}}{\partial \rho} = - c_{19} c_4 M_{42} k_{42}$$

$$\frac{\partial X_{42}}{\partial T} = c_{22} M_{42} k_{42} \frac{dK_{42}}{dT} - \left[n_{42} - \frac{b_{42}}{T}\right] \frac{X_{42}}{T}$$

Reaction 43, $AlCl_2 + M \rightleftharpoons AlCl + Cl + M$

$$k_{43} = a_{43} T^{-n_{43}} e^{-b_{43}/T}$$

$$M_{43} = \sum_{i=1}^{57} m_{43,i} c_i$$

$$X_{43} = \left[K_{43} c_{23} - \rho c_{22} c_{14}\right] M_{43} k_{43}$$

$$\frac{\partial X_{43}}{\partial c_j} = \frac{X_{43}}{M_{43}} m_{43,j} + \delta_{23,j} K_{43} M_{43} k_{43} - \delta_{22,j} \rho c_{14} M_{43} k_{43}$$

$$- \delta_{14,j} \rho c_{22} M_{43} k_{43} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{43}}{\partial \rho} = - c_{22} c_{14} M_{43} k_{43}$$

$$\frac{\partial X_{43}}{\partial T} = c_{23} M_{43} k_{43} \frac{dK_{43}}{dT} - \left[n_{43} - \frac{b_{43}}{T}\right] \frac{X_{43}}{T}$$

Reaction 44, $AlOCl + M \rightleftharpoons AlO + Cl + M$

$$k_{44} = a_{44} T^{-n_{44}} e^{-b_{44}/T}$$

$$M_{44} = \sum_{i=1}^{57} m_{44,i} c_i$$

$$X_{44} = \left[K_{44} c_{24} - \rho c_{20} c_{14}\right] M_{44} k_{44}$$

$$\frac{\partial X_{44}}{\partial c_j} = \frac{X_{44}}{M_{44}} m_{44,j} + \delta_{24,j} K_{44} M_{44} k_{44} - \delta_{20,j} \rho c_{14} M_{44} k_{44}$$

$$-\delta_{14,j} \rho c_{20} M_{44} k_{44} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{44}}{\partial \rho} = -c_{20} c_{14} M_{44} k_{44}$$

$$\frac{\partial X_{44}}{\partial T} = c_{24} M_{44} k_{44} \frac{dK_{44}}{dT} - \left[n_{44} - \frac{b_{44}}{T}\right] \frac{X_{44}}{T}$$

Reaction 45, $AlOCl + M \rightleftharpoons AlCl + O + M$

$$k_{45} = a_{45} T^{-n_{45}} e^{-b_{45}/T}$$

$$M_{45} = \sum_{i=1}^{57} m_{45,i} c_i$$

$$X_{45} = \left[K_{45} c_{24} - \rho c_{22} c_{18}\right] M_{45} k_{45}$$

$$\frac{\partial X_{45}}{\partial c_j} = \frac{X_{45}}{M_{45}} m_{45,j} + \delta_{24,j} K_{45} M_{45} k_{45} - \delta_{22,j} \rho c_{18} M_{45} k_{45}$$

$$-\delta_{18,j} \rho c_{22} M_{45} k_{45} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{45}}{\partial \rho} = -c_{22} c_{18} M_{45} k_{45}$$

$$\frac{\partial X_{45}}{\partial T} = c_{24} M_{45} k_{45} \frac{dK_{45}}{dT} - \left[n_{45} - \frac{b_{45}}{T}\right] \frac{X_{45}}{T}$$

Reaction 46, $AlF + M \rightleftharpoons Al + F + M$

$$k_{46} = a_{46} T^{-n_{46}} e^{-b_{46}/T}$$

$$M_{46} = \sum_{i=1}^{57} m_{46,i} c_i$$

$$X_{46} = \left[K_{46} c_{25} - \rho c_{19} c_{15}\right] M_{46} k_{46}$$

$$\frac{\partial X_{46}}{\partial c_j} = \frac{X_{46}}{M_{46}} m_{46,j} + \delta_{25,j} K_{46} M_{46} k_{46} - \delta_{19,j} \rho c_{15} M_{46} k_{46}$$

$$- \delta_{15,j} \rho c_{19} M_{46} k_{46} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{46}}{\partial \rho} = - c_{19} c_{15} M_{46} k_{46}$$

$$\frac{\partial X_{46}}{\partial T} = c_{25} M_{46} k_{46} \frac{dK_{46}}{dT} - \left[n_{46} - \frac{b_{46}}{T}\right] \frac{X_{46}}{T}$$

Reaction 47, $AlF_2 + M \rightleftharpoons AlF + F + M$

$$k_{47} = a_{47} T^{-n_{47}} e^{-b_{47}/T}$$

$$M_{47} = \sum_{i=1}^{57} m_{47,i} c_i$$

$$X_{47} = \left[K_{47} c_{26} - \rho c_{25} c_{15}\right] M_{47} k_{47}$$

$$\frac{\partial X_{47}}{\partial c_j} = \frac{X_{47}}{M_{47}} m_{47,j} + \delta_{26,j} K_{47} M_{47} k_{47} - \delta_{25,j} \rho c_{15} M_{47} k_{47}$$

$$- \delta_{15,j} \rho c_{25} M_{47} k_{47} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{47}}{\partial \rho} = - c_{25} c_{15} M_{47} k_{47}$$

$$\frac{\partial X_{47}}{\partial T} = c_{26} M_{47} k_{47} \frac{dK_{47}}{dT} - \left[n_{47} - \frac{b_{47}}{T}\right] \frac{X_{47}}{T}$$

Reaction 48, $AlOF + M \rightleftharpoons AlO + F + M$

$$k_{48} = a_{48} T^{-n_{48}} e^{-b_{48}/T}$$

$$M_{48} = \sum_{i=1}^{57} m_{48,i} c_i$$

$$X_{48} = \left[K_{48} c_{27} - \rho c_{20} c_{15}\right] M_{48} k_{48}$$

$$\frac{\partial X_{48}}{\partial c_j} = \frac{X_{48}}{M_{48}} m_{48,j} + \delta_{27,j} K_{48} M_{48} k_{48} - \delta_{20,j} \rho c_{15} M_{48} k_{48}$$

$$- \delta_{15,j} \rho c_{20} M_{48} k_{48} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{48}}{\partial \rho} = - c_{20} c_{15} M_{48} k_{48}$$

$$\frac{\partial X_{48}}{\partial T} = c_{27} M_{48} k_{48} \frac{dK_{48}}{dT} - \left[n_{48} - \frac{b_{48}}{T}\right] \frac{X_{48}}{T}$$

Reaction 49, $AlOF + M \rightleftharpoons AlF + O + M$

$$k_{49} = a_{49} T^{-n_{49}} e^{-b_{49}/T}$$

$$M_{49} = \sum_{i=1}^{57} m_{49,i} c_i$$

$$X_{49} = \left[K_{49} c_{27} - \rho c_{25} c_{18}\right] M_{49} k_{49}$$

$$\frac{\partial X_{49}}{\partial c_j} = \frac{X_{49}}{M_{49}} m_{49,j} + \delta_{27,j} K_{49} M_{49} k_{49} - \delta_{25,j} \rho c_{18} M_{49} k_{49}$$

$$- \delta_{18,j} \rho c_{25} M_{49} k_{49} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{49}}{\partial \rho} = - c_{25} c_{18} M_{49} k_{49}$$

$$\frac{\partial X_{49}}{\partial T} = c_{27} M_{49} k_{49} \frac{dK_{49}}{dT} - \left[n_{49} - \frac{b_{49}}{T}\right] \frac{X_{49}}{T}$$

Reaction 50, $Al + CO_2 \rightleftharpoons AlO + CO$

$$K_{50} = \frac{K_1}{K_{40}}$$

$$k_{50} = a_{50} T^{-n_{50}} e^{-b_{50}/T}$$

$$X_{50} = \left[K_{50} c_{19} c_1 - c_{20} c_3\right] k_{50}$$

$$\frac{\partial X_{50}}{\partial c_j} = \left[\delta_{1,j} K_{50} c_{19} - \delta_{3,j} c_{20} + \delta_{19,j} K_{50} c_1 - \delta_{20,j} c_3\right] k_{50}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{50}}{\partial T} = \left[\frac{1}{K_1}\frac{dK_1}{dT} - \frac{1}{K_{40}}\frac{dK_{40}}{dT}\right] K_{50} c_{19} c_1 k_{50} - \left[n_{50} - \frac{b_{50}}{T}\right]\frac{X_{50}}{T}$$

Reaction 51, $Al + CO \rightleftharpoons AlO + C$

$$K_{51} = \frac{K_3}{K_{40}}$$

$$k_{51} = a_{51} T^{-n_{51}} e^{-b_{51}/T}$$

$$X_{51} = \left[K_{51} c_{19} c_3 - c_{20} c_{13}\right] k_{51}$$

$$\frac{\partial X_{51}}{\partial c_j} = \left[\delta_{3,j} K_{51} c_{19} - \delta_{13,j} c_{20} + \delta_{19,j} K_{51} c_3 - \delta_{20,j} c_{13}\right] k_{51}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{51}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_{40}}\frac{dK_{40}}{dT}\right] K_{51} c_{19} c_3 k_{51} - \left[n_{51} - \frac{b_{51}}{T}\right]\frac{X_{51}}{T}$$

Reaction 52, $Al + NO \rightleftharpoons AlO + N$

$$K_{52} = \frac{K_{10}}{K_{40}}$$

$$k_{52} = a_{52} T^{-n_{52}} e^{-b_{52}/T}$$

$$X_{52} = \left[K_{52} c_{19} c_{10} - c_{20} c_{17}\right] k_{52}$$

$$\frac{\partial X_{52}}{\partial c_j} = \left[\delta_{10,j} K_{52} c_{19} - \delta_{17,j} c_{20} + \delta_{19,j} K_{52} c_{10} - \delta_{20,j} c_{17}\right] k_{52}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{52}}{\partial T} = \left[\frac{1}{K_{10}} \frac{dK_{10}}{dT} - \frac{1}{K_{40}} \frac{dK_{40}}{dT}\right] K_{52} c_{19} c_{10} k_{52} - \left[n_{52} - \frac{b_{52}}{T}\right] \frac{X_{52}}{T}$$

Reaction 53, $Al + O_2 \rightleftharpoons AlO + O$

$$K_{53} = \frac{K_{12}}{K_{40}}$$

$$k_{53} = a_{53} T^{-n_{53}} e^{-b_{53}/T}$$

$$X_{53} = \left[K_{53} c_{19} c_{12} - c_{20} c_{18}\right] k_{53}$$

$$\frac{\partial X_{53}}{\partial c_j} = \left[\delta_{12,j} K_{53} c_{19} - \delta_{18,j} c_{20} + \delta_{19,j} K_{53} c_{12} - \delta_{20,j} c_{18}\right] k_{53}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{53}}{\partial T} = \left[\frac{1}{K_{12}} \frac{dK_{12}}{dT} - \frac{1}{K_{40}} \frac{dK_{40}}{dT}\right] K_{53} c_{19} c_{12} k_{53} - \left[n_{53} - \frac{b_{53}}{T}\right] \frac{X_{53}}{T}$$

Reaction 54, $Al + AlOCl \rightleftharpoons Al_2O + Cl$

$$K_{54} = \frac{K_{44}}{K_{41}}$$

$$k_{54} = a_{54} T^{-n_{54}} e^{-b_{54}/T}$$

$$X_{54} = \left[K_{54} c_{19} c_{24} - c_{21} c_{14} \right] K_{54}$$

$$\frac{\partial X_{54}}{\partial c_j} = \left[-\delta_{14,j} c_{21} + \delta_{19,j} K_{54} c_{24} - \delta_{21,j} c_{14} + \delta_{24,j} K_{54} c_{19} \right] k_{54}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{54}}{\partial T} = \left[\frac{1}{K_{44}} \frac{dK_{44}}{dT} - \frac{1}{K_{41}} \frac{dK_{41}}{dT} \right] K_{54} c_{19} c_{24} k_{54} - \left[n_{54} - \frac{b_{54}}{T} \right] \frac{X_{54}}{T}$$

Reaction 55, $Al + AlOCl \rightleftharpoons AlO + AlCl$

$$K_{55} = \frac{K_{44}}{K_{42}}$$

$$k_{55} = a_{55} T^{-n_{55}} e^{-b_{55}/T}$$

$$X_{55} = \left[K_{55} c_{19} c_{24} - c_{20} c_{22} \right] k_{55}$$

$$\frac{\partial X_{55}}{\partial c_j} = \left[\delta_{19,j} K_{55} c_{24} - \delta_{20,j} c_{22} - \delta_{22,j} c_{20} + \delta_{24,j} K_{55} c_{19} \right] k_{55}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{55}}{\partial T} = \left[\frac{1}{K_{44}} \frac{dK_{44}}{dT} - \frac{1}{K_{42}} \frac{dK_{42}}{dT} \right] K_{55} c_{19} c_{24} k_{55} - \left[n_{55} - \frac{b_{55}}{T} \right] \frac{X_{55}}{T}$$

Reaction 56, $Al + AlOF \rightleftharpoons Al_2O + F$

$$K_{56} = \frac{K_{48}}{K_{41}}$$

$$k_{56} = a_{56}T^{-n_{56}} e^{-b_{56}/T}$$

$$X_{56} = \left[K_{56}c_{19}c_{27} - c_{21}c_{15}\right] k_{56}$$

$$\frac{\partial X_{56}}{\partial c_j} = \left[-\delta_{15,j}c_{21} + \delta_{19,j}K_{56}c_{27} - \delta_{21,j}c_{15} + \delta_{27,j}K_{56}c_{19}\right] k_{56}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{56}}{\partial T} = \left[\frac{1}{K_{48}} \frac{dK_{48}}{dT} - \frac{1}{K_{41}} \frac{dK_{41}}{dT}\right] K_{56}c_{19}c_{27}k_{56} - \left[n_{56} - \frac{b_{56}}{T}\right] \frac{X_{56}}{T}$$

Reaction 57, $AlO + HF \rightleftharpoons AlF + OH$

$$K_{57} = \frac{K_7K_{40}}{K_{11}K_{46}}$$

$$k_{57} = a_{57}T^{-n_{57}} e^{-b_{57}/T}$$

$$X_{57} = \left[K_{57}c_{20}c_7 - c_{25}c_{11}\right] k_{57}$$

$$\frac{\partial X_{57}}{\partial c_j} = \left[\delta_{7,j}K_{57}c_{20} - \delta_{11,j}c_{25} + \delta_{20,j}K_{57}c_7 - \delta_{25,j}c_{11}\right] k_{57}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{57}}{\partial T} = \left[\frac{1}{K_7} \frac{dK_7}{dT} + \frac{1}{K_{40}} \frac{dK_{40}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT} - \frac{1}{K_{46}} \frac{dK_{46}}{dT}\right] K_{57}c_{20}c_7k_{57} - \left[n_{57} - \frac{b_{57}}{T}\right] \frac{X_{57}}{T}$$

Reaction 58, $AlO + F \rightleftharpoons AlF + O$

$$K_{58} = \frac{K_{40}}{K_{46}}$$

$$k_{58} = a_{58} T^{-n_{58}} e^{-b_{58}/T}$$

$$X_{58} = \left[K_{58} c_{20} c_{15} - c_{25} c_{18}\right] k_{58}$$

$$\frac{\partial X_{58}}{\partial c_j} = \left[\delta_{15,j} K_{58} c_{20} - \delta_{18,j} c_{25} + \delta_{20,j} K_{58} c_{15} - \delta_{25,j} c_{18}\right] k_{58}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{58}}{\partial T} = \left[\frac{1}{K_{40}} \frac{dK_{40}}{dT} - \frac{1}{K_{46}} \frac{dK_{46}}{dT}\right] K_{58} c_{20} c_{15} k_{58} - \left[n_{58} - \frac{b_{58}}{T}\right] \frac{X_{58}}{T}$$

Reaction 59, $AlO + H \rightleftharpoons Al + OH$

$$K_{59} = \frac{K_{40}}{K_{11}}$$

$$k_{59} = a_{59} T^{-n_{59}} e^{-b_{59}/T}$$

$$X_{59} = \left[K_{59} c_{20} c_{16} - c_{19} c_{11}\right] k_{59}$$

$$\frac{\partial X_{59}}{\partial c_j} = \left[-\delta_{11,j} c_{19} + \delta_{16,j} K_{59} c_{20} - \delta_{19,j} c_{11} + \delta_{20,j} K_{59} c_{16}\right] k_{59}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{59}}{\partial T} = \left[\frac{1}{K_{40}} \frac{dK_{40}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{59} c_{20} c_{16} k_{59} - \left[n_{59} - \frac{b_{59}}{T}\right] \frac{X_{59}}{T}$$

Reaction 60, $AlO + AlF \rightleftharpoons Al_2O + F$

$$K_{60} = \frac{K_{46}}{K_{41}}$$

$$k_{60} = a_{60} T^{-n_{60}} e^{-b_{60}/T}$$

$$X_{60} = \left[K_{60} c_{20} c_{25} - c_{21} c_{15}\right] k_{60}$$

$$\frac{\partial X_{60}}{\partial c_j} = \left[-\delta_{15,j} c_{21} + \delta_{20,j} K_{60} c_{25} - \delta_{21,j} c_{15} + \delta_{25,j} K_{60} c_{20}\right] k_{60}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{60}}{\partial T} = \left[\frac{1}{K_{46}} \frac{dK_{46}}{dT} - \frac{1}{K_{41}} \frac{dK_{41}}{dT}\right] K_{60} c_{20} c_{25} k_{60} - \left[n_{60} - \frac{b_{60}}{T}\right] \frac{X_{60}}{T}$$

Reaction 61, $AlO + AlF \rightleftharpoons Al + AlOF$

$$K_{61} = \frac{K_{46}}{K_{48}}$$

$$k_{61} = a_{61} T^{-n_{61}} e^{-b_{61}/T}$$

$$X_{61} = \left[K_{61} c_{20} c_{25} - c_{19} c_{27}\right] k_{61}$$

$$\frac{\partial X_{61}}{\partial c_j} = \left[-\delta_{19,j} c_{27} + \delta_{20,j} K_{61} c_{25} + \delta_{25,j} K_{61} c_{20} - \delta_{27,j} c_{19}\right] k_{61}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{61}}{\partial T} = \left[\frac{1}{K_{46}} \frac{dK_{46}}{dT} - \frac{1}{K_{48}} \frac{dK_{48}}{dT}\right] K_{61} c_{20} c_{25} k_{61} - \left[n_{61} - \frac{b_{61}}{T}\right] \frac{X_{61}}{T}$$

Reaction 62, $Al_2O + Cl \rightleftharpoons AlO + AlCl$

$$K_{62} = \frac{K_{41}}{K_{42}}$$

$$k_{62} = a_{62} T^{-n_{62}} e^{-b_{62}/T}$$

$$X_{62} = \left[K_{62} c_{21} c_{14} - c_{20} c_{22}\right] k_{62}$$

$$\frac{\partial X_{62}}{\partial c_j} = \left[\delta_{14,j} K_{62} c_{21} - \delta_{20,j} c_{22} + \delta_{21,j} K_{62} c_{14} - \delta_{22,j} c_{20}\right] k_{62}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{62}}{\partial T} = \left[\frac{1}{K_{41}} \frac{dK_{41}}{dT} - \frac{1}{K_{42}} \frac{dK_{42}}{dT}\right] K_{62} c_{21} c_{14} k_{62} - \left[n_{62} - \frac{b_{62}}{T}\right] \frac{X_{62}}{T}$$

Reaction 63, $Al_2O + O \rightleftharpoons 2AlO$

$$K_{63} = \frac{K_{41}}{K_{40}}$$

$$k_{63} = a_{63} T^{-n_{63}} e^{-b_{63}/T}$$

$$X_{63} = \left[K_{63} c_{21} c_{18} - c_{20}^2\right] k_{63}$$

$$\frac{\partial X_{63}}{\partial c_j} = \left[\delta_{18,j} K_{63} c_{21} - 2\delta_{20,j} c_{20} + \delta_{21,j} K_{63} c_{18}\right] k_{63}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{63}}{\partial T} = \left[\frac{1}{K_{41}} \frac{dK_{41}}{dT} - \frac{1}{K_{40}} \frac{dK_{40}}{dT}\right] K_{63} c_{21} c_{18} k_{63} - \left[n_{63} - \frac{b_{63}}{T}\right] \frac{X_{63}}{T}$$

Reaction 64, $AlCl + CO \rightleftharpoons AlOCl + C$

$$K_{64} = \frac{K_{51}}{K_{55}}$$

$$k_{64} = a_{64}T^{-n_{64}} e^{-b_{64}/T}$$

$$X_{64} = \left[K_{64}c_3c_{22} - c_{13}c_{24}\right] k_{64}$$

$$\frac{\partial X_{64}}{\partial c_j} = \left[\delta_{3,j}K_{64}c_{22} - \delta_{13,j}c_{24} + \delta_{22,j}K_{64}c_3 - \delta_{24,j}c_{13}\right] k_{64}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{64}}{\partial T} = \left[\frac{1}{K_{51}} \frac{dK_{51}}{dT} - \frac{1}{K_{55}} \frac{dK_{55}}{dT}\right] K_{64}c_3c_{22}k_{64} - \left[n_{64} - \frac{b_{64}}{T}\right] \frac{X_{64}}{T}$$

Reaction 65, $AlCl + HCl \rightleftharpoons AlCl_2 + H$

$$K_{65} = \frac{K_6}{K_{43}}$$

$$k_{65} = a_{65}T^{-n_{65}} e^{-b_{65}/T}$$

$$X_{65} = \left[K_{65}c_6c_{22} - c_{16}c_{23}\right] k_{65}$$

$$\frac{\partial X_{65}}{\partial c_j} = \left[\delta_{6,j}K_{65}c_{22} - \delta_{16,j}c_{23} + \delta_{22,j}K_{65}c_6 - \delta_{23,j}c_{16}\right] k_{65}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{65}}{\partial T} = \left[\frac{1}{K_6} \frac{dK_6}{dT} - \frac{1}{K_{43}} \frac{dK_{43}}{dT}\right] K_{65}c_6c_{22}k_{65} - \left[n_{65} - \frac{b_{65}}{T}\right] \frac{X_{65}}{T}$$

Reaction 66, $AlCl + NO \rightleftharpoons AlOCl + N$

$$K_{66} = \frac{K_{52}}{K_{55}}$$

$$k_{66} = a_{66}T^{-n_{66}} e^{-b_{66}/T}$$

$$X_{66} = \left[K_{66}c_{10}c_{22} - c_{17}c_{24}\right] k_{66}$$

$$\frac{\partial X_{66}}{\partial c_j} = \left[\delta_{10,j}K_{66}c_{22} - \delta_{17,j}c_{24} + \delta_{22,j}K_{66}c_{10} - \delta_{24,j}c_{17}\right] k_{66}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{66}}{\partial T} = \left[\frac{1}{K_{52}}\frac{dK_{52}}{dT} - \frac{1}{K_{55}}\frac{dK_{55}}{dT}\right] K_{66}c_{10}c_{22}k_{66} - \left[n_{66} - \frac{b_{66}}{T}\right]\frac{X_{66}}{T}$$

Reaction 67, $AlCl + OH \rightleftharpoons AlO + HCl$

$$K_{67} = \frac{K_{11}K_{42}}{K_6K_{40}}$$

$$k_{67} = a_{67}T^{-n_{67}} e^{-b_{67}/T}$$

$$X_{67} = \left[K_{67}c_{11}c_{22} - c_6c_{20}\right] k_{67}$$

$$\frac{\partial X_{67}}{\partial c_j} = \left[-\delta_{6,j}c_{20} + \delta_{11,j}K_{67}c_{22} - \delta_{20,j}c_6 + \delta_{22,j}K_{67}c_{11}\right] k_{67}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{67}}{\partial T} = \left[\frac{1}{K_{11}}\frac{dK_{11}}{dT} + \frac{1}{K_{42}}\frac{dK_{42}}{dT} - \frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{40}}\frac{dK_{40}}{dT}\right] K_{67}c_{11}c_{22}k_{67}$$

$$- \left[n_6 - \frac{b_{67}}{T}\right]\frac{X_{67}}{T}$$

Reaction 68, $AlCl + Cl \rightleftharpoons Al + Cl_2$

$$K_{68} = \frac{K_{42}}{K_4}$$

$$k_{68} = a_{68} T^{-n_{68}} e^{-b_{68}/T}$$

$$X_{68} = \left[K_{68} c_{14} c_{22} - c_4 c_{19}\right] k_{68}$$

$$\frac{\partial X_{68}}{\partial c_j} = \left[-\delta_{4,j} c_{19} + \delta_{14,j} K_{68} c_{22} - \delta_{19,j} c_4 + \delta_{22,j} K_{68} c_{14}\right] k_{68}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{68}}{\partial T} = \left[\frac{1}{K_{42}} \frac{dK_{42}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{68} c_{14} c_{22} k_{68} - \left[n_{68} - \frac{b_{68}}{T}\right] \frac{X_{68}}{T}$$

Reaction 69, $AlCl + H \rightleftharpoons Al + HCl$

$$K_{69} = \frac{K_{42}}{K_6}$$

$$k_{69} = a_{69} T^{-n_{69}} e^{-b_{69}/T}$$

$$X_{69} = \left[K_{69} c_{16} c_{22} - c_6 c_{19}\right] k_{69}$$

$$\frac{\partial X_{69}}{\partial c_j} = \left[-\delta_{6,j} c_{19} + \delta_{16,j} K_{69} c_{22} - \delta_{19,j} c_6 + \delta_{22,j} K_{69} c_{16}\right] k_{69}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{69}}{\partial T} = \left[\frac{1}{K_{42}} \frac{dK_{42}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{69} c_{16} c_{22} k_{69} - \left[n_{69} - \frac{b_{69}}{T}\right] \frac{X_{69}}{T}$$

Reaction 70, $AlCl + O \rightleftharpoons AlO + Cl$

$$K_{70} = \frac{K_{42}}{K_{40}}$$

$$k_{70} = a_{70} T^{-n_{70}} e^{-b_{70}/T}$$

$$X_{70} = \left[K_{70} c_{18} c_{22} - c_{14} c_{20}\right] k_{70}$$

$$\frac{\partial X_{70}}{\partial c_j} = \left[\delta_{14,j} c_{20} + \delta_{18,j} K_{70} c_{22} - \delta_{20,j} c_{14} + \delta_{22,j} K_{70} c_{18}\right] k_{70}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{70}}{\partial T} = \left[\frac{1}{K_{42}} \frac{dK_{42}}{dT} - \frac{1}{K_{40}} \frac{dK_{40}}{dT}\right] K_{70} c_{18} c_{22} k_{70} - \left[n_{70} - \frac{b_{70}}{T}\right] \frac{X_{70}}{T}$$

Reaction 71, $2AlCl \rightleftharpoons Al + AlCl_2$

$$K_{71} = \frac{K_{42}}{K_{43}}$$

$$k_{71} = a_{71} T^{-n_{71}} e^{-b_{71}/T}$$

$$X_{71} = \left[K_{71} c_{22}^2 - c_{19} c_{23}\right] k_{71}$$

$$\frac{\partial X_{71}}{\partial c_j} = \left[-\delta_{19,j} c_{23} + 2\delta_{22,j} K_{71} c_{22} - \delta_{23,j} c_{19}\right] k_{71}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{71}}{\partial T} = \left[\frac{1}{K_{42}} \frac{dK_{42}}{dT} - \frac{1}{K_{43}} \frac{dK_{43}}{dT}\right] K_{71} c_{22}^2 k_{71} - \left[n_{71} - \frac{b_{71}}{T}\right] \frac{X_{71}}{T}$$

Reaction 72, $AlCl + AlOCl \rightleftharpoons Al_2O + Cl_2$

$$K_{72} = K_{54}K_{68}$$

$$k_{72} = a_{72}T^{-n_{72}} e^{-b_{72}/T}$$

$$X_{72} = \left[K_{72}c_{22}c_{24} - c_4c_{21}\right] k_{72}$$

$$\frac{\partial X_{72}}{\partial c_j} = \left[-\delta_{4,j}c_{21} - \delta_{21,j}c_4 + \delta_{22,j}K_{72}c_{24} + \delta_{24,j}K_{72}c_{22}\right] k_{72}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{72}}{\partial T} = \left[\frac{1}{K_{54}} \frac{dK_{54}}{dT} + \frac{1}{K_{68}} \frac{dK_{68}}{dT}\right] K_{72}c_{22}c_{24}k_{72} - \left[n_{72} - \frac{b_{72}}{T}\right]\frac{X_{72}}{T}$$

Reaction 73, $AlCl + AlOCl \rightleftharpoons AlO + AlCl_2$

$$K_{73} = \frac{K_{44}}{K_{43}}$$

$$k_{73} = a_{73}T^{-n_{73}} e^{-b_{73}/T}$$

$$X_{73} = \left[K_{73}c_{22}c_{24} - c_{20}c_{23}\right] k_{73}$$

$$\frac{\partial X_{73}}{\partial c_j} = \left[-\delta_{20,j}c_{23} + \delta_{22,j}K_{73}c_{24} - \delta_{23,j}c_{20} + \delta_{24,j}K_{73}c_{22}\right] k_{73}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{73}}{\partial T} = \left[\frac{1}{K_{44}} \frac{dK_{44}}{dT} - \frac{1}{K_{43}} \frac{dK_{43}}{dT}\right] K_{73}c_{22}c_{24}k_{73} - \left[n_{73} - \frac{b_{73}}{T}\right] \frac{X_{73}}{T}$$

Reaction 74, $AlCl + AlOF \rightleftharpoons AlF + AlOCl$

$$K_{74} = \frac{K_{49}}{K_{45}}$$

$$k_{74} = a_{74} T^{-n_{74}} e^{-b_{74}/T}$$

$$X_{74} = \left[K_{74} c_{22} c_{27} - c_{24} c_{25}\right] k_{74}$$

$$\frac{\partial X_{74}}{\partial c_j} = \left[\delta_{22,j} K_{74} c_{27} - \delta_{24,j} c_{25} - \delta_{25,j} c_{24} + \delta_{27,j} K_{74} c_{22}\right] k_{74}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{74}}{\partial T} = \left[\frac{1}{K_{49}} \frac{dK_{49}}{dT} - \frac{1}{K_{45}} \frac{dK_{45}}{dT}\right] K_{74} c_{22} c_{27} k_{74} - \left[n_{74} - \frac{b_{74}}{T}\right] \frac{X_{74}}{T}$$

Reaction 75, $AlCl_2 + Cl \rightleftharpoons AlCl + Cl_2$

$$K_{75} = \frac{K_{43}}{K_4}$$

$$k_{75} = a_{75} T^{-n_{75}} e^{-b_{75}/T}$$

$$X_{75} = \left[K_{75} c_{14} c_{23} - c_4 c_{22}\right] k_{75}$$

$$\frac{\partial X_{75}}{\partial c_j} = \left[-\delta_{4,j} c_{22} + \delta_{14,j} K_{75} c_{23} - \delta_{22,j} c_4 + \delta_{23,j} K_{75} c_{14}\right] k_{75}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{75}}{\partial T} = \left[\frac{1}{K_{43}} \frac{dK_{43}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{75} c_{14} c_{23} k_{75} - \left[n_{75} - \frac{b_{75}}{T}\right] \frac{X_{75}}{T}$$

Reaction 76, $AlOCl + CO \rightleftharpoons AlCl + CO_2$

$$K_{76} = \frac{K_{55}}{K_{50}}$$

$$k_{76} = a_{76} T^{-n_{76}} e^{-b_{76}/T}$$

$$X_{76} = \left[K_{76} c_3 c_{24} - c_1 c_{22}\right] k_{76}$$

$$\frac{\partial X_{76}}{\partial c_j} = \left[-\delta_{1,j} c_{22} + \delta_{3,j} K_{76} c_{24} - \delta_{22,j} c_1 + \delta_{24,j} K_{76} c_3\right] k_{76}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{76}}{\partial T} = \left[\frac{1}{K_{55}} \frac{dK_{55}}{dT} - \frac{1}{K_{50}} \frac{dK_{50}}{dT}\right] K_{76} c_3 c_{24} k_{76} - \left[n_{76} - \frac{b_{76}}{T}\right] \frac{X_{76}}{T}$$

Reaction 77, $AlOCl + HCl \rightleftharpoons AlCl_2 + OH$

$$K_{77} = \frac{K_{73}}{K_{67}}$$

$$k_{77} = a_{77} T^{-n_{77}} e^{-b_{77}/T}$$

$$X_{77} = \left[K_{77} c_6 c_{24} - c_{11} c_{23}\right] k_{77}$$

$$\frac{\partial X_{77}}{\partial c_j} = \left[\delta_{6,j} K_{77} c_{24} - \delta_{11,j} c_{23} - \delta_{23,j} c_{11} + \delta_{24,j} K_{77} c_6\right] k_{77}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{77}}{\partial T} = \left[\frac{1}{K_{73}} \frac{dK_{73}}{dT} - \frac{1}{K_{67}} \frac{dK_{67}}{dT}\right] K_{77} c_6 c_{24} k_{77} - \left[n_{77} - \frac{b_{77}}{T}\right] \frac{X_{77}}{T}$$

Reaction 78, $AlOCl + Cl \rightleftharpoons AlO + Cl_2$

$$K_{78} = \frac{K_{44}}{K_4}$$

$$k_{78} = a_{78} T^{-n_{78}} e^{-b_{78}/T}$$

$$X_{78} = \left[K_{78} c_{14} c_{24} - c_4 c_{20}\right] k_{78}$$

$$\frac{\partial X_{78}}{\partial c_j} = \left[-\delta_{4,j} c_{20} + \delta_{14,j} K_{78} c_{24} - \delta_{20,j} c_4 + \delta_{24,j} K_{78} c_{14}\right] k_{78}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{78}}{\partial T} = \left[\frac{1}{K_{44}} \frac{dK_{44}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{78} c_{14} c_{24} k_{78} - \left[n_{78} - \frac{b_{78}}{T}\right] \frac{X_{78}}{T}$$

Reaction 79, $AlOCl + Cl \rightleftharpoons AlCl_2 + O$

$$K_{79} = \frac{K_{73}}{K_{70}}$$

$$k_{79} = a_{79} T^{-n_{79}} e^{-b_{79}/T}$$

$$X_{79} = \left[K_{79} c_{14} c_{24} - c_{18} c_{23}\right] k_{79}$$

$$\frac{\partial X_{79}}{\partial c_j} = \left[\delta_{14,j} K_{79} c_{24} - \delta_{18,j} c_{23} - \delta_{23,j} c_{18} + \delta_{24,j} K_{79} c_{14}\right] k_{79}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{79}}{\partial T} = \left[\frac{1}{K_{73}} \frac{dK_{73}}{dT} - \frac{1}{K_{70}} \frac{dK_{70}}{dT}\right] K_{79} c_{14} c_{24} k_{79} - \left[n_{79} - \frac{b_{79}}{T}\right] \frac{X_{79}}{T}$$

Reaction 80, $AlOCl + H \rightleftharpoons AlO + HCl$

$$K_{80} = \frac{K_{44}}{K_6}$$

$$k_{80} = a_{80} T^{-n_{80}} e^{-b_{80}/T}$$

$$X_{80} = \left[K_{80} c_{16} c_{24} - c_6 c_{20}\right] k_{80}$$

$$\frac{\partial X_{80}}{\partial c_j} = \left[-\delta_{6,j} c_{20} + \delta_{16,j} K_{80} c_{24} - \delta_{20,j} c_6 + \delta_{24,j} K_{80} c_{16}\right] k_{80}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{80}}{\partial T} = \left[\frac{1}{K_{44}} \frac{dK_{44}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{80} c_{16} c_{24} k_{80} - \left[n_{80} - \frac{b_{80}}{T}\right] \frac{X_{80}}{T}$$

Reaction 81, $AlOCl + H \rightleftharpoons AlCl + OH$

$$K_{81} = K_{55} K_{59}$$

$$k_{81} = a_{81} T^{-n_{81}} e^{-b_{81}/T}$$

$$X_{81} = \left[K_{81} c_{16} c_{24} - c_{11} c_{22}\right] k_{81}$$

$$\frac{\partial X_{81}}{\partial c_j} = \left[-\delta_{11,j} c_{22} + \delta_{16,j} K_{81} c_{24} - \delta_{22,j} c_{11} + \delta_{24,j} K_{81} c_{16}\right] k_{81}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{81}}{\partial T} = \left[\frac{1}{K_{55}} \frac{dK_{55}}{dT} + \frac{1}{K_{59}} \frac{dK_{59}}{dT}\right] K_{81} c_{16} c_{24} k_{81} - \left[n_{81} - \frac{b_{81}}{T}\right] \frac{X_{81}}{T}$$

Reaction 82, $AlOCl + O \rightleftharpoons AlCl + O_2$

$$K_{82} = \frac{K_{55}}{K_{53}}$$

$$k_{82} = a_{82} T^{-n_{82}} e^{-b_{82}/T}$$

$$X_{82} = \left[K_{82} c_{18} c_{24} - c_{12} c_{22}\right] k_{82}$$

$$\frac{\partial X_{82}}{\partial c_j} = \left[-\delta_{12,j} c_{22} + \delta_{18,j} K_{82} c_{24} - \delta_{22,j} c_{12} + \delta_{24,j} K_{82} c_{18}\right] k_{82}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{82}}{\partial T} = \left[\frac{1}{K_{55}} \frac{dK_{55}}{dT} - \frac{1}{K_{53}} \frac{dK_{53}}{dT}\right] K_{82} c_{18} c_{24} k_{82} - \left[n_{82} - \frac{b_{82}}{T}\right] \frac{X_{82}}{T}$$

Reaction 83, $2AlF \rightleftharpoons Al + AlF_2$

$$K_{83} = \frac{K_{46}}{K_{47}}$$

$$k_{83} = a_{83} T^{-n_{83}} e^{-b_{83}/T}$$

$$X_{83} = \left[K_{83} c_{25}^2 - c_{19} c_{26}\right] k_{83}$$

$$\frac{\partial X_{83}}{\partial c_j} = \left[-\delta_{19,j} c_{26} + 2\delta_{25,j} c_{25} - \delta_{26,j} c_{19}\right] k_{83}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{83}}{\partial T} = \left[\frac{1}{K_{46}} \frac{dK_{46}}{dT} - \frac{1}{K_{47}} \frac{dK_{47}}{dT}\right] K_{83} c_{25}^2 k_{83} - \left[n_{83} - \frac{b_{83}}{T}\right] \frac{X_{83}}{T}$$

Reaction 84, $AlF + HCl \rightleftharpoons AlCl + HF$

$$K_{84} = \frac{K_{46}}{K_7 K_{69}}$$

$$k_{84} = a_{84} T^{-n_{84}} e^{-b_{84}/T}$$

$$X_{84} = \left[K_{84} c_6 c_{25} - c_7 c_{22}\right] k_{84}$$

$$\frac{\partial X_{84}}{\partial c_j} = \left[\delta_{6,j} K_{84} c_{25} - \delta_{7,j} c_{22} - \delta_{22,j} c_7 + \delta_{25,j} K_{84} c_6\right] k_{84}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{84}}{\partial T} = \left[\frac{1}{K_{46}} \frac{dK_{46}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT} - \frac{1}{K_{69}} \frac{dK_{69}}{dT}\right] K_{84} c_6 c_{25} k_{84} - \left[n_{84} - \frac{b_{84}}{T}\right] \frac{X_{84}}{T}$$

Reaction 85, $AlF + HF \rightleftharpoons AlF_2 + H$

$$K_{85} = \frac{K_7}{K_{47}}$$

$$k_{85} = a_{85} T^{-n_{85}} e^{-b_{85}/T}$$

$$X_{85} = \left[K_{85} c_7 c_{25} - c_{16} c_{26}\right] k_{85}$$

$$\frac{\partial X_{85}}{\partial c_j} = \left[\delta_{7,j} K_{85} c_{25} - \delta_{16,j} c_{26} + \delta_{25,j} K_{85} c_7 - \delta_{26,j} c_{16}\right] k_{85}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{85}}{\partial T} = \left[\frac{1}{K_7} \frac{dK_7}{dT} - \frac{1}{K_{47}} \frac{dK_{47}}{dT}\right] K_{85} c_7 c_{25} k_{85} - \left[n_{85} - \frac{b_{85}}{T}\right] \frac{X_{85}}{T}$$

Reaction 86, $AlF + NO \rightleftharpoons AlOF + N$

$$K_{86} = \frac{K_{10}}{K_{49}}$$

$$k_{86} = a_{86} T^{-n_{86}} e^{-b_{86}/T}$$

$$X_{86} = \left[K_{86} c_{10} c_{25} - c_{17} c_{27}\right] k_{86}$$

$$\frac{\partial X_{86}}{\partial c_j} = \left[\delta_{10,j} K_{86} c_{25} - \delta_{17,j} c_{27} + \delta_{25,j} K_{86} c_{10} - \delta_{27,j} c_{17}\right] k_{86}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{86}}{\partial T} = \left[\frac{1}{K_{10}} \frac{dK_{10}}{dT} - \frac{1}{K_{49}} \frac{dK_{49}}{dT}\right] K_{86} c_{10} c_{25} k_{86} - \left[n_{86} - \frac{b_{86}}{T}\right] \frac{X_{86}}{T}$$

Reaction 87, $AlF + Cl \rightleftharpoons AlCl + F$

$$K_{87} = \frac{K_{46}}{K_{42}}$$

$$k_{87} = a_{87} T^{-n_{87}} e^{-b_{87}/T}$$

$$X_{87} = \left[K_{87} c_{14} c_{25} - c_{15} c_{22}\right] k_{87}$$

$$\frac{\partial X_{87}}{\partial c_j} = \left[\delta_{14,j} K_{87} c_{25} - \delta_{15,j} c_{22} - \delta_{22,j} c_{15} + \delta_{25,j} K_{87} c_{14}\right] k_{87}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{87}}{\partial T} = \left[\frac{1}{K_{46}} \frac{dK_{46}}{dT} - \frac{1}{K_{42}} \frac{dK_{42}}{dT}\right] K_{87} c_{14} c_{25} k_{87} - \left[n_{87} - \frac{b_{87}}{T}\right] \frac{X_{87}}{T}$$

Reaction 88, $AlF + F \rightleftharpoons Al + F_2$

$$K_{88} = \frac{K_{46}}{K_5}$$

$$k_{88} = a_{88} T^{-n_{88}} e^{-b_{88}/T}$$

$$X_{88} = \left[K_{88} c_{15} c_{25} - c_5 c_{19}\right] k_{88}$$

$$\frac{\partial X_{88}}{\partial c_j} = \left[-\delta_{5,j} c_{19} + \delta_{15,j} K_{88} c_{25} - \delta_{19,j} c_5 + \delta_{25,j} K_{88} c_{15}\right] k_{88}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{88}}{\partial T} = \left[\frac{1}{K_{46}} \frac{dK_{46}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{88} c_{15} c_{25} k_{88} - \left[n_{88} - \frac{b_{88}}{T}\right] \frac{X_{88}}{T}$$

Reaction 89, $AlF + H \rightleftharpoons Al + HF$

$$K_{89} = \frac{K_{46}}{K_7}$$

$$k_{89} = a_{89} T^{-n_{89}} e^{-b_{89}/T}$$

$$X_{89} = \left[K_{89} c_{16} c_{25} - c_7 c_{19}\right] k_{89}$$

$$\frac{\partial X_{89}}{\partial c_j} = \left[-\delta_{7,j} c_{19} + \delta_{16,j} K_{89} c_{25} - \delta_{19,j} c_7 + \delta_{25,j} K_{89} c_{16}\right] k_{89}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{89}}{\partial_T} = \left[\frac{1}{k_{46}} \frac{dk_{46}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{89} c_{16} c_{25} k_{89} - \left[n_{89} - \frac{b_{89}}{T}\right] \frac{X_{89}}{T}$$

Reaction 90, $AlF + AlOF \rightleftharpoons AlO + AlF_2$

$$K_{90} = \frac{K_{48}}{K_{47}}$$

$$k_{90} = a_{90} T^{-n_{90}} e^{-b_{90}/T}$$

$$X_{90} = \left[K_{90} c_{25} c_{27} - c_{20} c_{26}\right] k_{90}$$

$$\frac{\partial X_{90}}{\partial c_j} = \left[- \delta_{20,j} c_{26} + \delta_{25,j} K_{90} c_{27} - \delta_{26,j} c_{20} + \delta_{27,j} K_{90} c_{25}\right] k_{90}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{90}}{\partial T} = \left[\frac{1}{K_{48}} \frac{dK_{48}}{dT} - \frac{1}{K_{47}} \frac{dK_{47}}{dT}\right] K_{90} c_{25} c_{27} k_{90} - \left[n_{90} - \frac{b_{90}}{T}\right] \frac{X_{90}}{T}$$

Reaction 91, $AlF_2 + F \rightleftharpoons AlF + F_2$

$$K_{91} = \frac{K_{47}}{K_5}$$

$$k_{91} = a_{91} T^{-n_{91}} e^{-n_{91}/T}$$

$$X_{91} = \left[K_{91} c_{15} c_{26} - c_5 c_{25}\right] k_{91}$$

$$\frac{\partial X_{91}}{\partial c_j} = \left[-\delta_{5,j} c_{25} + \delta_{15,j} K_{91} c_{26} - \delta_{25,j} c_5 + \delta_{26,j} K_{91} c_{15}\right] k_{91}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{91}}{\partial T} = \left[\frac{1}{K_{47}} \frac{dK_{47}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{91} c_{15} c_{26} k_{91} - \left[n_{91} - \frac{b_{91}}{T}\right] \frac{X_{91}}{T}$$

Reaction 92, $AlOF + HCl \rightleftharpoons AlOCl + HF$

$$K_{92} = \frac{K_{48}}{K_7 K_{80}}$$

$$k_{92} = a_{92} T^{-n_{92}} e^{-b_{92}/T}$$

$$X_{92} = \left[K_{92} c_6 c_{27} - c_7 c_{24} \right] k_{92}$$

$$\frac{\partial X_{92}}{\partial c_j} = \left[\delta_{6,j} K_{92} c_{27} - \delta_{7,j} c_{24} - \delta_{24,j} c_7 + \delta_{27,j} K_{92} c_6 \right] k_{92}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{92}}{\partial T} = \left[\frac{1}{K_{48}} \frac{dK_{48}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT} - \frac{1}{K_{80}} \frac{dK_{80}}{dT} \right] K_{92} c_6 c_{27} k_{92}$$

$$- \left[n_{92} - \frac{b_{92}}{T} \right] \frac{X_{92}}{T}$$

Reaction 93, $AlOF + Cl \rightleftharpoons AlOCl + F$

$$K_{93} = \frac{K_{59} K_{90}}{K_{80}}$$

$$k_{93} = a_{93} T^{-n_{93}} e^{-b_{93}/T}$$

$$X_{93} = \left[K_{93} c_7 c_{27} - c_{11} c_{26} \right] k_{93}$$

$$\frac{\partial X_{93}}{\partial c_j} = \left[\delta_{7,j} K_{93} c_{27} - \delta_{11,j} c_{26} - \delta_{26,j} c_{11} + \delta_{27,j} K_{93} c_7 \right] k_{93}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{93}}{\partial T} = \left[\frac{1}{K_{59}}\frac{dK_{59}}{dT} + \frac{1}{K_{90}}\frac{dK_{90}}{dT} - \frac{1}{K_{89}}\frac{dK_{89}}{dT}\right] K_{93}c_7c_{27}k_{93}$$

$$- \left[n_{93} - \frac{b_{93}}{T}\right]\frac{X_{93}}{T}$$

Reaction 94, $AlOF + Cl \rightleftharpoons AlOCl + F$

$$K_{94} = \frac{K_{48}}{K_{44}}$$

$$k_{94} = a_{94}T^{-n_{94}} e^{-b_{94}/T}$$

$$X_{94} = \left[K_{94}c_{14}c_{27} - c_{15}c_{24}\right] k_{94}$$

$$\frac{\partial X_{94}}{\partial c_j} = \left[\delta_{14,j}K_{94}c_{27} - \delta_{15,j}c_{24} - \delta_{24,j}c_{15} + \delta_{27,j}K_{94}c_{14}\right] k_{94}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{94}}{\partial T} = \left[\frac{1}{K_{48}}\frac{dK_{48}}{dT} - \frac{1}{K_{44}}\frac{dK_{44}}{dT}\right] K_{94}c_{14}c_{27}k_{94} - \left[n_{94} - \frac{b_{94}}{T}\right]\frac{X_{94}}{T}$$

Reaction 95, $AlOF + F \rightleftharpoons AlO + F_2$

$$K_{95} = \frac{K_{48}}{K_5}$$

$$k_{95} = a_{95}T^{-n_{95}} e^{-b_5/T}$$

$$X_{95} = \left[K_{95}c_{15}c_{27} - c_5c_{20}\right] k_{95}$$

$$\frac{\partial X_{95}}{\partial c_j} = \left[-\delta_{5,j}c_{20} + \delta_{15,j}K_{95}c_{27} - \delta_{20,j}c_5 + \delta_{27,j}K_{95}c_{15}\right] k_{95}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{95}}{\partial T} = \left[\frac{1}{K_{48}}\frac{dK_{48}}{dT} - \frac{1}{K_5}\frac{dK_5}{dT}\right]K_{95}c_{15}c_{27}k_{95} - \left[n_{95} - \frac{b_{95}}{T}\right]\frac{X_{95}}{T}$$

Reaction 96, $AlOF + F \rightleftharpoons AlF_2 + O$

$$K_{96} = K_{58}K_{90}$$

$$k_{96} = a_{96}T^{-n_{96}} e^{-b_{96}/T}$$

$$X_{96} = \left[K_{96}c_{15}c_{27} - c_{18}c_{26}\right]k_{96}$$

$$\frac{\partial X_{96}}{\partial c_j} = \left[\delta_{15,j}K_{96}c_{27} - \delta_{18,j}c_{26} - \delta_{26,j}c_{18} + \delta_{27,j}K_{96}c_{15}\right]k_{96}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{96}}{\partial T} = \left[\frac{1}{K_{58}}\frac{dK_{58}}{dT} + \frac{1}{K_{90}}\frac{dK_{90}}{dT}\right]K_{96}c_{15}c_{27}k_{96} - \left[n_{96} - \frac{b_{96}}{T}\right]\frac{X_{96}}{T}$$

Reaction 97, $AlOF + H \rightleftharpoons AlO + HF$

$$K_{97} = \frac{K_{48}}{K_7}$$

$$k_{97} = a_{97}T^{-n_{97}} e^{-b_{97}/T}$$

$$X_{97} = \left[K_{97}c_{16}c_{27} - c_7c_{20}\right] K_{97}$$

$$\frac{\partial X_{97}}{\partial c_j} = \left[-\delta_{7,j}c_{20} + \delta_{16,j}K_{97}c_{27} - \delta_{20,j}c_7 + \delta_{27,j}K_{97}c_{16}\right]K_{97}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{97}}{\partial T} = \left[\frac{1}{K_{48}}\frac{dK_{48}}{dT} - \frac{1}{K_7}\frac{dK_7}{dT}\right]K_{97}c_{16}c_{27}k_{97} - \left[n_{97} - \frac{b_{97}}{T}\right]\frac{X_{97}}{T}$$

Reaction 98, $AlOF + H \rightleftharpoons AlF + OH$

$$K_{98} = \frac{K_{59}}{K_{61}}$$

$$k_{98} = a_{98} T^{-n_{98}} e^{-b_{98}/T}$$

$$X_{98} = \left[K_{98} c_{16} c_{27} - c_{11} c_{25} \right] k_{98}$$

$$\frac{\partial X_{98}}{\partial c_j} = \left[-\delta_{11,j} c_{25} + \delta_{16,j} K_{98} c_{27} - \delta_{25,j} c_{11} + \delta_{27,j} K_{98} c_{16} \right] k_{98}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{98}}{\partial T} = \left[\frac{1}{K_{59}} \frac{dK_{59}}{dT} - \frac{1}{K_{61}} \frac{dK_{61}}{dT} \right] K_{98} c_{16} c_{27} k_{98} - \left[n_{98} - \frac{b_{98}}{T} \right] \frac{X_{98}}{T}$$

Reaction 99, $AlOF + O \rightleftharpoons AlF + O_2$

$$K_{99} = \frac{K_{49}}{K_{12}}$$

$$k_{99} = a_{99} T^{-n_{99}} e^{-b_{99}/T}$$

$$X_{99} = \left[K_{99} c_{18} c_{27} - c_{12} c_{25} \right] k_{99}$$

$$\frac{\partial X_{99}}{\partial c_j} = \left[-\delta_{12,j} c_{25} + \delta_{18,j} K_{99} c_{27} - \delta_{25,j} c_{12} + \delta_{27,j} K_{99} c_{18} \right] k_{99}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{99}}{\partial T} = \left[\frac{1}{K_{49}} \frac{dK_{49}}{dT} - \frac{1}{K_{12}} \frac{dK_{12}}{dT} \right] K_{99} c_{18} c_{27} k_{99} - \left[n_{99} - \frac{b_{99}}{T} \right] \frac{X_{99}}{T}$$

Reaction 100, $BeCl_2 + M \rightleftharpoons BeCl + Cl + M$

$$k_{100} = a_{100} T^{-n_{100}} e^{-b_{100}/T}$$

$$M_{100} = \sum_{i=1}^{57} m_{100,i} c_i$$

$$X_{100} = \left[K_{100} c_{45} - \rho c_{14} c_{44} \right] M_{100} k_{100}$$

$$\frac{\partial X_{100}}{\partial c_j} = \frac{X_{100}}{M_{100}} m_{100,j} + \delta_{45,j} K_{100} M_{100} k_{100} - \delta_{14,j} \rho c_{44} M_{100} k_{100}$$

$$- \delta_{44,j} \rho c_{14} M_{100} k_{100} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{100}}{\partial \rho} = -c_{14} c_{44} M_{100} k_{100}$$

$$\frac{\partial X_{100}}{\partial T} = c_{44} M_{100} k_{100} \frac{dK_{100}}{dT} - \left[n_{100} - \frac{b_{100}}{T} \right] \frac{X_{100}}{T}$$

Reaction 101, $BeF_2 + M \rightleftharpoons BeF + F + M$

$$k_{101} = a_{101} T^{-n_{101}} e^{-b_{101}/T}$$

$$M_{101} = \sum_{i=1}^{57} m_{101,i} c_i$$

$$X_{101} = \left[K_{101} c_{47} - \rho c_{15} c_{46} \right] M_{101} k_{101}$$

$$\frac{\partial X_{101}}{\partial c_j} = \frac{X_{101}}{M_{101}} m_{101,j} + \delta_{47,j} K_{101} M_{101} k_{101} - \delta_{15,j} \rho c_{46} M_{101} k_{101}$$

$$- \delta_{46,j} \rho c_{15} M_{101} k_{101} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{101}}{\partial \rho} = -c_{15}c_{46}M_{101}k_{101}$$

$$\frac{\partial X_{101}}{\partial T} = c_{47}M_{101}k_{101}\frac{dK_{101}}{dT} - \left[n_{101} - \frac{b_{101}}{T}\right]\frac{X_{101}}{T}$$

Reaction 102, $BeOH + M \rightleftharpoons Be + OH + M$

$$k_{102} = a_{102}T^{-n_{102}}e^{-b_{102}/T}$$

$$M_{102} = \sum_{i=1}^{57} m_{102,i}c_i$$

$$X_{102} = \left[K_{102}c_{43} - \rho c_{11}c_{40}\right]M_{102}k_{102}$$

$$\frac{\partial X_{102}}{\partial c_j} = \frac{X_{102}}{M_{102}} m_{102,j} + \delta_{43,j}K_{102}M_{102}k_{102} - \delta_{11,j}\rho c_{40}M_{102}k_{102}$$

$$-\delta_{40,j}\rho c_{11}M_{102}k_{102} \quad , \qquad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{102}}{\partial \rho} = -c_{11}c_{40}M_{102}k_{102}$$

$$\frac{\partial X_{102}}{\partial T} = c_{43}M_{102}k_{102}\frac{dK_{102}}{dT} - \left[n_{102} - \frac{b_{102}}{T}\right]\frac{X_{102}}{T}$$

Reaction 103, $BeOH + M \rightleftharpoons BeO + H + M$

$$k_{103} = a_{103}T^{-n_{103}}e^{-b_{103}/T}$$

$$M_{103} = \sum_{i=1}^{57} m_{103,i}c_i$$

$$X_{103} = \left[K_{103}c_{43} - \rho c_{16}c_{41}\right]M_{103}k_{103}$$

$$\frac{\partial X_{103}}{\partial c_j} = \frac{X_{103}}{M_{103}} m_{103,j} + \delta_{43,j} K_{103} M_{103} k_{103} - \delta_{16,j} \rho c_{41} M_{103} k_{103}$$

$$- \delta_{41,j} \rho c_{16} M_{103} k_{103} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{103}}{\partial \rho} = -c_{16} c_{41} M_{103} k_{103}$$

$$\frac{\partial X_{103}}{\partial T} = c_{43} M_{103} k_{103} \frac{dK_{103}}{dT} - \left[n_{103} - \frac{b_{103}}{T} \right] \frac{X_{103}}{T}$$

Reaction 104, $BeCl + M \rightleftharpoons Be + Cl + M$

$$k_{104} = a_{104} T^{-n_{104}} e^{-b_{104}/T}$$

$$M_{104} = \sum_{i=1}^{57} m_{104,i} c_i$$

$$X_{104} = \left[K_{104} c_{44} - \rho c_{14} c_{40} \right] M_{104} k_{104}$$

$$\frac{\partial X_{104}}{\partial c_j} = \frac{X_{104}}{M_{104}} m_{104,j} + \delta_{44,j} K_{104} M_{104} k_{104} - \delta_{14,j} \rho c_{40} M_{104} k_{104}$$

$$- \delta_{40,j} \rho c_{14} M_{104} k_{104} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{104}}{\partial \rho} = -c_{14} c_{40} M_{104} k_{104}$$

$$\frac{\partial X_{104}}{\partial T} = c_{44} M_{104} k_{104} \frac{dK_{104}}{dT} - \left[n_{104} - \frac{b_{104}}{T} \right] \frac{X_{104}}{T}$$

Reaction 105, $BeF + M \rightleftharpoons Be + F + M$

$$k_{105} = a_{105} T^{-n_{105}} e^{-b_{105}/T}$$

$$M_{105} = \sum_{i=1}^{57} m_{105,i} c_i$$

$$X_{105} = \left[K_{105} c_{46} - \rho c_{15} c_{40}\right] M_{105} k_{105}$$

$$\frac{\partial X_{105}}{\partial c_j} = \frac{X_{105}}{M_{105}} m_{105,j} + \delta_{46,j} K_{105} M_{105} k_{105} - \delta_{15,j} \rho c_{40} M_{105} k_{105}$$

$$-\delta_{40,j} \rho c_{15} M_{105} k_{105} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{105}}{\partial \rho} = -c_{15} c_{40} M_{105} k_{105}$$

$$\frac{\partial X_{105}}{\partial T} = c_{46} M_{105} k_{105} \frac{dK_{105}}{dT} - \left[n_{105} - \frac{b_{105}}{T}\right] \frac{X_{105}}{T}$$

Reaction 106, $BeO + M \rightleftharpoons Be + O + M$

$$k_{106} = a_{106} T^{-n_{106}} e^{-b_{106}/T}$$

$$M_{106} = \sum_{i=1}^{57} m_{106,i} c_i$$

$$X_{106} = \left[K_{106} c_{41} - \rho c_{18} c_{40}\right] M_{106} k_{106}$$

$$\frac{\partial X_{106}}{\partial c_j} = \frac{X_{106}}{M_{106}} m_{106,j} + \delta_{41,j} K_{106} M_{106} k_{106} - \delta_{18,j} \rho c_{40} M_{106} k_{106}$$

$$-\delta_{40,j} \rho c_{18} M_{106} k_{106} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{106}}{\partial \rho} = -c_{18}c_{40}M_{106}k_{106}$$

$$\frac{\partial X_{106}}{\partial T} = c_{41}M_{106}k_{106}\frac{dK_{106}}{dT} - \left[n_{106} - \frac{b_{106}}{T}\right]\frac{X_{106}}{T}$$

Reaction 107, $Be_2O + M \rightleftharpoons Be + BeO + M$

$$k_{107} = a_{107}T^{-n_{107}}e^{-b_{107}/T}$$

$$M_{107} = \sum_{i=1}^{57} m_{107,i}c_i$$

$$X_{107} = \left[K_{107}c_{42} - \rho c_{40}c_{41}\right] M_{107}k_{107}$$

$$\frac{\partial X_{107}}{\partial c_j} = \frac{X_{107}}{M_{107}} m_{107,j} + \delta_{42,j}K_{107}M_{107}k_{107} - \delta_{40,j}\rho c_{41}M_{107}k_{107}$$

$$- \delta_{41,j}\rho c_{40}M_{107}k_{107} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{107}}{\partial \rho} = - c_{40}c_{41}M_{107}k_{107}$$

$$\frac{\partial X_{107}}{\partial T} = c_{42}M_{107}k_{107}\frac{dK_{107}}{dT} - \left[n_{10} - \frac{b_{107}}{T}\right]\frac{X_{107}}{T}$$

Reaction 108, $BeO_2H_2 + M \rightleftharpoons BeOH + OH + M$

$$k_{108} = a_{108}T^{-n_{108}}e^{-b_{108}/T}$$

$$M_{108} = \sum_{i=1}^{57} m_{108,i}c_i$$

$$X_{108} = \left[K_{108}c_{48} - \rho c_{11}c_{43}\right] M_{108}k_{108}$$

$$\frac{\partial X_{108}}{\partial c_j} = \frac{X_{108}}{M_{108}} \; m_{108,j} - \delta_{11,j}\rho c_{43} M_{108} k_{108} - \delta_{43,j}\rho c_{11} M_{108} k_{108}$$

$$+ \delta_{48,j} K_{108} M_{108} k_{108} \quad , \qquad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{108}}{\partial \rho} = -c_{11} c_{43} M_{108} k_{108}$$

$$\frac{\partial X_{108}}{\partial T} = c_{48} M_{108} k_{108} \frac{dK_{108}}{dT} - \left[n_{108} - \frac{b_{108}}{T} \right] \frac{X_{108}}{T}$$

Reaction 109, $Be + BeF_2 \rightleftarrows 2BeF$

$$K_{109} = \frac{K_{101}}{K_{105}}$$

$$k_{109} = a_{109} T^{-n_{109}} e^{-b_{109}/T}$$

$$X_{109} = \left[K_{109} c_{40} c_{47} - c_{46}^2 \right] k_{109}$$

$$\frac{\partial X_{109}}{\partial c_j} = \left[\delta_{40,j} K_{109} c_{47} - 2\delta_{46,j} c_{46} + \delta_{47,j} K_{109} c_{40} \right] k_{109}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{109}}{\partial T} = \left[\frac{1}{K_{101}} \frac{dK_{101}}{dT} - \frac{1}{K_{105}} \frac{dK_{105}}{dT} \right] K_{109} c_{40} c_{47} k_{109}$$

$$- \left[n_{109} - \frac{b_{109}}{T} \right] \frac{X_{109}}{T}$$

Reaction 110, $BeO + H_2O \rightleftharpoons BeOH + OH$

$$K_{110} = \frac{K_2}{K_{103}}$$

$$k_{110} = a_{110}T^{-n_{110}} e^{-b_{110}/T}$$

$$X_{110} = \left[K_{110}c_2c_{41} - c_{11}c_{43}\right] k_{110}$$

$$\frac{\partial X_{110}}{\partial c_j} = \left[\delta_{2,j}K_{110}c_{41} - \delta_{11,j}c_{43} + \delta_{41,j}K_{110}c_2 - \delta_{43,j}c_{11}\right]k_{110}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{110}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_{103}}\frac{dK_{103}}{dT}\right] K_{110}c_2c_{41}k_{110} - \left[n_{110} - \frac{b_{110}}{T}\right]\frac{X_{110}}{T}$$

Reaction 111, $BeO + CO \rightleftharpoons Be + CO_2$

$$K_{111} = \frac{K_{106}}{K_1}$$

$$k_{111} = a_{111}T^{-n_{111}} e^{-b_{111}/T}$$

$$X_{111} = \left[K_{111}c_3c_{41} - c_1c_{40}\right] k_{111}$$

$$\frac{\partial X_{111}}{\partial c_j} = \left[-\delta_{1,j}c_{40} + \delta_{3,j}K_{111}c_{41} - \delta_{40,j}c_1 + \delta_{41,j}K_{111}c_3\right] k_{111}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{111}}{\partial T} = \left[\frac{1}{K_{106}}\frac{dK_{106}}{dT} - \frac{1}{K_1}\frac{dK_1}{dT}\right] K_{111}c_3c_{41}k_{111} - \left[n_{111} - \frac{b_{111}}{T}\right]\frac{X_{111}}{T}$$

Reaction 112, $BeO + HCl \rightleftharpoons BeCl + OH$

$$K_{112} = \frac{K_6 K_{106}}{K_{11} K_{104}}$$

$$k_{112} = a_{112} T^{-n_{112}} e^{-b_{112}/T}$$

$$X_{112} = \left[K_{112} c_6 c_{41} - c_{11} c_{44}\right] k_{112}$$

$$\frac{\partial X_{112}}{\partial c_j} = \left[\delta_{6,j} K_{112} c_{41} - \delta_{11,j} c_{44} + \delta_{41,j} K_{112} c_6 - \delta_{44,j} c_{11}\right] k_{112}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{112}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT} - \frac{1}{K_{104}}\frac{dK_{104}}{dT} + \frac{1}{K_{106}}\frac{dK_{106}}{dT}\right] \cdot$$

$$K_{112} c_6 c_{41} k_{112} - \left[n_{112} - \frac{b_{112}}{T}\right]\frac{X_{112}}{T}$$

Reaction 113, $BeO + HF \rightleftharpoons BeOH + F$

$$K_{113} = \frac{K_7}{K_{103}}$$

$$k_{113} = a_{113} T^{-n_{113}} e^{-b_{113}/T}$$

$$X_{113} = \left[K_{113} c_7 c_{41} - c_{15} c_{43}\right] k_{113}$$

$$\frac{\partial X_{113}}{\partial c_j} = \left[\delta_{7,j} K_{113} c_{41} - \delta_{15,j} c_{43} + \delta_{41,j} K_{113} c_7 - \delta_{43,j} c_{15}\right] k_{113}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{113}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{103}}\frac{dK_{103}}{dT}\right] K_{113} c_7 c_{41} k_{113} - \left[n_{113} - \frac{b_{113}}{T}\right]\frac{X_{113}}{T}$$

Reaction 114, $BeO + C \rightleftharpoons Be + CO$

$$K_{114} = \frac{K_{106}}{K_3}$$

$$k_{114} = a_{114} T^{-n_{114}} e^{-b_{114}/T}$$

$$X_{114} = \left[K_{114} c_{13} c_{41} - c_3 c_{40}\right] k_{114}$$

$$\frac{\partial X_{114}}{\partial c_j} = \left[-\delta_{3,j} c_{40} + \delta_{13,j} K_{114} c_{41} - \delta_{40,j} c_3 + \delta_{41,j} K_{114} c_{13}\right] k_{114}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{114}}{\partial T} = \left[\frac{1}{K_{106}} \frac{dK_{106}}{dT} - \frac{1}{K_3} \frac{dK_3}{dT}\right] K_{114} c_3 c_{41} k_{114} - \left[n_{114} - \frac{b_{114}}{T}\right] \frac{X_{114}}{T}$$

Reaction 115, $BeO + Cl \rightleftharpoons BeCl + O$

$$K_{115} = \frac{K_{106}}{K_{104}}$$

$$k_{115} = a_{115} T^{-n_{115}} e^{-b_{115}/T}$$

$$X_{115} = \left[K_{115} c_{14} c_{41} - c_{18} c_{44}\right] k_{115}$$

$$\frac{\partial X_{115}}{\partial c_j} = \left[\delta_{14,j} K_{115} c_{41} - \delta_{18,j} c_{44} + \delta_{41,j} K_{115} c_{14} - \delta_{44,j} c_{18}\right] k_{115}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{115}}{\partial T} = \left[\frac{1}{K_{106}} \frac{dK_{106}}{dT} - \frac{1}{K_{104}} \frac{dK_{104}}{dT}\right] K_{115} c_{14} c_{41} k_{115} - \left[n_{115} - \frac{b_{115}}{T}\right] \frac{X_{115}}{T}$$

Reaction 116, $BeO + H \rightleftharpoons Be + OH$

$$K_{116} = \frac{K_{106}}{K_{11}}$$

$$k_{116} = a_{116} T^{-n_{116}} e^{-b_{116}/T}$$

$$X_{116} = \left[K_{116} c_{16} c_{41} - c_{11} c_{40}\right] k_{116}$$

$$\frac{\partial X_{116}}{\partial c_j} = \left[-\delta_{11,j} c_{40} + \delta_{16,j} K_{116} c_{41} - \delta_{40,j} c_{11} + \delta_{41,j} K_{116} c_{16}\right] k_{116}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{116}}{\partial T} = \left[\frac{1}{K_{106}} \frac{dK_{106}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{116} c_{16} c_{41} k_{116} - \left[n_{116} - \frac{b_{116}}{T}\right] \frac{X_{116}}{T}$$

Reaction 117, $BeO + N \rightleftharpoons Be + NO$

$$K_{117} = \frac{K_{106}}{K_{10}}$$

$$k_{117} = a_{117} T^{-n_{117}} e^{-b_{117}/T}$$

$$X_{117} = \left[K_{117} c_{17} c_{41} - c_{10} c_{40}\right] k_{117}$$

$$\frac{\partial X_{117}}{\partial c_j} = \left[-\delta_{10,j} c_{40} + \delta_{17,j} K_{117} c_{41} - \delta_{40,j} c_{10} + \delta_{41,j} K_{117} c_{17}\right] k_{117}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{117}}{\partial T} = \left[\frac{1}{K_{106}} \frac{dK_{106}}{dT} - \frac{1}{K_{10}} \frac{dK_{10}}{dT}\right] K_{117} c_{17} c_{41} k_{117} - \left[n_{117} - \frac{b_{117}}{T}\right] \frac{X_{117}}{T}$$

Reaction 118, $BeO + O \rightleftharpoons Be + O_2$

$$K_{118} = \frac{K_{106}}{K_{12}}$$

$$k_{118} = a_{118} T^{-n_{118}} e^{-b_{118}/T}$$

$$X_{118} = \left[K_{118} c_{18} c_{41} - c_{12} c_{40}\right] k_{118}$$

$$\frac{\partial X_{118}}{\partial c_j} = \left[-\delta_{12,j} c_{40} + \delta_{18,j} K_{118} c_{41} - \delta_{40,j} c_{12} + \delta_{41,j} K_{118} c_{18}\right] k_{118}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{118}}{\partial T} = \left[\frac{1}{K_{106}} \frac{dK_{106}}{dT} - \frac{1}{K_{12}} \frac{dK_{12}}{dT}\right] K_{118} c_{18} c_{41} k_{118} - \left[n_{118} - \frac{b_{118}}{T}\right] \frac{X_{118}}{T}$$

Reaction 119, $BeO + BeF \rightleftharpoons Be_2O + F$

$$K_{119} = \frac{K_{105}}{K_{107}}$$

$$k_{119} = a_{119} T^{-n_{119}} e^{-b_{119}/T}$$

$$X_{119} = \left[K_{119} c_{41} c_{46} - c_{15} c_{42}\right] k_{119}$$

$$\frac{\partial X_{119}}{\partial c_j} = \left[-\delta_{15,j} c_{42} + \delta_{41,j} K_{119} c_{46} - \delta_{42,j} c_{15} + \delta_{46,j} K_{119} c_{41}\right] k_{119}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{119}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_{107}} \frac{dK_{107}}{dT}\right] K_{119} c_{41} c_{46} k_{119} - \left[n_{119} - \frac{b_{119}}{T}\right] \frac{X_{119}}{T}$$

Reaction 120, $Be_2O + H_2O \rightleftharpoons 2BeOH$

$$K_{120} = \frac{K_{107}K_{110}}{K_{103}K_{116}}$$

$$k_{120} = a_{120}T^{-n_{120}} e^{-b_{120}/T}$$

$$X_{120} = \left[K_{120}c_2c_{42} - c_{43}^2\right] k_{120}$$

$$\frac{\partial X_{120}}{\partial c_j} = \left[\delta_{2,j}K_{120}c_{42} + \delta_{42,j}K_{120}c_2 - 2\delta_{43,j}c_{43}\right] k_{120}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{120}}{\partial T} = \left[-\frac{1}{K_{103}}\frac{dK_{103}}{dT} + \frac{1}{K_{107}}\frac{dK_{107}}{dT} + \frac{1}{K_{110}}\frac{dK_{110}}{dT} - \frac{1}{K_{116}}\frac{dK_{116}}{dT}\right] \cdot$$

$$K_{120}c_2c_{42}k_{120} - \left[n_{120} - \frac{b_{120}}{T}\right]\frac{X_{120}}{T}$$

Reaction 121, $Be_2O + HCl \rightleftharpoons BeCl + BeOH$

$$K_{121} = \frac{K_6K_{109}}{K_{104}K_{105}}$$

$$k_{121} = a_{121}T^{-n_{121}} e^{-b_{121}/T}$$

$$X_{121} = \left[K_{121}c_6c_{42} - c_{43}c_{44}\right] k_{121}$$

$$\frac{\partial X_{121}}{\partial c_j} = \left[\delta_{6,j}K_{121}c_{42} + \delta_{42,j}K_{121}c_6 - \delta_{43,j}c_{44} + \delta_{44,j}c_{43}\right] k_{121}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{121}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{104}}\frac{dK_{104}}{dT} - \frac{1}{K_{105}}\frac{dK_{105}}{dT} + \frac{1}{K_{109}}\frac{dK_{109}}{dT}\right] \cdot$$

$$K_{121}c_6c_{42}k_{121} - \left[n_{121} - \frac{b_{121}}{T}\right]\frac{X_{121}}{T}$$

Reaction 122, $Be_2O + HF \rightleftharpoons BeF + BeOH$

$$K_{122} = \frac{K_{113}}{K_{119}}$$

$$k_{122} = a_{122} T^{-n_{122}} e^{-b_{122}/T}$$

$$X_{122} = \left[K_{122} c_7 c_{42} - c_{43} c_{46}\right] k_{122}$$

$$\frac{\partial X_{122}}{\partial c_j} = \left[\delta_{7,j} K_{122} c_{42} + \delta_{42,j} K_{122} c_7 - \delta_{43,j} c_{46} - \delta_{46,j} c_{43}\right] k_{122}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{122}}{\partial T} = \left[\frac{1}{K_{113}} \frac{dK_{13}}{dT} - \frac{1}{K_{119}} \frac{dK_{119}}{dT}\right] K_{122} c_7 c_{42} k_{122} - \left[n_{122} - \frac{b_{122}}{T}\right] \frac{X_{122}}{T}$$

Reaction 123, $Be_2O + OH \rightleftharpoons BeO + BeOH$

$$K_{123} = \frac{K_{11} K_{107}}{K_{103} K_{106}}$$

$$k_{123} = a_{123} T^{-n_{123}} e^{-b_{123}/T}$$

$$X_{123} = \left[K_{123} c_{11} c_{42} - c_{41} c_{43}\right] k_{123}$$

$$\frac{\partial X_{123}}{\partial c_j} = \left[\delta_{11,j} K_{123} c_{42} - \delta_{41,j} c_{43} + \delta_{42,j} K_{123} c_{11} - \delta_{43,j} c_{41}\right] k_{123}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{123}}{\partial T} = \left[\frac{1}{K_{11}} \frac{dK_{11}}{dT} + \frac{1}{K_{107}} \frac{dK_{107}}{dT} - \frac{1}{K_{103}} \frac{dK_{103}}{dT} - \frac{1}{K_{106}} \frac{dK_{106}}{dT}\right] \cdot K_{123} c_{11} c_{42} k_{123} - \left[n_{123} - \frac{b_{123}}{T}\right] \frac{X_{123}}{T}$$

Reaction 124, $Be_2O + Cl \rightleftharpoons BeO + BeCl$

$$K_{124} = \frac{K_{107}}{K_{104}}$$

$$k_{124} = a_{124} T^{-n_{124}} e^{-b_{124}/T}$$

$$X_{124} = \left[K_{124} c_{14} c_{42} - c_{41} c_{44}\right] k_{124}$$

$$\frac{\partial X_{124}}{\partial c_j} = \left[\delta_{14,j} K_{124} c_{42} - \delta_{41,j} c_{44} + \delta_{42,j} K_{124} c_{14} - \delta_{44,j} c_{41}\right] k_{124}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{124}}{\partial T} = \left[\frac{1}{K_{107}} \frac{dK_{107}}{dT} - \frac{1}{K_{104}} \frac{dK_{104}}{dT}\right] K_{124} c_{14} c_{42} k_{124} - \left[n_{124} - \frac{b_{124}}{T}\right] \frac{X_{124}}{T}$$

Reaction 125, $Be_2O + H \rightleftharpoons Be + BeOH$

$$K_{125} = \frac{K_{107}}{K_{103}}$$

$$k_{125} = a_{125} T^{-n_{125}} e^{-b_{125}/T}$$

$$X_{125} = \left[K_{125} c_{16} c_{42} - c_{40} c_{43}\right] k_{125}$$

$$\frac{\partial X_{125}}{\partial c_j} = \left[\delta_{16,j} K_{125} c_{42} - \delta_{40,j} c_{43} + \delta_{42,j} K_{125} c_{16} - \delta_{43,j} c_{40}\right] k_{125}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{125}}{\partial T} = \left[\frac{1}{K_{107}} \frac{dK_{107}}{dT} - \frac{1}{K_{103}} \frac{dK_{103}}{dT}\right] K_{125} c_{16} c_{42} k_{125} - \left[n_{125} - \frac{b_{125}}{T}\right] \frac{X_{125}}{T}$$

Reaction 126, $Be_2O + O \rightleftharpoons 2BeO$

$$K_{126} = \frac{K_{107}}{K_{106}}$$

$$k_{126} = a_{126}T^{-n_{126}} e^{-b_{126}/T}$$

$$X_{126} = \left[K_{126}c_{18}c_{42} - c_{41}^2\right]k_{126}$$

$$\frac{\partial X_{126}}{\partial c_j} = \left[\delta_{18,j}K_{126}c_{42} - 2\delta_{41,j}c_{41} + \delta_{42,j}K_{126}c_{18}\right]k_{126}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{126}}{\partial T} = \left[\frac{1}{K_{107}}\frac{dK_{107}}{dT} - \frac{1}{K_{106}}\frac{dK_{106}}{dT}\right]K_{126}c_{18}c_{42}k_{126}$$

$$- \left[n_{126} - \frac{b_{126}}{T}\right]\frac{X_{126}}{T}$$

Reaction 127, $2BeOH \rightleftharpoons Be + BeO_2H_2$

$$K_{127} = \frac{K_{102}}{K_{108}}$$

$$k_{127} = a_{127}T^{-n_{127}} e^{-b_{127}/T}$$

$$X_{127} = \left[K_{127}c_{43}^2 - c_{40}c_{48}\right]k_{127}$$

$$\frac{\partial X_{127}}{\partial c_j} = \left[-\delta_{40,j}c_{48}k_{127} + 2\delta_{43,j}K_{127}c_{43} - \delta_{48,j}c_{40}\right]k_{127}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{127}}{\partial T} = \left[\frac{1}{K_{102}}\frac{dK_{102}}{dT} - \frac{1}{K_{108}}\frac{dK_{108}}{dT}\right]K_{127}c_{43}^2k_{127}$$

$$- \left[n_{127} - \frac{b_{127}}{T}\right]\frac{X_{127}}{T}$$

Reaction 128, $BeOH + Cl \rightleftharpoons BeO + HCl$

$$K_{128} = \frac{K_{103}}{K_6}$$

$$k_{128} = a_{128} T^{-n_{128}} e^{-b_{128}/T}$$

$$X_{128} = \left[K_{128} c_{14} c_{43} - c_6 c_{41}\right] k_{128}$$

$$\frac{\partial X_{128}}{\partial c_j} = \left[-\delta_{6,j} c_{41} + \delta_{14,j} K_{128} c_{43} - \delta_{41,j} c_6 + \delta_{43,j} K_{128} c_{14}\right] k_{128}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{128}}{\partial T} = \left[\frac{1}{K_{103}} \frac{dK_{103}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{128} c_{14} c_{43} k_{128}$$

$$- \left[n_{128} - \frac{b_{128}}{T}\right] \frac{X_{128}}{T}$$

Reaction 129, $BeOH + Cl \rightleftharpoons BeCl + OH$

$$K_{129} = \frac{K_{102}}{K_{104}}$$

$$k_{129} = a_{129} T^{-n_{129}} e^{-b_{129}/T}$$

$$X_{129} = \left[K_{129} c_{14} c_{43} - c_{11} c_{44}\right] k_{129}$$

$$\frac{\partial X_{129}}{\partial c_j} = \left[-\delta_{11,j} c_{44} + \delta_{14,j} K_{129} c_{43} + \delta_{43,j} K_{129} c_{14} - \delta_{14,j} c_{11}\right] k_{129}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{129}}{\partial T} = \left[\frac{1}{K_{102}} \frac{dK_{102}}{dT} - \frac{1}{K_{104}} \frac{dK_{104}}{dT}\right] K_{129} c_{14} c_{43} k_{129}$$

$$- \left[n_{129} - \frac{b_{129}}{T}\right] \frac{X_{129}}{T}$$

Reaction 130, $BeOH + H \rightleftarrows Be + H_2O$

$$K_{130} = \frac{K_{102}}{K_2}$$

$$k_{130} = a_{130} T^{-n_{130}} e^{-b_{130}/T}$$

$$X_{130} = \left[K_{130} c_{16} c_{43} - c_2 c_{40}\right] k_{130}$$

$$\frac{\partial X_{130}}{\partial c_j} = \left[-\delta_{2,j} c_{40} + \delta_{16,j} K_{130} c_{43} - \delta_{40,j} c_2 + \delta_{43,j} K_{130} c_{16}\right] k_{130}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{130}}{\partial T} = \left[\frac{1}{K_{102}} \frac{dK_{102}}{dT} - \frac{1}{K_{129}} \frac{dK_{129}}{dT}\right] K_{130} c_{16} c_{43} k_{130}$$

$$- \left[n_{130} - \frac{b_{130}}{T}\right] \frac{X_{130}}{T}$$

Reaction 131, $BeOH + H \rightleftarrows BeO + H_2$

$$K_{131} = \frac{K_{103}}{K_8}$$

$$k_{131} = a_{131} T^{-n_{131}} e^{-b_{131}/T}$$

$$X_{131} = \left[K_{131} c_{16} c_{43} - c_8 c_{41}\right] k_{131}$$

$$\frac{\partial X_{131}}{\partial c_j} = \left[-\delta_{8,j} c_{41} + \delta_{16,j} K_{131} c_{43} - \delta_{41,j} c_8 + \delta_{43,j} K_{131} c_{16}\right] k_{131}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{131}}{\partial T} = \left[\frac{1}{K_{103}} \frac{dK_{103}}{dT} - \frac{1}{K_8} \frac{dK_8}{dT}\right] K_{131} c_{16} c_{43} k_{131}$$

$$- \left[n_{131} - \frac{b_{131}}{T}\right] \frac{X_{131}}{T}$$

Reaction 132, $BeOH + O \rightleftharpoons BeO + OH$

$$K_{132} = \frac{K_{103}}{K_{11}}$$

$$k_{132} = a_{132}T^{-n_{132}} e^{-b_{132}/T}$$

$$X_{132} = \left[K_{132}c_{18}c_{43} - c_{11}c_{41}\right] k_{132}$$

$$\frac{\partial X_{132}}{\partial c_j} = \left[-\delta_{11,j}c_{41} + \delta_{18,j}K_{132}c_{43} - \delta_{41,j}c_{11} + \delta_{43,j}K_{132}c_{18}\right]k_{132}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{132}}{\partial T} = \left[\frac{1}{K_{103}}\frac{dK_{103}}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT}\right] K_{132}c_{18}c_{43}k_{132}$$

$$-\left[n_{132} - \frac{b_{132}}{T}\right]\frac{X_{132}}{T}$$

Reaction 133, $2BeCl \rightleftharpoons Be + BeCl_2$

$$K_{133} = \frac{K_{104}}{K_{100}}$$

$$k_{133} = a_{133}T^{-n_{133}} e^{-b_{133}/T}$$

$$X_{133} = \left[K_{133}c_{44}^2 - c_{40}c_{45}\right]k_{133}$$

$$\frac{\partial X_{133}}{\partial c_j} = \left[-\delta_{40,j}c_{45} + 2\delta_{44,j}K_{133}c_{44} - \delta_{45,j}c_{40}\right]k_{133}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{133}}{\partial T} = \left[\frac{1}{K_{104}}\frac{dK_{104}}{dT} - \frac{1}{K_{100}}\frac{dK_{100}}{dT}\right] K_{133}c_{44}^2k_{133} - \left[n_{133} - \frac{b_{133}}{T}\right]\frac{X_{133}}{T}$$

Reaction 134, $BeCl + H_2O \rightleftharpoons BeOH + HCl$

$$K_{134} = \frac{K_2}{K_6 K_{129}}$$

$$k_{134} = a_{134} T^{-n_{134}} e^{-b_{134}/T}$$

$$X_{134} = \left[K_{134} c_2 c_{44} - c_6 c_{43}\right] k_{134}$$

$$\frac{\partial X_{134}}{\partial c_j} = \left[\delta_{2,j} K_{134} c_{44} - \delta_{6,j} c_{43} - \delta_{43,j} c_6 + \delta_{44,j} K_{134} c_2\right] k_{134}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{134}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{129}}\frac{dK_{129}}{dT}\right] K_{134} c_2 c_{44} k_{134}$$

$$- \left[n_{134} - \frac{b_{134}}{T}\right] \frac{X_{134}}{T}$$

Reaction 135, $BeCl + HCl \rightleftharpoons BeCl_2 + H$

$$K_{133} = \frac{K_6}{K_{100}}$$

$$k_{135} = a_{135} T^{-n_{135}} e^{-b_{135}/T}$$

$$X_{135} = \left[K_{135} c_6 c_{44} - c_{16} c_{45}\right] k_{135}$$

$$\frac{\partial X_{135}}{\partial c_j} = \left[\delta_{6,j} K_{135} c_{44} - \delta_{16,j} c_{45} + \delta_{44,j} K_{135} c_6 - \delta_{45,j} c_{16}\right] k_{135}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{135}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{100}}\frac{dK_{100}}{dT}\right] K_{135} c_6 c_{44} k_{135} - \left[n_{135} - \frac{b_{135}}{T}\right] \frac{X_{135}}{T}$$

Reaction 136, $BeCl + Cl \rightleftharpoons Be + Cl_2$

$$K_{136} = \frac{K_{104}}{K_4}$$

$$k_{136} = a_{136} T^{-n_{136}} e^{-n_{136}/T}$$

$$X_{136} = \left[K_{136} c_{14} c_{44} - c_4 c_{40}\right] k_{136}$$

$$\frac{\partial X_{136}}{\partial c_j} = \left[-\delta_{4,j} c_{40} + \delta_{14,j} K_{136} c_{44} - \delta_{40,j} c_4 + \delta_{44,j} K_{136} c_{14}\right] k_{136}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{136}}{\partial T} = \left[\frac{1}{K_{104}} \frac{dK_{104}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{136} c_{14} c_{44} k_{136} - \left[n_{136} - \frac{b_{136}}{T}\right] \frac{X_{136}}{T}$$

Reaction 137, $BeCl + H \rightleftharpoons Be + HCl$

$$K_{137} = \frac{K_{104}}{K_6}$$

$$k_{137} = a_{137} T^{-n_{137}} e^{-b_{137}/T}$$

$$X_{137} = \left[K_{137} c_{16} c_{44} - c_6 c_{40}\right] k_{137}$$

$$\frac{\partial X_{137}}{\partial c_j} = \left[-\delta_{6,j} c_{40} + \delta_{16,j} K_{137} c_{44} - \delta_{40,j} c_6 + \delta_{44,j} K_{137} c_{16}\right] k_{137}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{137}}{\partial T} = \left[\frac{1}{K_{104}} \frac{dK_{104}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{137} c_{16} c_{44} k_{137}$$

$$- \left[n_{137} - \frac{b_{137}}{T}\right] \frac{X_{137}}{T}$$

Reaction 138, $BeF + H_2O \rightleftharpoons BeOH + HF$

$$K_{138} = \frac{K_2 K_{105}}{K_7 K_{102}}$$

$$k_{138} = a_{138} T^{-n_{138}} e^{-b_{138}/T}$$

$$X_{138} = \left[K_{138} c_2 c_{46} - c_7 c_{43}\right] k_{138}$$

$$\frac{\partial X_{138}}{\partial c_j} = \left[\delta_{2,j} K_{138} c_{46} - \delta_{7,j} c_{43} - \delta_{43,j} c_7 + \delta_{46,j} K_{138} c_2\right] k_{138}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{138}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{102}}\frac{dK_{102}}{dT} + \frac{1}{K_{105}}\frac{dK_{105}}{dT}\right] K_{138} c_2 c_{46} k_{138}$$

$$- \left[n_{138} - \frac{b_{138}}{T}\right] \frac{X_{138}}{T}$$

Reaction 139, $BeF + HCl \rightleftharpoons BeCl + HF$

$$K_{139} = \frac{K_{105}}{K_7 K_{137}}$$

$$k_{139} = a_{139} T^{-n_{139}} e^{-b_{139}/T}$$

$$X_{139} = \left[K_{139} c_6 c_{46} - c_7 c_{44}\right] k_{139}$$

$$\frac{\partial X_{139}}{\partial c_j} = \left[\delta_{6,j} K_{139} c_{46} - \delta_{7,j} c_{44} - \delta_{44,j} c_7 + \delta_{46,j} K_{139} c_6\right] k_{139}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{139}}{\partial T} = \left[\frac{1}{K_{105}}\frac{dK_{105}}{dT} - \frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{137}}\frac{dK_{137}}{dT}\right] K_{139} c_6 c_{46} k_{139}$$

$$- \left[n_{139} - \frac{b_{139}}{T}\right] \frac{X_{139}}{T}$$

Reaction 140, $BeF + OH \rightleftharpoons BeO + HF$

$$K_{140} = \frac{K_{105}}{K_7 K_{116}}$$

$$k_{140} = a_{140} T^{-n_{140}} e^{-b_{140}/T}$$

$$X_{140} = \left[K_{140} c_{11} c_{46} - c_7 c_{41}\right] k_{140}$$

$$\frac{\partial X_{140}}{\partial c_j} = \left[-\delta_{7,j} c_{41} + \delta_{11,j} K_{140} c_{46} - \delta_{41,j} c_7 + \delta_{46,j} K_{140} c_{11}\right] k_{140}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{140}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT} - \frac{1}{K_{116}} \frac{dK_{116}}{dT}\right] K_{140} c_{11} c_{46} k_{140}$$

$$- \left[n_{140} - \frac{b_{140}}{T}\right] \frac{X_{140}}{T}$$

Reaction 141, $BeF + OH \rightleftharpoons BeOH + F$

$$K_{141} = \frac{K_{105}}{K_{102}}$$

$$k_{141} = a_{141} T^{-n_{141}} e^{-b_{141}/T}$$

$$X_{141} = \left[K_{141} c_{11} c_{46} - c_{15} c_{43}\right] k_{141}$$

$$\frac{\partial X_{141}}{\partial c_j} = \left[\delta_{11,j} K_{141} c_{46} - \delta_{15,j} c_{43} - \delta_{43,j} c_{15} + \delta_{46,j} K_{141} c_{11}\right] k_{141}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{141}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_{102}} \frac{dK_{102}}{dT}\right] K_{141} c_{11} c_{46} k_{141}$$

$$- \left[n_{141} - \frac{b_{141}}{T}\right] \frac{X_{141}}{T}$$

Reaction 142, $BeF + Cl \rightleftharpoons BeCl + F$

$$K_{142} = \frac{K_{105}}{K_{104}}$$

$$k_{142} = a_{142} T^{-n_{142}} e^{-b_{142}/T}$$

$$X_{142} = \left[K_{142} c_{14} c_{46} - c_{15} c_{44}\right] k_{142}$$

$$\frac{\partial X_{142}}{\partial c_j} = \left[\delta_{14,j} K_{142} c_{46} - \delta_{15,j} c_{44} - \delta_{44,j} c_{15} + \delta_{46,j} K_{142} c_{14}\right] k_{142}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{142}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_{104}} \frac{dK_{104}}{dT}\right] K_{142} c_{14} c_{46} k_{142} - \left[n_{142} - \frac{b_{142}}{T}\right] \frac{X_{142}}{T}$$

Reaction 143, $BeF + F \rightleftharpoons Be + F_2$

$$K_{143} = \frac{K_{105}}{K_5}$$

$$k_{143} = a_{143} T^{-n_{143}} e^{-b_{143}/T}$$

$$X_{143} = \left[K_{143} c_{15} c_{46} - c_5 c_{40}\right] k_{143}$$

$$\frac{\partial X_{143}}{\partial c_j} = \left[-\delta_{5,j} c_{40} + \delta_{15,j} K_{143} c_{46} - \delta_{40,j} c_5 + \delta_{46,j} K_{143} c_{15}\right] k_{143}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{143}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{143} c_{15} c_{46} k_{143} - \left[n_{143} - \frac{b_{143}}{T}\right] \frac{X_{143}}{T}$$

Reaction 144, $BeF + H \rightleftharpoons Be + HF$

$$K_{144} = \frac{K_{105}}{K_7}$$

$$k_{144} = a_{144} T^{-n_{144}} e^{-b_{144}/T}$$

$$X_{144} = \left[K_{144} c_{16} c_{46} - c_7 c_{40}\right] k_{144}$$

$$\frac{\partial X_{144}}{\partial c_j} = \left[-\delta_{7,j} c_{40} + \delta_{16,j} K_{144} c_{46} - \delta_{40,j} c_7 + \delta_{46,j} K_{144} c_{16}\right] k_{144}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{144}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{144} c_{16} c_{46} k_{144} - \left[n_{144} - \frac{b_{144}}{T}\right] \frac{X_{144}}{T}$$

Reaction 145, $BeF + O \rightleftharpoons BeO + F$

$$K_{145} = \frac{K_{105}}{K_{106}}$$

$$k_{145} = a_{145} T^{-n_{145}} e^{-b_{145}/T}$$

$$X_{145} = \left[K_{145} c_{18} c_{46} - c_{15} c_{41}\right] k_{145}$$

$$\frac{\partial X_{145}}{\partial c_j} = \left[-\delta_{15,j} c_{41} + \delta_{18,j} K_{145} c_{46} - \delta_{41,j} c_{15} + \delta_{46,j} K_{145} c_{18}\right] k_{145}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{145}}{\partial T} = \left[\frac{1}{K_{105}} \frac{dK_{105}}{dT} - \frac{1}{K_{106}} \frac{dK_{106}}{dT}\right] K_{145} c_{18} c_{46} k_{145}$$

$$- \left[n_{145} - \frac{b_{145}}{T}\right] \frac{X_{145}}{T}$$

Reaction 146, $BeF_2 + H \rightleftharpoons BeF + HF$

$$K_{146} = \frac{K_{101}}{K_7}$$

$$k_{146} = a_{146} T^{-n_{146}} e^{-b_{146}/T}$$

$$X_{146} = \left[K_{146} c_{16} c_{47} - c_7 c_{46}\right] k_{146}$$

$$\frac{\partial X_{146}}{\partial c_j} = \left[-\delta_{7,j} c_{46} + \delta_{16,j} K_{146} c_{47} - \delta_{46,j} c_7 + \delta_{47,j} K_{146} c_{16}\right] k_{146}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{146}}{\partial T} = \left[\frac{1}{K_{101}} \frac{dK_{101}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{146} c_{16} c_{47} k_{146}$$

$$- \left[n_{146} - \frac{b_{146}}{T}\right] \frac{X_{146}}{T}$$

Reaction 147, $BeO_2H_2 + H \rightleftharpoons BeOH + H_2O$

$$K_{147} = \frac{K_{108}}{K_2}$$

$$k_{147} = a_{147} T^{-n_{147}} e^{-b_{147}/T}$$

$$X_{147} = \left[K_{147} c_{16} c_{48} - c_2 c_{43}\right] k_{147}$$

$$\frac{\partial X_{147}}{\partial c_j} = \left[-\delta_{2,j} c_{43} + \delta_{16,j} K_{147} c_{48} - \delta_{43,j} c_2 + \delta_{48,j} K_{147} c_{16}\right] k_{147}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{147}}{\partial T} = \left[\frac{1}{K_{108}} \frac{dK_{108}}{dT} - \frac{1}{K_2} \frac{dK_2}{dT}\right] K_{147} c_{16} c_{48} k_{147}$$

$$- \left[n_{147} - \frac{b_{147}}{T}\right] \frac{X_{147}}{T}$$

Reaction 148, $BN + M \rightleftharpoons B + N + M$

$$k_{148} = a_{148} T^{-n_{148}} e^{-b_{148}/T}$$

$$M_{148} = \sum_{i=1}^{57} m_{148,i} c_i$$

$$X_{148} = \left[K_{148} c_{29} - \rho c_{17} c_{28}\right] M_{148} k_{148}$$

$$\frac{\partial X_{148}}{\partial c_j} = \frac{X_{148}}{M_{148}} m_{148,j} + \delta_{29,j} K_{148} M_{148} k_{148} - \delta_{17,j} \rho c_{28} M_{148} k_{148}$$

$$-\delta_{28,j} \rho c_{17} M_{148} k_{148} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{148}}{\partial \rho} = -c_{17} c_{28} M_{148} k_{148}$$

$$\frac{\partial X_{148}}{\partial T} = c_{29} M_{148} k_{148} \frac{dK_{148}}{dT} - \left[n_{148} - \frac{b_{148}}{T}\right] \frac{X_{148}}{T}$$

Reaction 149, $BO + M \rightleftharpoons B + O + M$

$$k_{149} = a_{149} T^{-n_{149}} e^{-b_{149}/T}$$

$$M_{149} = \sum_{i=1}^{57} m_{149,i} c_i$$

$$X_{149} = \left[K_{149} c_{30} - \rho c_{18} c_{28}\right] M_{149} k_{149}$$

$$\frac{\partial X_{149}}{\partial c_j} = \frac{X_{149}}{M_{149}} m_{149,j} + \delta_{30,j} K_{149} M_{149} k_{149} - \delta_{18,j} \rho c_{28} M_{149} k_{149}$$

$$-\delta_{28,j} \rho c_{18} M_{149} k_{149} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{149}}{\partial \rho} = -c_{18} c_{28} M_{149} k_{149}$$

$$\frac{\partial X_{149}}{\partial T} = c_{30} M_{149} k_{149} \frac{dK_{149}}{dT} - \left[n_{149} - \frac{b_{149}}{T}\right] \frac{X_{149}}{T}$$

Reaction 150, $BO_2 + M \rightleftharpoons BO + O + M$

$$k_{150} = a_{150}T^{-n_{150}} e^{-b_{150}/T}$$

$$M_{150} = \sum_{i=1}^{57} m_{150,i}c_i$$

$$X_{150} = \left[K_{150}c_{31} - \rho c_{18}c_{30}\right] M_{150}k_{150}$$

$$\frac{\partial X_{150}}{\partial c_j} = \frac{X_{150}}{M_{150}} m_{150,j} + \delta_{31,j}K_{150}M_{150}k_{150} - \delta_{18,j}\rho c_{30}M_{150}k_{150}$$
$$-\delta_{30,j}\rho c_{18}M_{150}k_{150} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{150}}{\partial \rho} = -c_{18}c_{30}M_{150}k_{150}$$

$$\frac{\partial X_{150}}{\partial T} = c_{31}M_{150}k_{150}\frac{dK_{150}}{dT} - \left[n_{150} - \frac{b_{150}}{T}\right]\frac{X_{150}}{T}$$

Reaction 151, $BCl + M \rightleftharpoons B + Cl + M$

$$k_{151} = a_{151}T^{-n_{148}} e^{-b_{151}/T}$$

$$M_{151} = \sum_{i=1}^{57} m_{151,i}c_i$$

$$X_{151} = \left[X_{151}c_{32} - \rho c_{14}c_{28}\right] M_{151}k_{151}$$

$$\frac{\partial X_{151}}{\partial c_j} = \frac{X_{151}}{M_{151}} m_{151,j} + \delta_{32,j}K_{151}M_{151}k_{151} - \delta_{14,j}\rho c_{28}M_{151}k_{151}$$
$$-\delta_{28,j}\rho c_{14}M_{151}k_{151} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{151}}{\partial \rho} = -c_{14}c_{28}M_{151}k_{151}$$

$$\frac{\partial X_{151}}{\partial T} = c_{32}M_{151}k_{151}\frac{dK_{151}}{dT} - \left[n_{151} - \frac{b_{151}}{T}\right]\frac{X_{151}}{T}$$

Reaction 152, $BCl_2 + M \rightleftarrows BCl + Cl + M$

$$k_{152} = a_{152} T^{-n_{152}} e^{-b_{152}/T}$$

$$M_{152} = \sum_{i=1}^{57} m_{152,i} c_i$$

$$X_{152} = \left[K_{152} c_{33} - \rho c_{14} c_{32}\right] M_{152} k_{152}$$

$$\frac{\partial X_{152}}{\partial c_j} = \frac{X_{152}}{M_{152}} m_{152,j} + \delta_{33,j} K_{152} M_{152} k_{152} - \delta_{14,j} \rho c_{32} M_{152} k_{152}$$

$$-\delta_{32,j} \rho c_{14} M_{152} k_{152} \quad , \quad j = 1, 2, \cdots , 57$$

$$\frac{\partial X_{152}}{\partial \rho} = -c_{14} c_{32} M_{152} k_{152}$$

$$\frac{\partial X_{152}}{\partial T} = c_{33} M_{152} k_{152} \frac{dK_{152}}{dT} - \left[n_{152} - \frac{b_{152}}{T}\right] \frac{X_{152}}{T}$$

Reaction 153, $BCl_3 + M \rightleftarrows BCl_2 + Cl + M$

$$k_{153} = a_{153} T^{-n_{153}} e^{-b_{153}/T}$$

$$M_{153} = \sum_{i=1}^{57} m_{153,i} c_i$$

$$X_{153} = \left[K_{153} c_{34} - \rho c_{14} c_{33}\right] M_{153} k_{153}$$

$$\frac{\partial X_{153}}{\partial c_j} = \frac{X_{153}}{M_{153}} m_{153,j} + \delta_{34,j} K_{153} M_{153} k_{153} - \delta_{14,j} \rho c_{33} M_{153} k_{153}$$

$$-\delta_{33,j} \rho c_{14} M_{153} k_{153} \quad , \quad j = 1, 2, \cdots , 57$$

$$\frac{\partial X_{153}}{\partial \rho} = -c_{14} c_{33} M_{153} k_{153}$$

$$\frac{\partial X_{153}}{\partial T} = c_{34} M_{153} k_{153} \frac{dK_{153}}{dT} - \left[n_{153} - \frac{b_{153}}{T}\right] \frac{X_{153}}{T}$$

Reaction 154, $BOCl + M \rightleftharpoons BCl + O + M$

$$k_{154} = a_{154} T^{-n_{154}} e^{-b_{154}/T}$$

$$M_{154} = \sum_{i=1}^{57} m_{154,i} c_i$$

$$X_{154} = \left[K_{154} c_{35} - \rho c_{18} c_{32} \right] M_{154} k_{154}$$

$$\frac{\partial X_{154}}{\partial c_j} = \frac{X_{154}}{M_{154}} m_{154,j} + \delta_{35,j} K_{154} M_{154} k_{154} - \delta_{18,j} \rho c_{32} M_{154} k_{154}$$
$$-\delta_{32,j} \rho c_{18} M_{154} k_{154} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{154}}{\partial \rho} = -c_{18} c_{32} M_{154} k_{154}$$

$$\frac{\partial X_{154}}{\partial T} = c_{35} M_{154} k_{154} \frac{dK_{154}}{dT} - \left[n_{154} - \frac{b_{154}}{T} \right] \frac{X_{154}}{T}$$

Reaction 155, $BF + M \rightleftharpoons B + F + M$

$$k_{155} = a_{155} T^{-n_{155}} e^{-b_{155}/T}$$

$$M_{155} = \sum_{i=1}^{57} m_{155,i} c_i$$

$$X_{155} = \left[K_{155} c_{36} - \rho c_{15} c_{28} \right] M_{155} k_{155}$$

$$\frac{\partial X_{155}}{\partial c_j} = \frac{X_{155}}{M_{155}} m_{155,j} + \delta_{36,j} K_{155} M_{155} k_{155} - \delta_{15,j} \rho c_{28} M_{155} k_{155}$$
$$-\delta_{28,j} \rho c_{15} M_{155} k_{155} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{155}}{\partial \rho} = -c_{15} c_{28} M_{155} k_{155}$$

$$\frac{\partial X_{155}}{\partial T} = c_{36} M_{155} k_{155} \frac{dK_{155}}{dT} - \left[n_{155} - \frac{b_{155}}{T} \right] \frac{X_{155}}{T}$$

Reaction 156, $BF_2 + M \rightleftharpoons BF + F + M$

$$k_{156} = a_{156} T^{-n_{156}} e^{-b_{156}/T}$$

$$M_{156} = \sum_{i=1}^{57} m_{156,i} c_i$$

$$X_{156} = \left[K_{156} c_{37} - \rho c_{15} c_{36}\right] M_{156} k_{156}$$

$$\frac{\partial X_{156}}{\partial c_j} = \frac{X_{156}}{M_{156}} m_{156,j} + \delta_{37,j} K_{156} M_{156} k_{156} - \delta_{15,j} \rho c_{36} M_{156} k_{156}$$
$$-\delta_{36,j} \rho c_{15} M_{156} k_{156} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{156}}{\partial \rho} = -c_{15} c_{36} M_{156} k_{156}$$

$$\frac{\partial X_{156}}{\partial T} = c_{37} M_{156} k_{156} \frac{dK_{156}}{dT} - \left[n_{156} - \frac{b_{156}}{T}\right] \frac{X_{156}}{T}$$

Reaction 157, $BF_3 + M \rightleftharpoons BF_2 + F + M$

$$k_{157} = a_{157} T^{-n_{157}} e^{-b_{157}/T}$$

$$M_{157} = \sum_{i=1}^{57} m_{157,i} c_i$$

$$X_{157} = \left[K_{157} c_{38} - \rho c_{15} c_{37}\right] M_{157} k_{157}$$

$$\frac{\partial X_{157}}{\partial c_j} = \frac{X_{157}}{M_{157}} m_{157,j} + \delta_{38,j} K_{157} M_{157} k_{157} - \delta_{15,j} \rho c_{37} M_{157} k_{157}$$
$$-\delta_{37,j} \rho c_{15} M_{157} k_{157} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{157}}{\partial \rho} = -c_{15} c_{37} M_{157} k_{157}$$

$$\frac{\partial X_{157}}{\partial T} = c_{38} M_{157} k_{157} \frac{dK_{157}}{dT} - \left[n_{157} - \frac{b_{157}}{T}\right] \frac{X_{157}}{T}$$

Reaction 158, $BOF + M \rightleftharpoons BO + F + M$

$$k_{158} = a_{158} T^{-n_{158}} e^{-b_{158}/T}$$

$$M_{158} = \sum_{i=1}^{57} m_{158,i} c_i$$

$$X_{158} = \left[K_{158} c_{39} - \rho c_{15} c_{30}\right] M_{158} k_{158}$$

$$\frac{\partial X_{158}}{\partial c_j} = \frac{X_{158}}{M_{158}} m_{158,j} + \delta_{39,j} K_{158} M_{158} k_{158} - \delta_{15,j} \rho c_{30} M_{158} k_{158}$$
$$- \delta_{30,j} \rho c_{15} M_{158} k_{158} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{158}}{\partial \rho} = -c_{15} c_{30} M_{158} k_{158}$$

$$\frac{\partial X_{158}}{\partial T} = c_{39} M_{158} k_{158} \frac{dK_{158}}{dT} - \left[n_{158} - \frac{b_{158}}{T}\right] \frac{X_{158}}{T}$$

Reaction 159, $BOF + M \rightleftharpoons BF + O + M$

$$k_{159} = a_{159} T^{-n_{159}} e^{-b_{159}/T}$$

$$M_{159} = \sum_{i=1}^{57} m_{159,i} c_i$$

$$X_{159} = \left[K_{159} c_{39} - \rho c_{18} c_{36}\right] M_{159} k_{159}$$

$$\frac{\partial X_{159}}{\partial c_j} = \frac{X_{159}}{M_{159}} m_{159,j} + \delta_{39,j} K_{159} M_{159} k_{159} - \delta_{18,j} \rho c_{36} M_{159} k_{159}$$
$$- \delta_{36,j} \rho c_{18} M_{159} k_{159}$$

$$\frac{\partial X_{159}}{\partial \rho} = -c_{18} c_{36} M_{159} k_{159}$$

$$\frac{\partial X_{159}}{\partial T} = c_{39} M_{159} k_{159} \frac{dK_{159}}{dT} - \left[n_{159} - \frac{b_{159}}{T}\right] \frac{X_{159}}{T}$$

Reaction 160, $B + N_2 \rightleftharpoons BN + N$

$$K_{160} = \frac{K_9}{K_{148}}$$

$$k_{160} = a_{160} T^{-n_{160}} e^{-b_{160}/T}$$

$$X_{160} = \left[K_{160} c_9 c_{28} - c_{17} c_{29}\right] k_{160}$$

$$\frac{\partial X_{160}}{\partial c_j} = \left[\delta_{9,j} K_{160} c_{28} - \delta_{17,j} c_{29} + \delta_{28,j} K_{160} c_9 - \delta_{29,j} c_{17}\right] k_{160}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{160}}{\partial T} = \left[\frac{1}{K_9}\frac{dK_9}{dT} - \frac{1}{K_{148}}\frac{dK_{148}}{dT}\right] K_{160} c_9 c_{28} k_{160} - \left[n_{160} - \frac{b_{160}}{T}\right]\frac{X_{160}}{T}$$

Reaction 161, $B + NO \rightleftharpoons BN + O$

$$K_{161} = \frac{K_{10}}{K_{148}}$$

$$k_{161} = a_{161} T^{-n_{161}} e^{-b_{161}/T}$$

$$X_{161} = \left[K_{161} c_{10} c_{28} - c_{18} c_{29}\right] k_{161}$$

$$\frac{\partial X_{161}}{\partial c_j} = \left[\delta_{10,j} K_{161} c_{28} - \delta_{18,j} c_{29} + \delta_{28,j} K_{161} c_{10} - \delta_{29,j} c_{18}\right] k_{161}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{161}}{\partial T} = \left[\frac{1}{K_{10}}\frac{dK_{10}}{dT} - \frac{1}{K_{148}}\frac{dK_{148}}{dT}\right] K_{161} c_{10} c_{28} k_{161}$$

$$- \left[n_{161} - \frac{b_{161}}{T}\right]\frac{X_{161}}{T}$$

Reaction 162, $B + NO \rightleftharpoons BO + N$

$$K_{162} = \frac{K_{10}}{K_{149}}$$

$$k_{162} = a_{162} T^{-n_{162}} e^{-b_{162}/T}$$

$$X_{162} = \left[K_{162} c_{10} c_{28} - c_{17} c_{30}\right] k_{162}$$

$$\frac{\partial X_{162}}{\partial c_j} = \left[\delta_{10,j} K_{162} c_{28} - \delta_{17,j} c_{30} + \delta_{28,j} K_{162} c_{10} - \delta_{30,j} c_{17}\right] k_{162}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{162}}{\partial T} = \left[\frac{1}{K_{10}} \frac{dK_{10}}{dT} - \frac{1}{K_{149}} \frac{dK_{149}}{dT}\right] K_{162} c_{10} c_{28} k_{162}$$

$$- \left[n_{162} - \frac{b_{162}}{T}\right] \frac{X_{162}}{T}$$

Reaction 163, $BN + NO \rightleftharpoons BO + N_2$

$$K_{163} = \frac{K_{162}}{K_{160}}$$

$$k_{163} = a_{163} T^{-n_{163}} e^{-b_{163}/T}$$

$$X_{163} = \left[K_{163} c_{10} c_{29} - c_9 c_{30}\right] k_{163}$$

$$\frac{\partial X_{163}}{\partial c_j} = \left[-\delta_{9,j} c_{30} + \delta_{10,j} K_{163} c_{29} + \delta_{29,j} K_{163} c_{10} - \delta_{30,j} c_9\right] k_{163}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{163}}{\partial T} = \left[\frac{1}{K_{162}} \frac{dK_{162}}{dT} - \frac{1}{K_{160}} \frac{dK_{160}}{dT}\right] K_{163} c_{10} c_{29} k_{163}$$

$$- \left[n_{163} - \frac{b_{163}}{T}\right] \frac{X_{163}}{T}$$

Reaction 164, $2BO \rightleftharpoons B + BO_2$

$$K_{164} = \frac{K_{149}}{K_{150}}$$

$$k_{164} = a_{164} T^{-n_{164}} e^{-b_{164}/T}$$

$$X_{164} = \left[K_{164} c_{30}^2 - c_{28} c_{31}\right] k_{164}$$

$$\frac{\partial X_{164}}{\partial c_j} = \left[-\delta_{28,j} c_{31} + \delta_{30,j} K_{164} c_{30} - \delta_{31,j} c_{28}\right] k_{164} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{164}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{164} c_{30}^2 k_{164} - \left[n_{164} - \frac{b_{164}}{T}\right] \frac{X_{164}}{T}$$

Reaction 165, $BO + CO_2 \rightleftharpoons BO_2 + CO$

$$K_{165} = \frac{K_1}{K_{150}}$$

$$k_{165} = a_{165} T^{-n_{165}} e^{-b_{165}/T}$$

$$X_{165} = \left[K_{165} c_1 c_{30} - c_3 c_{31}\right] k_{165}$$

$$\frac{\partial X_{165}}{\partial c_j} = \left[\delta_{1,j} K_{165} c_{30} - \delta_{3,j} c_{31} + \delta_{30,j} K_{165} c_1 - \delta_{31,j} c_3\right] k_{165}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{165}}{\partial T} = \left[\frac{1}{K_1} \frac{dK_1}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{165} c_1 c_{30} k_{165}$$

$$- \left[n_{165} - \frac{b_{165}}{T}\right] \frac{X_{165}}{T}$$

Reaction 166, $BO + CO \rightleftharpoons B + CO_2$

$$K_{166} = \frac{K_{149}}{K_1}$$

$$k_{166} = a_{166} T^{-n_{166}} e^{-b_{166}/T}$$

$$X_{166} = \left[K_{166} c_3 c_{30} - c_1 c_{28}\right] k_{166}$$

$$\frac{\partial X_{166}}{\partial c_j} = \left[-\delta_{1,j} c_{28} + \delta_{3,j} K_{166} c_{30} - \delta_{28,j} c_1 + \delta_{30,j} K_{166} c_3\right] k_{166}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{166}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_1} \frac{dK_1}{dT}\right] K_{166} c_3 c_{30} k_{166}$$

$$- \left[n_{166} - \frac{b_{166}}{T}\right] \frac{X_{166}}{T}$$

Reaction 167, $BO + CO \rightleftharpoons BO_2 + C$

$$K_{167} = \frac{K_3}{K_{150}}$$

$$k_{167} = a_{167} T^{-n_{167}} e^{-b_{167}/T}$$

$$X_{167} = \left[K_{167} c_3 c_{30} - c_{13} c_{31}\right] k_{167}$$

$$\frac{\partial X_{167}}{\partial c_j} = \left[\delta_{3,j} K_{167} c_{30} - \delta_{13,j} c_{31} + \delta_{30,j} K_{167} c_3 - \delta_{31,j} c_{13}\right] k_{167}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{167}}{\partial T} = \left[\frac{1}{K_3} \frac{dK_3}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{167} c_3 c_{30} k_{167}$$

$$- \left[n_{167} - \frac{b_{167}}{T}\right] \frac{X_{167}}{T}$$

Reaction 168, $BO + HCl \rightleftharpoons BCl + OH$

$$K_{168} = \frac{K_6 K_{149}}{K_{11} K_{151}}$$

$$k_{168} = a_{168} T^{-n_{168}} e^{-b_{168}/T}$$

$$X_{168} = \left[K_{168} c_6 c_{30} - c_{11} c_{32}\right] k_{168}$$

$$\frac{\partial X_{168}}{\partial c_j} = \left[\delta_{6,j} K_{168} c_{30} - \delta_{11,j} c_{32} + \delta_{30,j} K_{168} c_6 - \delta_{32,j} c_{11}\right] k_{168}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{168}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT} + \frac{1}{K_{149}}\frac{dK_{149}}{dT} - \frac{1}{K_{151}}\frac{dK_{151}}{dT}\right]$$

$$K_{168} c_6 c_{30} k_{168} - \left[n_{168} - \frac{b_{168}}{T}\right]\frac{X_{168}}{T}$$

Reaction 169, $BO + HF \rightleftharpoons BF + OH$

$$K_{169} = \frac{K_7 K_{149}}{K_{11} K_{155}}$$

$$k_{169} = a_{169} T^{-n_{169}} e^{-b_{169}/T}$$

$$X_{169} = \left[K_{169} c_7 c_{30} - c_{11} c_{36}\right] k_{169}$$

$$\frac{\partial X_{169}}{\partial c_j} = \left[\delta_{7,j} K_{169} c_{30} - \delta_{11,j} c_{36} + \delta_{30,j} K_{169} c_7 - \delta_{36,j} c_{11}\right] k_{169}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{169}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT} + \frac{1}{K_{149}}\frac{dK_{149}}{dT} - \frac{1}{K_{155}}\frac{dK_{155}}{dT}\right] K_{169} c_7 c_{30} k_{169}$$

$$- \left[n_{169} - \frac{b_{169}}{T}\right]\frac{X_{169}}{T}$$

Reaction 170, $BO + NO \rightleftharpoons BN + O_2$

$$K_{170} = \frac{K_{10}K_{149}}{K_{12}K_{148}}$$

$$k_{170} = a_{170}T^{-n_{170}} e^{-b_{170}/T}$$

$$X_{170} = \left[K_{170}c_{10}c_{30} - c_{12}c_{29}\right] k_{170}$$

$$\frac{\partial X_{170}}{\partial c_j} = \left[\delta_{10,j}K_{170}c_{30} - \delta_{12,j}c_{29} - \delta_{29,j}c_{12} + \delta_{30,j}K_{170}c_{10}\right] k_{170}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{170}}{\partial T} = \left[\frac{1}{K_{10}} \frac{dK_{10}}{dT} - \frac{1}{K_{12}} \frac{dK_{12}}{dT} - \frac{1}{K_{148}} \frac{dK_{148}}{dT} + \frac{1}{K_{149}} \frac{dK_{149}}{dT}\right] \cdot$$

$$K_{170}c_{10}c_{30}k_{170} - \left[n_{170} - \frac{b_{170}}{T}\right] \frac{X_{170}}{T}$$

Reaction 171, $BO + NO \rightleftharpoons BO_2 + N$

$$K_{171} = \frac{K_{10}}{K_{150}}$$

$$k_{171} = a_{171}T^{-n_{171}} e^{-b_{171}/T}$$

$$X_{171} = \left[K_{171}c_{10}c_{30} - c_{17}c_{31}\right] k_{171}$$

$$\frac{\partial X_{171}}{\partial c_j} = \left[\delta_{10,j}K_{171}c_{30} - \delta_{17,j}c_{31} + \delta_{30,j}K_{171}c_{10} - \delta_{31,j}c_{17}\right] k_{171}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{171}}{\partial T} = \left[\frac{1}{K_{10}} \frac{dK_{10}}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{171}c_{10}c_{30}k_{171}$$

$$- \left[n_{171} - \frac{b_{171}}{T}\right] \frac{X_{171}}{T}$$

Reaction 172, $BO + C \rightleftharpoons B + CO$

$$K_{172} = \frac{K_{149}}{K_3}$$

$$k_{172} = a_{172}T^{-n_{172}} e^{-b_{172}/T}$$

$$X_{172} = \left[K_{172}c_{13}c_{30} - c_3c_{28}\right]k_{172}$$

$$\frac{\partial X_{172}}{\partial c_j} = \left[-\delta_{3,j}c_{28} + \delta_{13,j}K_{172}c_{30} - \delta_{28,j}c_3 + \delta_{30,j}K_{172}c_{13}\right]k_{172}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{172}}{\partial T} = \left[\frac{1}{K_{149}}\frac{dK_{149}}{dT} - \frac{1}{K_3}\frac{dK_3}{dT}\right]K_{172}c_{13}c_{30}k_{172} - \left[n_{172} - \frac{b_{172}}{T}\right]\frac{X_{172}}{T}$$

Reaction 173, $BO + Cl \rightleftharpoons BCl + O$

$$K_{173} = \frac{K_{149}}{K_{151}}$$

$$k_{173} = a_{173}T^{-n_{173}} e^{-b_{173}/T}$$

$$X_{173} = \left[K_{173}c_{14}c_{30} - c_{18}c_{32}\right]k_{173}$$

$$\frac{\partial X_{173}}{\partial c_j} = \left[\delta_{14,j}K_{173}c_{30} - \delta_{18,j}c_{32} + \delta_{30,j}K_{173}c_{14} - \delta_{32,j}c_{18}\right]k_{173}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{173}}{\partial T} = \left[\frac{1}{K_{149}}\frac{dK_{149}}{dT} - \frac{1}{K_{151}}\frac{dK_{151}}{dT}\right]K_{173}c_{14}c_{30}k_{173}$$

$$- \left[n_{173} - \frac{b_{173}}{T}\right]\frac{X_{173}}{T}$$

Reaction 174, $BO + F \rightleftarrows BF + O$

$$K_{174} = \frac{K_{149}}{K_{155}}$$

$$k_{174} = a_{174} T^{-n_{174}} e^{-b_{174}/T}$$

$$X_{174} = \left[K_{174} c_{15} c_{30} - c_{18} c_{36}\right] k_{174}$$

$$\frac{\partial X_{174}}{\partial c_j} = \left[\delta_{15,j} K_{174} c_{30} - \delta_{18,j} c_{36} + \delta_{30,j} K_{174} c_{15} - \delta_{36,j} k_{18}\right] k_{174}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{174}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_{155}} \frac{dK_{155}}{dT}\right] K_{174} c_{15} c_{30} k_{174} - \left[n_{174} - \frac{b_{174}}{T}\right] \frac{X_{174}}{T}$$

Reaction 175, $BO + H \rightleftarrows B + OH$

$$K_{175} = \frac{K_{149}}{K_{11}}$$

$$k_{175} = a_{175} T^{-n_{175}} e^{-b_{175}/T}$$

$$X_{175} = \left[K_{175} c_{16} c_{30} - c_{11} c_{28}\right] k_{175}$$

$$\frac{\partial X_{175}}{\partial c_j} = \left[-\delta_{11,j} c_{28} + \delta_{16,j} K_{175} c_{30} - \delta_{28,j} c_{11} + \delta_{30,j} K_{175} c_{16}\right] k_{175}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{175}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{175} c_{16} c_{30} k_{175} - \left[n_{175} - \frac{b_{175}}{T}\right] \frac{X_{175}}{T}$$

Reaction 176, $BO + N \rightleftharpoons BN + O$

$$K_{176} = \frac{K_{149}}{K_{148}}$$

$$k_{176} = a_{176} T^{-n_{176}} e^{-b_{176}/T}$$

$$X_{176} = \left[K_{176} c_{17} c_{30} - c_{18} c_{29}\right] k_{176}$$

$$\frac{\partial X_{176}}{\partial c_j} = \left[\delta_{17,j} K_{176} c_{30} - \delta_{18,j} c_{29} - \delta_{29,j} c_{18} + \delta_{30,j} K_{176} c_{17}\right] k_{176}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{176}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_{148}} \frac{dK_{148}}{dT}\right] K_{176} c_{17} c_{30} k_{176}$$

$$- \left[n_{176} - \frac{b_{176}}{T}\right] \frac{X_{176}}{T}$$

Reaction 177, $BO + O \rightleftharpoons B + O_2$

$$K_{177} = \frac{K_{149}}{K_{12}}$$

$$k_{177} = a_{177} T^{-n_{177}} e^{-b_{177}/T}$$

$$X_{177} = \left[K_{177} c_{18} c_{30} - c_{12} c_{28}\right] k_{177}$$

$$\frac{\partial X_{177}}{\partial c_j} = \left[-\delta_{12,j} c_{28} + \delta_{18,j} K_{177} c_{30} - \delta_{28,j} c_{12} + \delta_{30,j} K_{177} c_{18}\right] k_{177}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{177}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_{12}} \frac{dK_{12}}{dT}\right] K_{177} c_{18} c_{30} k_{177} - \left[n_{177} - \frac{b_{177}}{T}\right] \frac{X_{177}}{T}$$

Reaction 178, $BO + BCl \rightleftharpoons B + BOCl$

$$K_{178} = \frac{K_{149}}{K_{154}}$$

$$k_{178} = a_{178} T^{-n_{178}} e^{-b_{178}/T}$$

$$X_{178} = \left[K_{178} c_{30} c_{32} - c_{28} c_{35}\right] k_{178}$$

$$\frac{\partial X_{178}}{\partial c_j} = \left[-\delta_{28,j} c_{35} + \delta_{30,j} K_{178} c_{32} + \delta_{32,j} K_{178} c_{30} - \delta_{35,j} c_{28}\right] k_{178}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{178}}{\partial T} = \left[\frac{1}{K_{149}} \frac{dK_{149}}{dT} - \frac{1}{K_{154}} \frac{dK_{154}}{dT}\right] K_{178} c_{30} c_{32} k_{178}$$

$$- \left[n_{178} - \frac{b_{178}}{T}\right] \frac{X_{178}}{T}$$

Reaction 179, $BO + BOCl \rightleftharpoons BO_2 + BCl$

$$K_{179} = \frac{K_{154}}{K_{150}}$$

$$k_{179} = a_{179} T^{-n_{179}} e^{-b_{179}/T}$$

$$X_{179} = \left[K_{179} c_{30} c_{35} - c_{31} c_{32}\right] k_{179}$$

$$\frac{\partial X_{179}}{\partial c_j} = \left[\delta_{30,j} K_{179} c_{35} - \delta_{31,j} c_{32} - \delta_{32,j} c_{31} + \delta_{35,j} K_{179} c_{30}\right] k_{179}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{179}}{\partial T} = \left[\frac{1}{K_{154}} \frac{dK_{154}}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{179} c_{30} c_{35} k_{179}$$

$$- \left[n_{179} - \frac{b_{179}}{T}\right] \frac{X_{179}}{T}$$

Reaction 180, $BO + BF \rightleftharpoons B + BOF$

$$K_{180} = \frac{K_{155}}{K_{158}}$$

$$k_{180} = a_{180} T^{-n_{180}} e^{-b_{180}/T}$$

$$X_{180} = \left[K_{180} c_{30} c_{36} - c_{28} c_{39}\right] k_{180}$$

$$\frac{\partial X_{180}}{\partial c_j} = \left[-\delta_{28,j} c_{39} + \delta_{30,j} K_{180} c_{36} + \delta_{36,j} K_{180} c_{30} - \delta_{39,j} c_{28}\right] k_{180}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{180}}{\partial T} = \left[\frac{1}{K_{155}} \frac{dK_{155}}{dT} - \frac{1}{K_{158}} \frac{dK_{158}}{dT}\right] K_{180} c_{30} c_{36} k_{180}$$

$$- \left[n_{180} - \frac{b_{180}}{T}\right] \frac{X_{180}}{T}$$

Reaction 181, $BO + BF_3 \rightleftharpoons BF_2 + BOF$

$$K_{181} = \frac{K_{157}}{K_{158}}$$

$$k_{181} = a_{181} T^{-n_{181}} e^{-b_{181}/T}$$

$$X_{181} = \left[K_{181} c_{30} c_{38} - c_{37} c_{39}\right] k_{181}$$

$$\frac{\partial X_{181}}{\partial c_j} = \left[\delta_{30,j} K_{181} c_{38} - \delta_{37,j} c_{39} + \delta_{38,j} K_{181} c_{30} - \delta_{39,j} c_{37}\right] k_{181}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{181}}{\partial T} = \left[\frac{1}{K_{157}} \frac{dK_{157}}{dT} - \frac{1}{K_{158}} \frac{dK_{158}}{dT}\right] K_{181} c_{30} c_{38} k_{181}$$

$$- \left[n_{181} - \frac{b_{181}}{T}\right] \frac{X_{181}}{T}$$

Reaction 182, $BO + BOF \rightleftharpoons BF + BO_2$

$$K_{182} = \frac{K_{159}}{K_{150}}$$

$$k_{182} = a_{182} T^{-n_{182}} e^{-b_{182}/T}$$

$$X_{182} = \left[K_{182} c_{30} c_{39} - c_{31} c_{36}\right] k_{182}$$

$$\frac{\partial X_{182}}{\partial c_j} = \left[\delta_{30,j} K_{182} c_{39} - \delta_{31,j} c_{36} - \delta_{36,j} c_{31} + \delta_{39,j} K_{182} c_{30}\right] k_{182}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{182}}{\partial T} = \left[\frac{1}{K_{159}} \frac{dK_{159}}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{182} c_{30} c_{39} k_{182}$$

$$- \left[n_{182} - \frac{b_{182}}{T}\right] \frac{X_{182}}{T}$$

Reaction 183, $BO_2 + HF \rightleftharpoons BOF + OH$

$$K_{183} = \frac{K_7 K_{150}}{K_{11} K_{158}}$$

$$k_{183} = a_{183} T^{-n_{183}} e^{-b_{183}/T}$$

$$X_{183} = \left[K_{183} c_7 c_{31} - c_{11} c_{39}\right] k_{183}$$

$$\frac{\partial X_{183}}{\partial c_j} = \left[\delta_{7,j} K_{183} c_{31} - \delta_{11,j} c_{39} + \delta_{31,j} K_{183} c_7 - \delta_{39,j} c_{11}\right] k_{183}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{183}}{\partial T} = \left[\frac{1}{K_7} \frac{dK_7}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT} + \frac{1}{K_{150}} \frac{dK_{150}}{dT} - \frac{1}{K_{158}} \frac{dK_{158}}{dT}\right] \cdot$$

$$K_{183} c_7 c_{31} k_{183} - \left[n_{183} - \frac{b_{183}}{T}\right] \frac{X_{183}}{T}$$

Reaction 184, $BO_2 + Cl \rightleftharpoons BOCl + O$

$$K_{184} = \frac{K_{173}}{K_{179}}$$

$$k_{184} = a_{184} T^{-n_{184}} e^{-b_{184}/T}$$

$$X_{184} = \left[K_{184} c_{14} c_{31} - c_{18} c_{35}\right] k_{184}$$

$$\frac{\partial X_{184}}{\partial c_j} = \left[\delta_{14,j} K_{184} c_{31} - \delta_{18,j} c_{35} + \delta_{31,j} K_{184} c_{14} - \delta_{35,j} c_{18}\right] k_{184}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{184}}{\partial T} = \left[\frac{1}{K_{173}} \frac{dK_{173}}{dT} - \frac{1}{K_{179}} \frac{dK_{179}}{dT}\right] K_{184} c_{14} c_{31} k_{184}$$

$$- \left[n_{184} - \frac{b_{184}}{T}\right] \frac{X_{184}}{T}$$

Reaction 185, $BO_2 + H \rightleftharpoons BO + OH$

$$K_{185} = \frac{K_{150}}{K_{11}}$$

$$k_{185} = a_{185} T^{-n_{185}} e^{-b_{185}/T}$$

$$X_{185} = \left[K_{185} c_{16} c_{31} - c_{11} c_{30}\right] k_{185}$$

$$\frac{\partial X_{185}}{\partial c_j} = \left[-\delta_{11,j} c_{30} + \delta_{16,j} K_{185} c_{31} - \delta_{30,j} c_{11} + \delta_{31,j} K_{185} c_{16}\right] k_{185}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{185}}{\partial T} = \left[\frac{1}{K_{150}} \frac{dK_{150}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{185} c_{16} c_{31} k_{185} - \left[n_{185} - \frac{b_{185}}{T}\right] \frac{X_{185}}{T}$$

Reaction 186, $BO_2 + O \rightleftharpoons BO + O_2$

$$K_{186} = \frac{K_{150}}{K_{12}}$$

$$k_{186} = a_{186} T^{-n_{186}} e^{-b_{186}/T}$$

$$X_{186} = \left[K_{186} c_{18} c_{31} - c_{12} c_{30}\right] k_{186}$$

$$\frac{\partial X_{186}}{\partial c_j} = \left[-\delta_{12,j} c_{30} + \delta_{18,j} K_{186} c_{31} - \delta_{30,j} c_{12} + \delta_{31,j} K_{186} c_{18}\right] k_{186}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{186}}{\partial T} = \left[\frac{1}{K_{150}} \frac{dK_{150}}{dT} - \frac{1}{K_{12}} \frac{dK_{12}}{dT}\right] K_{186} c_{18} c_{31} k_{186}$$

$$- \left[n_{186} - \frac{b_{186}}{T}\right] \frac{X_{186}}{T}$$

Reaction 187, $2BCl \rightleftharpoons B + BCl_2$

$$K_{187} = \frac{K_{151}}{K_{152}}$$

$$k_{187} = a_{187} T^{-n_{187}} e^{-b_{187}/T}$$

$$X_{187} = \left[K_{187} c_{32}^2 - c_{28} c_{33}\right] k_{187}$$

$$\frac{\partial X_{187}}{\partial c_j} = \left[-\delta_{28,j} c_{33} + 2\delta_{32,j} K_{187} c_{32} - \delta_{33,j} c_{28}\right] k_{187}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{187}}{\partial T} = \left[\frac{1}{K_{151}} \frac{dK_{151}}{dT} - \frac{1}{K_{152}} \frac{dK_{152}}{dT}\right] K_{187} c_{32}^2 k_{187} - \left[n_{187} - \frac{b_{187}}{T}\right] \frac{X_{187}}{T}$$

Reaction 188, $BCl + Cl \rightleftharpoons B + Cl_2$

$$K_{188} = \frac{K_{151}}{K_4}$$

$$k_{188} = a_{188} T^{-n_{188}} e^{-b_{188}/T}$$

$$X_{188} = \left[K_{188} c_{14} c_{32} - c_4 c_{28}\right] k_{188}$$

$$\frac{\partial X_{188}}{\partial c_j} = \left[-\delta_{4,j} c_{28} + \delta_{14,j} K_{188} c_{32} - \delta_{28,j} c_4 + \delta_{32,j} K_{188} c_{14}\right] k_{188}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{188}}{\partial T} = \left[\frac{1}{K_{151}} \frac{dK_{151}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{188} c_{14} c_{32} k_{188} - \left[n_{188} - \frac{b_{188}}{T}\right] \frac{X_{188}}{T}$$

Reaction 189, $BCl + H \rightleftharpoons B + HCl$

$$K_{189} = \frac{K_{151}}{K_6}$$

$$k_{189} = a_{189} T^{-n_{189}} e^{-b_{189}/T}$$

$$X_{189} = \left[K_{189} c_{16} c_{32} - c_6 c_{28}\right] k_{189}$$

$$\frac{\partial X_{189}}{\partial c_j} = \left[-\delta_{6,j} c_{28} + \delta_{16,j} K_{189} c_{32} - \delta_{28,j} c_6 + \delta_{32,j} K_{189} c_{16}\right] k_{189}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{189}}{\partial T} = \left[\frac{1}{K_{151}} \frac{dK_{151}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{189} c_{16} c_{32} k_{189}$$

$$- \left[n_{189} - \frac{b_{189}}{T}\right] \frac{X_{189}}{T}$$

Reaction 190, $BCl + N \rightleftharpoons BN + Cl$

$$K_{190} = \frac{K_{151}}{K_{148}}$$

$$k_{190} = a_{190} T^{-n_{190}} e^{-b_{190}/T}$$

$$X_{190} = \left[K_{190} c_{17} c_{32} - c_{14} c_{29}\right] k_{190}$$

$$\frac{\partial X_{190}}{\partial c_j} = \left[-\delta_{14,j} c_{29} + \delta_{17,j} K_{190} c_{32} - \delta_{29,j} c_{14} + \delta_{32,j} K_{190} c_{17}\right] k_{190}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{190}}{\partial T} = \left[\frac{1}{K_{151}} \frac{dK_{151}}{dT} - \frac{1}{K_{148}} \frac{dK_{148}}{dT}\right] K_{190} c_{17} c_{32} k_{190} - \left[n_{190} - \frac{b_{190}}{T}\right] \frac{X_{190}}{T}$$

Reaction 191, $BCl + BOF \rightleftharpoons BOCl + BF$

$$K_{191} = \frac{K_{159}}{K_{154}}$$

$$k_{191} = a_{191} T^{-n_{191}} e^{-b_{191}/T}$$

$$X_{191} = \left[K_{191} c_{32} c_{39} - c_{35} c_{36}\right] k_{191}$$

$$\frac{\partial X_{191}}{\partial c_j} = \left[\delta_{32,j} K_{191} c_{39} - \delta_{35,j} c_{36} - \delta_{36,j} c_{35} + \delta_{39,j} K_{191} c_{32}\right] k_{191}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{191}}{\partial T} = \left[\frac{1}{K_{159}} \frac{dK_{159}}{dT} - \frac{1}{K_{154}} \frac{dK_{154}}{dT}\right] K_{191} c_{32} c_{39} k_{191} - \left[n_{191} - \frac{b_{191}}{T}\right] \frac{X_{191}}{T}$$

Reaction 192, $BCl_2 + Cl \rightleftharpoons BCl + Cl_2$

$$K_{192} = \frac{K_{152}}{K_4}$$

$$k_{192} = a_{192} T^{-n_{192}} e^{-b_{192}/T}$$

$$X_{192} = \left[K_{192} c_{14} c_{33} - c_4 c_{32}\right] k_{192}$$

$$\frac{\partial X_{192}}{\partial c_j} = \left[-\delta_{4,j} c_{32} + \delta_{14,j} K_{192} c_{33} - \delta_{32,j} c_4 + \delta_{33,j} K_{192} c_{14}\right] k_{192}$$

$$j = 1, 2, \cdots, 56$$

$$\frac{\partial X_{192}}{\partial T} = \left[\frac{1}{K_{152}} \frac{dK_{152}}{dT} - \frac{1}{K_4} \frac{dK_{14}}{dT}\right] K_{192} c_{14} c_{33} k_{192} - \left[n_{192} - \frac{b_{192}}{T}\right] \frac{X_{192}}{T}$$

Reaction 193, $BCl_3 + Cl \rightleftharpoons BCl_2 + Cl_2$

$$K_{193} = \frac{K_{153}}{K_4}$$

$$k_{193} = a_{193} T^{-n_{193}} e^{-b_{193}/T}$$

$$X_{193} = \left[K_{193} c_{14} c_{34} - c_4 c_{33}\right] k_{193}$$

$$\frac{\partial X_{193}}{\partial c_j} = \left[-\delta_{4,j} c_{33} + \delta_{14,j} K_{193} c_{34} - \delta_{33,j} c_4 + \delta_{34,j} K_{193} c_{14}\right] k_{193}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{193}}{\partial T} = \left[\frac{1}{K_{153}} \frac{dK_{153}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{193} c_{14} c_{34} k_{193} - \left[n_{193} - \frac{b_{193}}{T}\right] \frac{X_{193}}{T}$$

Reaction 194, $BOCl + HCl \rightleftharpoons BCl_2 + OH$

$$K_{194} = \frac{K_6 K_{154}}{K_{11} K_{152}}$$

$$k_{194} = a_{194} T^{-n_{194}} e^{-b_{194}/T}$$

$$X_{194} = \left[K_{194} c_6 c_{35} - c_{11} c_{33}\right] k_{194}$$

$$\frac{\partial X_{194}}{\partial c_j} = \left[\delta_{6,j} K_{194} c_{35} - \delta_{11,j} c_{33} - \delta_{33,j} c_{11} + \delta_{35,j} K_{194} c_6\right] k_{194}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{194}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{11}}\frac{dK_{11}}{dT} - \frac{1}{K_{152}}\frac{dK_{152}}{dT} + \frac{1}{K_{154}}\frac{dK_{154}}{dT}\right] \cdot$$

$$K_{194} c_6 c_{35} k_{194} - \left[n_{194} - \frac{b_{194}}{T}\right] \frac{X_{194}}{T}$$

Reaction 195, $BOCl + OH \rightleftharpoons BO_2 + HCl$

$$K_{195} = \frac{K_{179} K_{189}}{K_{175}}$$

$$k_{195} = a_{195} T^{-n_{195}} e^{-b_{195}/T}$$

$$X_{195} = \left[K_{195} c_{11} c_{35} - c_6 c_{31}\right] k_{195}$$

$$\frac{\partial X_{195}}{\partial c_j} = \left[-\delta_{6,j} c_{31} + \delta_{11,j} K_{195} c_{35} - \delta_{31,j} c_6 + \delta_{35,j} K_{195} c_{11}\right] k_{195}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{195}}{\partial T} = \left[-\frac{1}{K_{175}}\frac{dK_{175}}{dT} + \frac{1}{K_{179}}\frac{dK_{179}}{dT} + \frac{1}{K_{189}}\frac{dK_{189}}{dT}\right] \cdot$$

$$K_{195} c_{11} c_{35} k_{195} - \left[n_{195} - \frac{b_{195}}{T}\right] \frac{X_{195}}{T}$$

Reaction 196, $BOCl + Cl \rightleftharpoons BO + Cl_2$

$$K_{196} = \frac{K_{188}}{K_{178}}$$

$$k_{196} = a_{196} T^{-n_{196}} e^{-b_{196}/T}$$

$$X_{196} = \left[K_{196} c_{14} c_{35} - c_4 c_{30}\right] k_{196}$$

$$\frac{\partial X_{196}}{\partial c_j} = \left[-\delta_{4,j} c_{30} + \delta_{14,j} K_{196} c_{35} - \delta_{30,j} c_4 + \delta_{35,j} K_{196} c_{14}\right] k_{196}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{196}}{\partial T} = \left[\frac{1}{K_{188}} \frac{dK_{188}}{dT} - \frac{1}{K_{178}} \frac{dK_{178}}{dT}\right] K_{196} c_{14} c_{35} k_{196}$$

$$- \left[n_{196} - \frac{b_{196}}{T}\right] \frac{X_{196}}{T}$$

Reaction 197, $BOCl + Cl \rightleftharpoons BCl_2 + O$

$$K_{197} = \frac{K_{154}}{K_{152}}$$

$$k_{197} = a_{197} T^{-n_{197}} e^{-b_{197}/T}$$

$$X_{197} = \left[K_{197} c_{14} c_{35} - c_{18} c_{33}\right] k_{197}$$

$$\frac{\partial X_{197}}{\partial c_j} = \left[\delta_{14,j} K_{197} c_{35} - \delta_{18,j} c_{33} - \delta_{33,j} c_{18} + \delta_{35,j} K_{197} c_{14}\right] k_{197}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{197}}{\partial T} = \left[\frac{1}{K_{154}} \frac{dK_{154}}{dT} - \frac{1}{K_{152}} \frac{dK_{152}}{dT}\right] K_{197} c_{14} c_{35} k_{197}$$

$$- \left[n_{197} - \frac{b_{197}}{T}\right] \frac{X_{197}}{T}$$

Reaction 198, $BOCl + H \rightleftharpoons BO + HCl$

$$K_{198} = \frac{K_{189}}{K_{178}}$$

$$k_{198} = a_{198} T^{-n_{198}} e^{-b_{198}/T}$$

$$X_{198} = \left[K_{198} c_{16} c_{35} - c_6 c_{30}\right] k_{198}$$

$$\frac{\partial X_{198}}{\partial c_j} = \left[-\delta_{6,j} c_{30} + \delta_{16,j} K_{198} c_{35} - \delta_{30,j} c_6 + \delta_{35,j} K_{198} c_{16}\right] k_{198}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{198}}{\partial T} = \left[\frac{1}{K_{189}} \frac{dK_{189}}{dT} - \frac{1}{K_{178}} \frac{dK_{178}}{dT}\right] K_{198} c_{16} c_{35} k_{198}$$

$$- \left[n_{198} - \frac{b_{198}}{T}\right] \frac{X_{198}}{T}$$

Reaction 199, $BOCl + H \rightleftharpoons BCl + OH$

$$K_{199} = \frac{K_{154}}{K_{11}}$$

$$k_{199} = a_{199} T^{-n_{199}} e^{-b_{199}/T}$$

$$X_{199} = \left[K_{199} c_{16} c_{35} - c_{11} c_{43}\right] k_{199}$$

$$\frac{\partial X_{199}}{\partial c_j} = \left[-\delta_{11,j} c_{32} + \delta_{16,j} K_{199} c_{35} - \delta_{32,j} c_{11} + \delta_{35,j} K_{199} c_{16}\right] k_{199}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{199}}{\partial T} = \left[\frac{1}{K_{154}} \frac{dK_{154}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{199} c_{16} c_{35} k_{199} - \left[n_{199} - \frac{b_{199}}{T}\right] \frac{X_{199}}{T}$$

Reaction 200, $BCCl + N \rightleftharpoons BCl + NO$

$$K_{200} = \frac{K_{154}}{K_{10}}$$

$$k_{200} = a_{200} T^{-n_{200}} e^{-b_{200}/T}$$

$$X_{200} = \left[K_{200} c_{17} c_{35} - c_{10} c_{32}\right] k_{200}$$

$$\frac{\partial X_{200}}{\partial c_j} = \left[-\delta_{10,j} c_{32} + \delta_{17,j} K_{200} c_{35} - \delta_{32,j} c_{10} + \delta_{35,j} K_{200} c_{17}\right] k_{200}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{200}}{\partial T} = \left[\frac{1}{K_{154}} \frac{dK_{154}}{dT} - \frac{1}{K_{10}} \frac{dK_{10}}{dT}\right] K_{200} c_{17} c_{35} k_{200} - \left[n_{200} - \frac{b_{200}}{T}\right] \frac{X_{200}}{T}$$

Reaction 201, $BOCl + O \rightleftharpoons BCl + O_2$

$$K_{201} = \frac{K_{154}}{K_{12}}$$

$$k_{201} = a_{201} T^{-n_{201}} e^{-b_{201}/T}$$

$$X_{201} = \left[K_{201} c_{18} c_{35} - c_{12} c_{32}\right] k_{201}$$

$$\frac{\partial X_{201}}{\partial c_j} = \left[-\delta_{12,j} c_{32} + \delta_{18,j} K_{201} c_{35} - \delta_{32,j} c_{12} + \delta_{35,j} K_{201} c_{18}\right] k_{201}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{201}}{\partial T} = \left[\frac{1}{K_{154}} \frac{dK_{154}}{dT} - \frac{1}{K_{12}} \frac{dK_{12}}{dT}\right] K_{201} c_{18} c_{35} k_{201} - \left[n_{201} - \frac{b_{201}}{T}\right] \frac{X_{201}}{T}$$

Reaction 202, $2BF \rightleftharpoons B + BF_2$

$$K_{202} = \frac{K_{155}}{K_{156}}$$

$$k_{202} = a_{202} T^{-n_{202}} e^{-b_{202}/T}$$

$$X_{202} = \left[K_{202} c_{36}^2 - c_{28} c_{37}\right] k_{202}$$

$$\frac{\partial X_{202}}{\partial c_j} = \left[-\delta_{28,j} c_{37} + 2\delta_{36,j} K_{202} c_{36} - \delta_{37,j} c_{28}\right] k_{202}$$

$$\frac{\partial X_{202}}{\partial c_j} = \left[-\delta_{28,j} c_{37} + 2\delta_{36,j} K_{202} c_{36} - \delta_{37,j} c_{28}\right] k_{202}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{202}}{\partial T} = \left[\frac{1}{K_{155}} \frac{dK_{155}}{dT} - \frac{1}{K_{156}} \frac{dK_{156}}{dT}\right] K_{202} c_{36}^2 k_{202} - \left[n_{202} - \frac{b_{202}}{T}\right] \frac{X_{202}}{T}$$

Reaction 203, $BF + CO_2 \rightleftharpoons BOF + CO$

$$K_{203} = \frac{K_1}{K_{159}}$$

$$k_{203} = a_{203} T^{-n_{203}} e^{-b_{203}/T}$$

$$X_{203} = \left[K_{203} c_1 c_{36} - c_3 c_{39}\right] k_{203}$$

$$\frac{\partial X_{203}}{\partial c_j} = \left[\delta_{1,j} K_{203} c_{36} - \delta_{3,j} c_{39} + \delta_{36,j} K_{203} c_1 - \delta_{39,j} c_3\right] k_{203}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{203}}{\partial T} = \left[\frac{1}{K_1} \frac{dK_1}{dT} \frac{1}{K_{159}} \frac{dK_{159}}{dT}\right] K_{203} c_1 c_{36} k_{203} - \left[n_{203} - \frac{b_{203}}{T}\right] \frac{X_{203}}{T}$$

Reaction 204, $BF + CO \rightleftharpoons BOF + C$

$$K_{204} = \frac{K_3}{K_{159}}$$

$$k_{204} = a_{204} T^{-n_{204}} e^{-b_{204}/T}$$

$$X_{204} = \left[K_{204} c_3 c_{36} - c_{13} c_{39}\right] k_{204}$$

$$\frac{\partial X_{204}}{\partial c_j} = \left[\delta_{3,j} K_{204} c_{36} - \delta_{13,j} c_{39} + \delta_{36,j} K_{204} c_3 - \delta_{39,j} c_{13}\right] k_{204}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{204}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_{159}}\frac{dK_{159}}{dT}\right] K_{204} c_3 c_{36} k_{204} - \left[n_{204} - \frac{b_{204}}{T}\right]\frac{X_{204}}{T}$$

Reaction 205, $BF + HCl \rightleftharpoons BCl + HF$

$$K_{205} = \frac{K_{155}}{K_7 K_{189}}$$

$$k_{205} = a_{205} T^{-n_{205}} e^{-b_{205}/T}$$

$$X_{205} = \left[K_{205} c_6 c_{36} - c_7 c_{32}\right] k_{205}$$

$$\frac{\partial X_{205}}{\partial c_j} = \left[\delta_{6,j} K_{205} c_{36} - \delta_{7,j} c_{32} - \delta_{32,j} c_7 + \delta_{36,j} K_{205} c_6\right] k_{205}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{205}}{\partial T} = \left[\frac{1}{K_{155}}\frac{dK_{155}}{dT} - \frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{189}}\frac{dK_{189}}{dT}\right] K_{205} c_6 c_{36} k_{205}$$

$$- \left[n_{205} - \frac{b_{205}}{T}\right]\frac{X_{205}}{T}$$

Reaction 206, $BF + HF \rightleftarrows BF_2 + H$

$$K_{206} = \frac{K_7}{K_{156}}$$

$$k_{206} = a_{206} T^{-n_{206}} e^{-b_{206}/T}$$

$$X_{206} = \left[K_{206} c_7 c_{36} - c_{16} c_{37}\right] k_{206}$$

$$\frac{\partial X_{206}}{\partial c_j} = \left[\delta_{7,j} K_{206} c_{36} - \delta_{16,j} c_{37} + \delta_{36,j} K_{206} c_7 - \delta_{37,j} c_{16}\right] k_{206}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{206}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{156}}\frac{dK_{156}}{dT}\right] K_{206} c_7 c_{36} k_{206} - \left[n_{206} - \frac{b_{206}}{T}\right] \frac{X_{206}}{T}$$

Reaction 207, $BF + Cl \rightleftarrows BCl + F$

$$K_{207} = \frac{K_{155}}{K_{151}}$$

$$k_{207} = a_{207} T^{-n_{207}} e^{-b_{207}/T}$$

$$X_{207} = \left[K_{207} c_{14} c_{36} - c_{15} c_{32}\right] k_{207}$$

$$\frac{\partial X_{207}}{\partial c_j} = \left[\delta_{14,j} K_{207} c_{36} - \delta_{15,j} c_{32} - \delta_{32,j} c_{15} + \delta_{36,j} K_{207} c_{14}\right] k_{207}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{207}}{\partial T} = \left[\frac{1}{K_{155}}\frac{dK_{155}}{dT} - \frac{1}{K_{151}}\frac{dK_{151}}{dT}\right] K_{207} c_{14} c_{36} k_{207}$$

$$- \left[n_{207} - \frac{b_{207}}{T}\right] \frac{X_{207}}{T}$$

Reaction 208, $BF + F \rightleftharpoons B + F_2$

$$K_{208} = \frac{K_{155}}{K_5}$$

$$k_{208} = a_{208} T^{-n_{208}} e^{-b_{208}/T}$$

$$X_{208} = \left[K_{208} c_{15} c_{36} - c_5 c_{28}\right] k_{208}$$

$$\frac{\partial X_{208}}{\partial c_j} = \left[-\delta_{5,j} c_{28} + \delta_{15,j} K_{208} c_{36} - \delta_{28,j} c_5 + \delta_{36,j} K_{208} c_{15}\right] k_{208}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{208}}{\partial T} = \left[\frac{1}{K_{155}} \frac{dK_{155}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{208} c_{15} c_{36} k_{208} - \left[n_{208} - \frac{b_{208}}{T}\right] \frac{X_{208}}{T}$$

Reaction 209, $BF + H \rightleftharpoons B + HF$

$$K_{209} = \frac{K_{155}}{K_7}$$

$$k_{209} = a_{209} T^{-n_{209}} e^{-b_{209}/T}$$

$$X_{209} = \left[K_{209} c_{16} c_{36} - c_7 c_{28}\right] k_{209}$$

$$\frac{\partial X_{209}}{\partial c_j} = \left[-\delta_{7,j} c_{28} + \delta_{16,j} K_{209} c_{36} - \delta_{28,j} c_7 + \delta_{36,j} K_{209} c_{16}\right] k_{209}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{209}}{\partial T} = \left[\frac{f}{K_{155}} \frac{dK_{155}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{209} c_{16} c_{36} k_{209} - \left[n_{209} - \frac{b_{209}}{T}\right] \frac{X_{209}}{T}$$

Reaction 210, $BF + N \rightleftharpoons BN + F$

$$K_{210} = \frac{K_{155}}{K_{148}}$$

$$k_{210} = a_{210} T^{-n_{210}} e^{-b_{210}/T}$$

$$X_{210} = \left[K_{210} c_{17} c_{36} - c_{15} c_{29}\right] k_{210}$$

$$\frac{\partial X_{210}}{\partial c_j} = \left[-\delta_{15,j} c_{29} + \delta_{17,j} K_{210} c_{36} - \delta_{29,j} c_{15} + \delta_{36,j} K_{210} c_{17}\right] k_{210}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{210}}{\partial T} = \left[\frac{1}{K_{155}} \frac{dK_{155}}{dT} - \frac{1}{K_{148}} \frac{dK_{148}}{dT}\right] K_{210} c_{17} c_{36} k_{210}$$

$$- \left[n_{210} - \frac{b_{210}}{T}\right] \frac{X_{210}}{T}$$

Reaction 211, $BF + BF_2 \rightleftharpoons B + BF_3$

$$K_{211} = \frac{K_{155}}{K_{157}}$$

$$k_{211} = a_{211} T^{-n_{211}} e^{-b_{211}/T}$$

$$X_{211} = \left[K_{211} c_{36} c_{37} - c_{28} c_{38}\right] k_{211}$$

$$\frac{\partial X_{211}}{\partial c_j} = \left[-\delta_{28,j} c_{38} + \delta_{36,j} K_{211} c_{37} + \delta_{37,j} K_{211} c_{36} - \delta_{38,j} c_{28}\right] k_{211}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{211}}{\partial T} = \left[\frac{1}{K_{155}} \frac{dK_{155}}{dT} - \frac{1}{K_{157}} \frac{dK_{157}}{dT}\right] K_{211} c_{36} c_{37} k_{211}$$

$$- \left[n_{211} - \frac{b_{211}}{T}\right] \frac{X_{211}}{T}$$

Reaction 212, $BF + BOF \rightleftharpoons BO + BF_2$

$$K_{212} = \frac{K_{158}}{K_{156}}$$

$$k_{212} = a_{212} T^{-n_{212}} e^{-b_{212}/T}$$

$$X_{212} = \left[K_{212} c_{36} c_{39} - c_{30} c_{37}\right] k_{212}$$

$$\partial X_{212} = \left[-\delta_{30,j} c_{37} + \delta_{36,j} K_{212} c_{39} - \delta_{37,j} c_{30} + \delta_{39,j} K_{212} c_{36}\right] k_{212}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{212}}{\partial T} = \left[\frac{1}{K_{158}} \frac{dK_{158}}{dT} - \frac{1}{K_{156}} \frac{dK_{156}}{dT}\right] K_{212} c_{36} c_{39} k_{212} - \left[n_{212} - \frac{b_{212}}{T}\right] \frac{X_{212}}{T}$$

Reaction 213, $BF_2 + F \rightleftharpoons BF + F_2$

$$K_{213} = \frac{K_{156}}{K_5}$$

$$k_{213} = a_{213} T^{-n_{213}} e^{-b_{213}/T}$$

$$X_{213} = \left[K_{213} c_{15} c_{37} - c_5 c_{36}\right] k_{213}$$

$$\frac{\partial X_{213}}{\partial c_j} = \left[-\delta_{5,j} c_{36} + \delta_{15,j} K_{213} c_{37} - \delta_{36,j} c_5 + \delta_{37,j} K_{213} c_{15}\right] k_{213}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{213}}{\partial T} = \left[\frac{1}{K_{156}} \frac{dK_{156}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{213} c_{15} c_{37} k_{213} - \left[n_{213} - \frac{b_{213}}{T}\right] \frac{X_{213}}{T}$$

Reaction 214, $BF_3 + F \rightleftarrows BF_2 + F_2$

$$K_{214} = \frac{K_{157}}{K_5}$$

$$k_{214} = a_{214} T^{-n_{214}} e^{-b_{214}/T}$$

$$X_{214} = \left[K_{214} c_{15} c_{38} - c_5 c_{37}\right] k_{214}$$

$$\frac{\partial X_{214}}{\partial c_j} = \left[-\delta_{5,j} c_{37} + \delta_{15,j} K_{214} c_{38} - \delta_{37,j} c_5 + \delta_{38,j} K_{214} c_{15}\right] k_{214}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{214}}{\partial T} = \left[\frac{1}{K_{157}} \frac{dK_{157}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{214} c_{15} c_{38} k_{214} - \left[n_{214} - \frac{b_{214}}{T}\right] \frac{X_{214}}{T}$$

Reaction 215, $BF_3 + H \rightleftarrows BF_2 + HF$

$$K_{215} = \frac{K_{157}}{K_7}$$

$$k_{215} = a_{215} T^{-n_{215}} e^{-b_{215}/T}$$

$$X_{215} = \left[K_{215} c_{16} c_{38} - c_7 c_{37}\right] k_{215}$$

$$\frac{\partial X_{215}}{\partial c_j} = \left[-\delta_{7,j} c_{37} + \delta_{16,j} K_{215} c_{38} - \delta_{37,j} c_7 + \delta_{38,j} K_{215} c_{16}\right] k_{215}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{215}}{\partial T} = \left[\frac{1}{K_{157}} \frac{dK_{157}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{215} c_{16} c_{38} k_{215}$$

$$- \left[n_{215} - \frac{b_{215}}{T}\right] \frac{X_{215}}{T}$$

Reaction 216, $2BOF \rightleftharpoons BO_2 + BF_2$

$$K_{216} = \frac{K_{164}K_{212}}{K_{180}}$$

$$k_{216} = a_{216}T^{-n_{216}} e^{-b_{216}/T}$$

$$X_{216} = \left[K_{216}c_{39}^2 - c_{31}c_{37}\right] k_{216}$$

$$\frac{\partial X_{216}}{\partial c_j} = \left[-\delta_{31,j}c_{37} - \delta_{37,j}c_{31} + 2\delta_{39,j}K_{216}c_{39}\right] k_{216}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{216}}{\partial T} = \left[\frac{1}{K_{164}} \frac{dK_{164}}{dT} - \frac{1}{K_{180}} \frac{dK_{180}}{T} + \frac{1}{K_{212}} \frac{dK_{212}}{dT}\right] K_{216}c_{39}^2 k_{216}$$

$$- \left[n_{216} - \frac{b_{216}}{T}\right] \frac{X_{216}}{T}$$

Reaction 217, $BOF + HCl \rightleftharpoons BOCl + HF$

$$K_{217} = K_{191}K_{205}$$

$$k_{217} = a_{217}T^{-n_{217}} e^{-b_{217}/T}$$

$$X_{217} = \left[K_{217}c_6c_{39} - c_7c_{35}\right]k_{217}$$

$$\frac{\partial X_{217}}{\partial c_j} = \left[\delta_{6,j}K_{217}c_{39} - \delta_{7,j}c_{35} - \delta_{35,j}c_7 + \delta_{39,j}K_{217}c_6\right] k_{217}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{217}}{\partial T} = \left[\frac{1}{K_{191}} \frac{dK_{191}}{dT} + \frac{1}{K_{205}} \frac{dK_{205}}{dT}\right] K_{217}c_6c_{39}k_{217}$$

$$- \left[n_{217} - \frac{b_{217}}{T}\right] \frac{X_{217}}{T}$$

Reaction 218, $BOF + HF \rightleftharpoons BF_2 + OH$

$$K_{218} = K_{169}K_{212}$$

$$k_{218} = a_{218}T^{-n_{218}} e^{-b_{218}/T}$$

$$X_{218} = \left[K_{218}c_7c_{39} - c_{11}c_{37}\right]k_{218}$$

$$\frac{\partial X_{218}}{\partial c_j} = \left[\delta_{7,j}K_{218}c_{39} - \delta_{11,j}c_{37} - \delta_{37,j}c_{11} + \delta_{39,j}K_{218}c_7\right]k_{218}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{218}}{\partial T} = \left[\frac{1}{K_{169}}\frac{dK_{169}}{dT} + \frac{1}{K_{212}}\frac{dK_{212}}{dT}\right]K_{218}c_7c_{39}k_{218}$$

$$- \left[n_{218} - \frac{b_{218}}{T}\right]\frac{X_{218}}{T}$$

Reaction 219, $BOF + Cl \rightleftharpoons BOCl + F$

$$K_{219} = \frac{K_{158}K_{178}}{K_{151}}$$

$$k_{219} = a_{219}T^{-n_{219}} e^{-b_{219}/T}$$

$$X_{219} = \left[K_{219}c_{14}c_{39} - c_{15}c_{35}\right]k_{219}$$

$$\frac{\partial X_{219}}{\partial c_j} = \left[\delta_{14,j}K_{219}c_{39} - \delta_{15,j}c_{35} - \delta_{35,j}c_{15} + \delta_{39,j}K_{219}c_{14}\right]k_{219}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{219}}{\partial T} = \left[-\frac{1}{K_{151}}\frac{dK_{151}}{dT} + \frac{1}{K_{158}}\frac{dK_{158}}{dT} + \frac{1}{K_{178}}\frac{dK_{178}}{dT}\right]K_{219}c_{14}c_{39}k_{219}$$

$$- \left[n_{219} - \frac{b_{219}}{T}\right]\frac{X_{219}}{T}$$

Reaction 220, $BOF + F \rightleftharpoons BO + F_2$

$$K_{220} = \frac{K_{158}}{K_5}$$

$$k_{220} = a_{220} T^{-n_{220}} e^{-b_{220}/T}$$

$$X_{220} = \left[K_{220} c_{15} c_{39} - c_5 c_{30}\right] k_{220}$$

$$\frac{\partial X_{220}}{\partial c_j} = \left[-\delta_{5,j} c_{30} + \delta_{15,j} K_{220} c_{39} - \delta_{30,j} c_5 + \delta_{39,j} K_{220} c_{15}\right] k_{220}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{220}}{\partial T} = \left[\frac{1}{K_{158}} \frac{dK_{158}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{220} c_{15} c_{39} k_{220} - \left[n_{220} - \frac{b_{220}}{T}\right] \frac{X_{220}}{T}$$

Reaction 221, $BOF + F \rightleftharpoons BF_2 + O$

$$K_{221} = \frac{K_{159}}{K_{156}}$$

$$k_{221} = a_{221} T^{-n_{221}} e^{-b_{221}/T}$$

$$X_{221} = \left[K_{221} c_{15} c_{39} - c_{18} c_{37}\right] k_{221}$$

$$\frac{\partial X_{221}}{\partial c_j} = \left[\delta_{15,j} K_{221} c_{39} - \delta_{18,j} c_{37} - \delta_{37,j} c_{18} + \delta_{39,j} K_{221} c_{15}\right] k_{221}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{221}}{\partial T} = \left[\frac{1}{K_{159}} \frac{dK_{159}}{dT} - \frac{1}{K_{156}} \frac{dK_{156}}{dT}\right] K_{221} c_{15} c_{39} k_{221}$$

$$- \left[n_{221} - \frac{b_{221}}{T}\right] \frac{X_{221}}{T}$$

Reaction 222, $BOF + H \rightleftarrows BO + HF$

$$K_{222} = \frac{K_{158}}{K_7}$$

$$k_{222} = a_{222} T^{-n_{222}} e^{-b_{222}/T}$$

$$X_{222} = \left[K_{222} c_{16} c_{39} - c_7 c_{30}\right] k_{222}$$

$$\frac{\partial X_{222}}{\partial c_j} = \left[-\delta_{7,j} c_{30} + \delta_{16,j} K_{222} c_{39} - \delta_{30,j} c_7 + \delta_{39,j} K_{222} c_{16}\right] k_{222}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{222}}{\partial T} = \left[\frac{1}{K_{158}} \frac{dK_{158}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{222} c_{16} c_{39} k_{222} - \left[n_{222} - \frac{b_{222}}{T}\right] \frac{X_{222}}{T}$$

Reaction 223, $BOF + H \rightleftarrows BF + OH$

$$K_{223} = \frac{K_{159}}{K_{11}}$$

$$k_{223} = a_{223} T^{-n_{223}} e^{-b_{223}/T}$$

$$X_{223} = \left[K_{223} c_{16} c_{39} - c_{11} c_{36}\right] k_{223}$$

$$\frac{\partial X_{223}}{\partial c_j} = \left[-\delta_{11,j} c_{36} + \delta_{16,j} K_{223} c_{39} - \delta_{36,j} c_{11} + \delta_{39,j} K_{223} c_{16}\right] k_{223}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{223}}{\partial T} = \left[\frac{1}{K_{159}} \frac{dK_{159}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{223} c_{16} c_{39} k_{223}$$

$$- \left[n_{223} - \frac{b_{223}}{T}\right] \frac{X_{223}}{T}$$

Reaction 224, $BOF + O \rightleftharpoons BO_2 + F$

$$K_{224} = \frac{K_{158}}{K_{150}}$$

$$k_{224} = a_{224} T^{-n_{224}} e^{-b_{224}/T}$$

$$X_{224} = \left[K_{224} c_{18} c_{39} - c_{15} c_{31}\right] k_{224}$$

$$\frac{\partial X_{224}}{\partial c_j} = \left[-\delta_{15,j} c_{31} + \delta_{18,j} K_{224} c_{39} - \delta_{31,j} c_{15} + \delta_{39,j} K_{224} c_{18}\right] k_{224}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{224}}{\partial T} = \left[\frac{1}{K_{158}} \frac{dK_{158}}{dT} - \frac{1}{K_{150}} \frac{dK_{150}}{dT}\right] K_{224} c_{18} c_{39} k_{224}$$

$$- \left[n_{224} - \frac{b_{224}}{T}\right] \frac{X_{224}}{T}$$

Reaction 225, $LiOH + M \rightleftharpoons Li + OH + M$

$$k_{225} = a_{225} T^{-n_{225}} e^{-b_{225}/T}$$

$$M_{225} = \sum_{i=1}^{57} m_{225,i} c_i$$

$$X_{225} = \left[K_{225} c_{53} - \rho c_{11} c_{49}\right] M_{225} k_{225}$$

$$\frac{\partial X_{225}}{\partial c_j} = \frac{X_{225}}{M_{225}} m_{225,j} - \delta_{11,j} \rho c_{49} M_{225} k_{225} - \delta_{49,j} \rho c_{11} M_{225} k_{225}$$

$$+ \delta_{53,j} K_{225} M_{225} k_{225} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{225}}{\partial \rho} = -c_{11} c_{49} M_{225} k_{225}$$

$$\frac{\partial X_{225}}{\partial T} = c_{53} M_{225} k_{225} \frac{dK_{225}}{dT} - \left[n_{225} - \frac{b_{225}}{T}\right] \frac{X_{225}}{T}$$

Reaction 226, $LiOH + M \rightleftarrows LiO + H + M$

$$k_{226} = a_{226}T^{-n_{226}} e^{-b_{226}/T}$$

$$M_{226} = \sum_{i=1}^{57} m_{226,i}c_i$$

$$X_{226} = \left[K_{226}c_{53} - \rho c_{16}c_{51}\right]M_{226}k_{226}$$

$$\frac{\partial X_{226}}{\partial c_j} = \frac{X_{226}}{M_{226}} m_{226,j} - \delta_{16,j}\rho c_{51}M_{226}k_{226} - \delta_{51,j}\rho c_{16}M_{226}k_{226} + \delta_{53,j}K_{226}M_{226}k_{226} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{226}}{\partial \rho} = -c_{16}c_{51}M_{226}k_{226}$$

$$\frac{\partial X_{226}}{\partial T} = c_{53}M_{226}k_{226}\frac{dK_{226}}{dT} - \left[n_{226} - \frac{b_{226}}{T}\right]\frac{X_{226}}{T}$$

Reaction 227, $LiCl + M \rightleftarrows Li + Cl + M$

$$k_{227} = a_{227}T^{-n_{227}} e^{-b_{227}/T}$$

$$M_{227} = \sum_{i=1}^{57} m_{227,i}c_i$$

$$X_{227} = \left[K_{227}c_{55} - \rho c_{14}c_{49}\right]M_{227}k_{227}$$

$$\frac{\partial X_{227}}{\partial c_j} = \frac{X_{227}}{M_{227}} m_{227,j} - \delta_{14,j}\rho c_{49}M_{227}k_{227} - \delta_{49,j}\rho c_{14}M_{227}k_{227} + \delta_{55,j}K_{227}M_{227}k_{227} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{227}}{\partial \rho} = -c_{14}c_{49}M_{227}k_{227}$$

$$\frac{\partial X_{227}}{\partial T} = c_{55}M_{227}k_{227}\frac{dK_{227}}{dT} - \left[n_{227} - \frac{b_{227}}{T}\right]\frac{X_{227}}{T}$$

Reaction 228, $LiF + M \rightleftharpoons Li + F + M$

$$k_{228} = a_{228} T^{-n_{228}} e^{-b_{228}/T}$$

$$M_{228} = \sum_{i=1}^{57} m_{228,i} c_i$$

$$X_{228} = \left[K_{228} c_{54} - \rho c_{15} c_{49}\right] M_{228} k_{228}$$

$$\frac{\partial X_{228}}{\partial c_j} = \frac{X_{228}}{M_{228}} m_{228,j} - \delta_{15,j} \rho c_{49} M_{228} k_{228} - \delta_{49,j} \rho c_{15} M_{228} k_{228} + \delta_{54,j} K_{228} M_{228} k_{228} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{228}}{\partial \rho} = -c_{15} c_{49} M_{228} k_{228}$$

$$\frac{\partial X_{228}}{\partial T} = c_{54} M_{228} k_{228} \frac{dK_{228}}{dT} - \left[n_{228} - \frac{b_{228}}{T}\right] \frac{X_{228}}{T}$$

Reaction 229, $LiH + M \rightleftharpoons Li + H + M$

$$k_{229} = a_{229} T^{-n_{229}} e^{-b_{229}/T}$$

$$M_{229} = \sum_{i=1}^{57} m_{229,i} c_i$$

$$X_{229} = \left[K_{229} c_{50} - \rho c_{16} c_{49}\right] M_{229} k_{229}$$

$$\frac{\partial X_{229}}{\partial c_j} = \frac{X_{229}}{M_{229}} m_{229,j} - \delta_{16,j} \rho c_{49} M_{229} k_{229} - \delta_{49,j} \rho c_{16} M_{229} k_{229} + \delta_{50,j} K_{229} M_{229} k_{229} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{229}}{\partial \rho} = -c_{16} c_{49} M_{229} k_{229}$$

$$\frac{\partial X_{229}}{\partial T} = c_{50} M_{229} k_{229} \frac{dK_{229}}{dT} - \left[n_{229} - \frac{b_{229}}{T}\right] \frac{X_{229}}{T}$$

Reaction 230, $LiO + M \rightleftharpoons Li + O + M$

$$k_{230} = a_{230} T^{-n_{230}} e^{-b_{230}/T}$$

$$M_{230} = \sum_{i=1}^{57} m_{230,i} c_i$$

$$X_{230} = \left[K_{230} c_{51} - \rho c_{18} c_{49}\right] M_{230} k_{230}$$

$$\frac{\partial X_{230}}{\partial c_j} = \frac{X_{230}}{M_{230}} m_{230,j} - \delta_{18,j} \rho c_{49} M_{230} k_{230} - \delta_{49,j} \rho c_{18} M_{230} k_{230}$$

$$+ \delta_{51,j} K_{230} M_{230} k_{230} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{230}}{\partial \rho} = -c_{18} c_{49} M_{230} k_{230}$$

$$\frac{\partial X_{230}}{\partial T} = c_{51} M_{230} k_{230} \frac{dK_{230}}{dT} - \left[n_{230} - \frac{b_{230}}{T}\right] \frac{X_{230}}{T}$$

Reaction 231, $Li_2O + M \rightleftharpoons Li + LiO + M$

$$k_{231} = a_{231} T^{-n_{231}} e^{-b_{231}/T}$$

$$M_{231} = \sum_{i=1}^{57} m_{231,i} c_i$$

$$X_{231} = \left[K_{231} c_{52} - \rho c_{49} c_{51}\right] M_{231} k_{231}$$

$$\frac{\partial X_{231}}{\partial c_j} = \frac{X_{231}}{M_{231}} m_{231,j} - \delta_{49,j} \rho c_{51} M_{231} k_{231} - \delta_{51,j} \rho c_{49} M_{231} k_{231}$$

$$+ \delta_{52,j} K_{231} M_{231} k_{231} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{231}}{\partial \rho} = -c_{49} c_{51} M_{231} k_{231}$$

$$\frac{\partial X_{231}}{\partial T} = c_{52} M_{231} k_{231} \frac{dK_{231}}{dT} - \left[n_{231} - \frac{b_{231}}{T}\right] \frac{X_{231}}{T}$$

Reaction 232, $Li_2F_2 + M \rightleftharpoons 2LiF + M$

$$k_{232} = a_{232}T^{-n_{232}} e^{-b_{232}/T}$$

$$M_{232} = \sum_{i=1}^{57} m_{232,i}c_i$$

$$X_{232} = \left[K_{232}c_{56} - \rho c_{54}^2\right] M_{232}k_{232}$$

$$\frac{\partial X_{232}}{\partial c_j} = \frac{X_{232}}{M_{232}} m_{232,j} - 2\delta_{54,j}\rho c_{54}M_{232}k_{232}$$

$$+ \delta_{56,j}K_{232}M_{232}k_{232} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{232}}{\partial \rho} = -c_{54}^2 M_{232}k_{232}$$

$$\frac{\partial X_{232}}{\partial T} = c_{56}M_{232}k_{232}\frac{dK_{232}}{dT} - \left[n_{232} - \frac{b_{232}}{T}\right]\frac{X_{232}}{T}$$

Reaction 233, $Li_2Cl_2 + M \rightleftharpoons 2LiCl + M$

$$k_{233} = a_{233}T^{-n_{233}} e^{-b_{233}/T}$$

$$M_{233} = \sum_{i=1}^{57} m_{233,i}c_i$$

$$X_{233} = \left[K_{233}c_{57} - \rho c_{55}^2\right] M_{233}k_{233}$$

$$\frac{\partial X_{233}}{\partial c_j} = \frac{X_{233}}{M_{233}} m_{233,j} - \partial\delta_{55,j}c_{55}M_{233}k_{233}$$

$$+ \delta_{57,j}K_{233}M_{233}k_{233} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{233}}{\partial \rho} = -c_{55}^2 M_{233}k_{233}$$

$$\frac{\partial X_{233}}{\partial T} = c_{57}M_{233}k_{233}\frac{dK_{233}}{dT} - \left[n_{233} - \frac{b_{233}}{T}\right]\frac{X_{233}}{T}$$

Reaction 234, Li + $H_2O \rightleftharpoons$ LiH + OH

$$K_{234} = \frac{K_2}{K_{229}}$$

$$k_{234} = a_{234} T^{-n_{234}} e^{-b_{234}/T}$$

$$X_{234} = \left[K_{234} c_2 c_{49} - c_{11} c_{50}\right] k_{234}$$

$$\frac{\partial X_{234}}{\partial c_j} = \left[\delta_{2,j} K_{234} c_{49} - \delta_{11,j} c_{50} + \delta_{49,j} K_{234} c_2 - \delta_{50,j} c_{11}\right] k_{234}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{234}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_{229}}\frac{dK_{229}}{dT}\right] K_{234} c_2 c_{49} k_{33}$$

$$- \left[n_{234} - \frac{b_{234}}{T}\right] \frac{X_{234}}{T}$$

Reaction 235, Li + $H_2O \rightleftharpoons$ LiOH + H

$$K_{235} = \frac{K_2}{K_{225}}$$

$$k_{235} = a_{234} T^{-n_{235}} e^{-b_{235}/T}$$

$$X_{235} = \left[K_{235} c_2 c_{49} - c_{16} c_{53}\right] k_{235}$$

$$\frac{\partial X_{235}}{\partial c_j} = \left[\delta_{2,j} K_{235} c_{49} - \delta_{16,j} c_{53} + \delta_{49,j} K_{235} c_2 - \delta_{53,j} c_{16}\right] k_{235}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{235}}{\partial T} = \left[\frac{1}{K_2}\frac{dK_2}{dT} - \frac{1}{K_{225}}\frac{dK_{225}}{dT}\right] K_{235} c_2 c_{49} k_{235}$$

$$- \left[n_{235} - \frac{b_{235}}{T}\right] \frac{X_{235}}{T}$$

Reaction 236, $Li + CO \rightleftarrows LiO + C$

$$K_{236} = \frac{K_3}{K_{230}}$$

$$k_{236} = a_{236} T^{-n_{236}} e^{-b_{236}/T}$$

$$X_{236} = \left[K_{236} c_3 c_{49} - c_{13} c_{51}\right] k_{236}$$

$$\frac{\partial X_{236}}{\partial c_j} = \left[\delta_{3,j} K_{236} c_{49} - \delta_{13,j} c_{51} + \delta_{49,j} K_{236} c_3 - \delta_{51,j} c_{13}\right] k_{236}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{236}}{\partial T} = \left[\frac{1}{K_3}\frac{dK_3}{dT} - \frac{1}{K_{230}}\frac{dK_{230}}{dT}\right] K_{236} c_3 c_{49} k_{236} - \left[n_{236} - \frac{b_{236}}{T}\right] \frac{X_{236}}{T}$$

Reaction 237, $Li + HF \rightleftarrows LiH + F$

$$K_{237} = \frac{K_7}{K_{229}}$$

$$k_{237} = a_{237} T^{-n_{237}} e^{-b_{237}/T}$$

$$X_{237} = \left[K_{237} c_7 c_{49} - c_{15} c_{50}\right] k_{237}$$

$$\frac{\partial X_{237}}{\partial c_j} = \left[\delta_{7,j} K_{237} c_{49} - \delta_{15,j} c_{50} + \delta_{49,j} K_{237} c_7 - \delta_{50,j} c_{15}\right] k_{237}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{237}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{229}}\frac{dK_{229}}{dT}\right] K_{237} c_7 c_{49} k_{237} - \left[n_{237} - \frac{b_{237}}{T}\right] \frac{X_{237}}{T}$$

Reaction 238, $Li + H_2 \rightleftharpoons LiH + H$

$$K_{238} = \frac{K_8}{K_{229}}$$

$$k_{238} = a_{238} T^{-n_{238}} e^{-b_{238}/T}$$

$$X_{238} = \left[K_{238} c_8 c_{49} - c_{16} c_{50}\right] k_{238}$$

$$\frac{\partial X_{238}}{\partial c_j} = \left[\delta_{8,j} K_{238} c_{49} - \delta_{16,j} c_{50} + \delta_{49,j} K_{238} c_8 - \delta_{50,j} c_{16}\right] k_{238}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{238}}{\partial T} = \left[\frac{1}{K_8}\frac{dK_8}{dT} - \frac{1}{K_{229}}\frac{dK_{229}}{dT}\right] K_{238} c_8 c_{49} k_{238} - \left[n_{238} - \frac{b_{238}}{T}\right]\frac{X_{238}}{T}$$

Reaction 239, $Li + OH \rightleftharpoons LiH + O$

$$K_{239} = \frac{K_{11}}{K_{229}}$$

$$k_{239} = a_{239} T^{-n_{239}} e^{-b_{239}/T}$$

$$X_{239} = \left[K_{239} c_{11} c_{49} - c_{18} c_{50}\right] k_{239}$$

$$\frac{\partial X_{239}}{\partial c_j} = \left[\delta_{11,j} K_{239} c_{49} - \delta_{18,j} c_{50} + \delta_{49,j} K_{239} c_{11} - \delta_{50,j} c_{18}\right] k_{239}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{239}}{\partial T} = \left[\frac{1}{K_{11}}\frac{dK_{11}}{dT} - \frac{1}{K_{229}}\frac{dK_{229}}{dT}\right] K_{239} c_{11} c_{48} k_{239} - \left[n_{239} - \frac{b_{239}}{T}\right]\frac{X_{239}}{T}$$

Reaction 240, $Li + OH \rightleftharpoons LiO + H$

$$K_{240} = \frac{K_{11}}{K_{230}}$$

$$k_{240} = a_{240} T^{-n_{240}} e^{-b_{240}/T}$$

$$X_{240} = \left[K_{240} c_{11} c_{49} - c_{16} c_{51}\right] k_{240}$$

$$\frac{\partial X_{240}}{\partial c_j} = \left[\delta_{11,j} K_{240} c_{49} - \delta_{16,j} c_{51} + \delta_{49,j} K_{240} c_{11} - \delta_{51,j} c_{16}\right] k_{240}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{240}}{\partial T} = \left[\frac{1}{K_{11}} \frac{dK_{11}}{dT} - \frac{1}{K_{230}} \frac{dK_{230}}{dT}\right] K_{240} c_{11} c_{49} k_{240} - \left[n_{240} - \frac{b_{240}}{T}\right] \frac{X_{240}}{T}$$

Reaction 241, $Li + O_2 \rightleftharpoons LiO + O$

$$K_{241} = \frac{K_{12}}{K_{230}}$$

$$k_{241} = a_{241} T^{-n_{241}} e^{-b_{241}/T}$$

$$X_{241} = \left[K_{241} c_{12} c_{49} - c_{18} c_{51}\right] k_{241}$$

$$\frac{\partial X_{241}}{\partial c_j} = \left[\delta_{12,j} K_{241} c_{49} - \delta_{18,j} c_{51} + \delta_{49,j} K_{241} c_{12} - \delta_{51,j} c_{18}\right] k_{241}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{241}}{\partial T} = \left[\frac{1}{K_{12}} \frac{dK_{12}}{dT} - \frac{1}{K_{230}} \frac{dK_{230}}{dT}\right] K_{241} c_{12} c_{49} k_{241}$$

$$- \left[n_{241} - \frac{b_{241}}{T}\right] \frac{X_{241}}{T}$$

Reaction 242, $Li + LiOH \rightleftharpoons LiH + LiO$

$$K_{242} = \frac{K_{226}}{K_{229}}$$

$$k_{242} = a_{242} T^{-n_{242}} e^{-b_{242}/T}$$

$$X_{242} = \left[K_{242} c_{49} c_{53} - c_{50} c_{51}\right] k_{242}$$

$$\frac{\partial X_{242}}{\partial c_j} = \left[\delta_{49,j} K_{242} c_{53} - \delta_{50,j} c_{51} - \delta_{51,j} c_{50} + \delta_{53,j} K_{242} c_{49}\right] k_{242}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{242}}{\partial T} = \left[\frac{1}{K_{226}} \frac{dK_{226}}{dT} - \frac{1}{K_{229}} \frac{dK_{229}}{dT}\right] K_{242} c_{49} c_{53} k_{242} - \left[n_{242} - \frac{b_{242}}{T}\right] \frac{X_{242}}{T}$$

Reaction 243, $Li + LiOH \rightleftharpoons Li_2O + H$

$$K_{243} = \frac{K_{226}}{K_{231}}$$

$$k_{243} = a_{243} T^{-n_{243}} e^{-b_{243}/T}$$

$$X_{243} = \left[K_{243} c_{49} c_{53} - c_{16} c_{52}\right] k_{243}$$

$$\frac{\partial X_{243}}{\partial c_j} = \left[-\delta_{16,j} c_{52} + \delta_{49,j} K_{243} c_{53} - \delta_{52,j} c_{16} + \delta_{53,j} K_{243} c_{49}\right] k_{243}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{243}}{\partial T} = \left[\frac{1}{K_{226}} \frac{dK_{226}}{dT} - \frac{1}{K_{231}} \frac{dK_{231}}{dT}\right] K_{243} c_{49} c_{53} k_{243} - \left[n_{243} - \frac{b_{243}}{T}\right] \frac{X_{243}}{T}$$

Reaction 244, $LiH + Cl \rightleftharpoons Li + HCl$

$$K_{244} = \frac{K_{229}}{K_6}$$

$$k_{244} = a_{244} T^{-n_{244}} e^{-b_{244}/T}$$

$$X_{244} = \left[K_{244} c_{14} c_{50} - c_6 c_{49}\right] k_{244}$$

$$\frac{\partial X_{244}}{\partial c_j} = \left[-\delta_{6,j} c_{49} + \delta_{14,j} K_{244} c_{50} - \delta_{49,j} c_6 + \delta_{50,j} K_{244} c_{14}\right] k_{244}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{244}}{\partial T} = \left[\frac{1}{K_{229}} \frac{dK_{229}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{244} c_{14} c_{50} k_{244} - \left[n_{244} - \frac{b_{244}}{T}\right] \frac{X_{244}}{T}$$

Reaction 245, $LiO + CO \rightleftharpoons Li + CO_2$

$$K_{245} = \frac{K_{230}}{K_1}$$

$$k_{245} = a_{245} T^{-n_{245}} e^{-b_{245}/T}$$

$$X_{245} = \left[K_{245} c_3 c_{51} - c_1 c_{49}\right] k_{245}$$

$$\frac{\partial X_{245}}{\partial c_j} = \left[-\delta_{1,j} c_{49} + \delta_{3,j} K_{245} c_{51} - \delta_{49,j} c_1 + \delta_{51,j} K_{245} c_3\right] k_{245}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{245}}{\partial T} = \left[\frac{1}{K_{230}} \frac{dK_{230}}{dT} - \frac{1}{K_1} \frac{dK_1}{dT}\right] K_{245} c_3 c_{51} k_{245} - \left[n_{245} - \frac{b_{245}}{T}\right] \frac{X_{245}}{T}$$

Reaction 246, $LiO + HCl \rightleftharpoons LiOH + Cl$

$$K_{246} = \frac{K_6}{K_{226}}$$

$$k_{246} = a_{246} T^{-n_{246}} e^{-b_{246}/T}$$

$$X_{246} = \left[K_{246} c_6 c_{51} - c_{14} c_{53}\right] k_{246}$$

$$\frac{\partial X_{246}}{\partial c_j} = \left[\delta_{6,j} K_{246} c_{51} - \delta_{14,j} c_{53} + \delta_{51,j} K_{246} c_6 - \delta_{53,j} c_{14}\right] k_{246}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{246}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{226}}\frac{dK_{226}}{dT}\right] K_{246} c_6 c_{51} k_{246} - \left[n_{246} - \frac{b_{246}}{T}\right]\frac{X_{246}}{T}$$

Reaction 247, $LiO + HF \rightleftharpoons LiOH + F$

$$K_{247} = \frac{K_7}{K_{226}}$$

$$k_{247} = a_{247} T^{-n_{247}} e^{-b_{247}/T}$$

$$X_{247} = \left[K_{247} c_7 c_{51} - c_{15} c_{53}\right] k_{247}$$

$$\frac{\partial X_{247}}{\partial c_j} = \left[\delta_{7,j} K_{247} c_{51} - \delta_{15,j} c_{53} + \delta_{51,j} K_{247} c_7 - \delta_{53,j} c_{15}\right] k_{247}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{247}}{\partial T} = \left[\frac{1}{K_7}\frac{dK_7}{dT} - \frac{1}{K_{226}}\frac{dK_{226}}{dT}\right] K_{247} c_7 c_{51} k_{247}$$

$$- \left[n_{247} - \frac{b_{247}}{T}\right]\frac{X_{247}}{T}$$

Reaction 248, $LiO + H_2 \rightleftharpoons LiH + OH$

$$K_{248} = \frac{K_{238}}{K_{239}}$$

$$k_{248} = a_{248} T^{-n_{248}} e^{-b_{248}/T}$$

$$X_{248} = \left[K_{248} c_8 c_{51} - c_{11} c_{50}\right] k_{248}$$

$$\frac{\partial X_{248}}{\partial c_j} = \left[\delta_{8,j} K_{248} c_{51} - \delta_{11,j} c_{50} - \delta_{50,j} c_{11} + \delta_{51,j} K_{248} c_8\right] k_{248}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{248}}{\partial T} = \left[\frac{1}{K_{238}} \frac{dK_{238}}{dT} - \frac{1}{K_{239}} \frac{dK_{239}}{dT}\right] K_{247} c_8 c_{51} k_{248} - \left[n_{248} - \frac{b_{248}}{T}\right] \frac{X_{248}}{T}$$

Reaction 249, $LiO + OH \rightleftharpoons LiH + O_2$

$$K_{249} = \frac{K_{238}}{K_{240}}$$

$$k_{249} = a_{249} T^{-n_{249}} e^{-b_{249}/T}$$

$$X_{249} = \left[K_{249} c_{11} c_{51} - c_{12} c_{50}\right] k_{249}$$

$$\frac{\partial X_{249}}{\partial c_j} = \left[\delta_{11,j} K_{249} c_{51} - \delta_{12,j} c_{50} - \delta_{50,j} c_{12} + \delta_{51,j} K_{249} c_{11}\right] k_{249}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{249}}{\partial T} = \left[\frac{1}{K_{238}} \frac{dK_{238}}{dT} - \frac{1}{K_{240}} \frac{dK_{240}}{dT}\right] K_{249} c_{11} c_{51} k_{249}$$

$$- \left[n_{249} - \frac{b_{249}}{T}\right] \frac{X_{249}}{T}$$

Reaction 250, $LiO + N \rightleftharpoons Li + NO$

$$K_{250} = \frac{K_{230}}{K_{10}}$$

$$k_{250} = a_{250} T^{-n_{250}} e^{-b_{250}/T}$$

$$X_{250} = \left[K_{250} c_{17} c_{51} - c_{10} c_{49}\right] k_{250}$$

$$\frac{\partial X_{250}}{\partial c_j} = \left[-\delta_{10,j} c_{49} + \delta_{17,j} K_{250} c_{51} - \delta_{49,j} c_{10} + \delta_{51,j} K_{250} c_{17}\right] k_{250}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{250}}{\partial T} = \left[\frac{1}{K_{230}} \frac{dK_{230}}{dT} - \frac{1}{K_{10}} \frac{dK_{10}}{dT}\right] K_{250} c_{17} c_{51} k_{250} - \left[n_{250} - \frac{b_{250}}{T}\right] \frac{X_{250}}{T}$$

Reaction 251, $LiO + LiOH \rightleftharpoons Li_2O + OH$

$$K_{251} = \frac{K_{225}}{K_{231}}$$

$$k_{251} = a_{251} T^{-n_{251}} e^{-b_{251}/T}$$

$$X_{251} = \left[K_{251} c_{51} c_{53} - c_{11} c_{52}\right] k_{251}$$

$$\frac{\partial X_{251}}{\partial c_j} = \left[-\delta_{11,j} c_{52} + \delta_{51,j} K_{251} c_{53} - \delta_{52,j} c_{11} + \delta_{53,j} K_{251} c_{51}\right] k_{251}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{251}}{\partial T} = \left[\frac{1}{K_{225}} \frac{dK_{225}}{dT} - \frac{1}{K_{231}} \frac{dK_{231}}{dT}\right] K_{251} c_{51} c_{53} k_{251}$$

$$- \left[n_{251} - \frac{b_{251}}{T}\right] \frac{X_{251}}{T}$$

Reaction 252, $LiO + LiF \rightleftharpoons Li_2O + F$

$$K_{252} = \frac{K_{228}}{K_{231}}$$

$$k_{252} = a_{252} T^{-n_{252}} e^{-b_{252}/T}$$

$$X_{252} = \left[K_{252} c_{51} c_{54} - c_{15} c_{52}\right] k_{252}$$

$$\frac{\partial X_{252}}{\partial c_j} = \left[-\delta_{15,j} c_{52} + \delta_{51,j} K_{252} c_{54} - \delta_{52,j} c_{15} + \delta_{54,j} K_{252} c_{51}\right] k_{252}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{252}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} - \frac{1}{K_{231}} \frac{dK_{231}}{dT}\right] K_{252} c_{51} c_{54} k_{252}$$

$$- \left[n_{252} - \frac{b_{252}}{T}\right] \frac{X_{252}}{T}$$

Reaction 253, $Li_2O + H_2O \rightleftharpoons 2LiOH$

$$K_{253} = \frac{K_{234}}{K_{242}}$$

$$k_{253} = a_{253} T^{-n_{253}} e^{-b_{253}/T}$$

$$X_{253} = \left[K_{253} c_2 c_{52} - c_{53}^2\right] k_{253}$$

$$\frac{\partial X_{253}}{\partial c_j} = \left[\delta_{2,j} K_{253} c_{52} + \delta_{52,j} K_{253} c_2 - 2\delta_{53,j} c_{53}\right] k_{253}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{253}}{\partial T} = \left[\frac{1}{K_{234}} \frac{dK_{234}}{dT} - \frac{1}{K_{242}} \frac{dK_{242}}{dT}\right] K_{253} c_2 c_{52} k_{253}$$

$$- \left[n_{253} - \frac{b_{253}}{T}\right] \frac{X_{253}}{T}$$

Reaction 254, $Li_2O + HF \rightleftharpoons LiOH + LiF$

$$K_{254} = \frac{K_{246}}{K_{251}}$$

$$k_{254} = a_{254} T^{-n_{254}} e^{-b_{254}/T}$$

$$X_{254} = \left[K_{254} c_7 c_{52} - c_{53} c_{54}\right] k_{254}$$

$$\frac{\partial X_{254}}{\partial c_j} = \left[\delta_{7,j} K_{254} c_{52} + \delta_{52,j} K_{254} c_7 - \delta_{53,j} c_{54} - \delta_{54,j} c_{53}\right] k_{254}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{254}}{\partial T} = \left[\frac{1}{K_{246}} \frac{dK_{246}}{dT} - \frac{1}{K_{251}} \frac{dK_{251}}{dT}\right] K_{254} c_7 c_{51} k_{254}$$

$$- \left[n_{254} - \frac{b_{254}}{T}\right] \frac{X_{254}}{T}$$

Reaction 255, $Li_2O + H_2 \rightleftharpoons LiH + LiOH$

$$K_{255} = \frac{K_{237}}{K_{242}}$$

$$k_{255} = a_{255} T^{-n_{255}} e^{-b_{255}/T}$$

$$X_{255} = \left[K_{255} c_8 c_{52} - c_{50} c_{53}\right] k_{255}$$

$$\frac{\partial X_{255}}{\partial c_j} = \left[\delta_{8,j} K_{255} c_{52} - \delta_{50,j} c_{53} + \delta_{52,j} K_{255} c_8 - \delta_{53,j} c_{50}\right] k_{255}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{255}}{\partial T} = \left[\frac{1}{K_{237}} \frac{dK_{237}}{dT} - \frac{1}{K_{242}} \frac{dK_{242}}{dT}\right] K_{255} c_8 c_{52} k_{255}$$

$$- \left[n_{255} - \frac{b_{255}}{T}\right] \frac{X_{255}}{T}$$

Reaction 256, $Li_2O + H \rightleftarrows LiH + LiO$

$$K_{256} = \frac{K_{231}}{K_{229}}$$

$$k_{256} = a_{256} T^{-n_{256}} e^{-b_{256}/T}$$

$$X_{256} = \left[K_{256} c_{16} c_{52} - c_{50} c_{51}\right] k_{256}$$

$$\frac{\partial X_{256}}{\partial c_j} = \left[\delta_{16,j} K_{256} c_{52} - \delta_{50,j} c_{51} - \delta_{51,j} c_{50} + \delta_{52,j} K_{256} c_{16}\right] k_{256}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{256}}{\partial T} = \left[\frac{1}{K_{231}} \frac{dK_{231}}{dT} - \frac{1}{K_{229}} \frac{dK_{229}}{dT}\right] K_{256} c_{16} c_{52} k_{256}$$

$$- \left[n_{256} - \frac{b_{256}}{T}\right] \frac{X_{256}}{T}$$

Reaction 257, $Li_2O + O \rightleftarrows 2LiO$

$$K_{257} = \frac{K_{231}}{K_{230}}$$

$$k_{257} = a_{257} T^{-n_{257}} e^{-b_{257}/T}$$

$$X_{257} = \left[K_{257} c_{18} c_{52} - c_{51}^2\right] k_{257}$$

$$\frac{\partial X_{257}}{\partial c_j} = \left[\delta_{18,j} K_{257} c_{52} - 2\delta_{51,j} c_{51} + \delta_{52,j} K_{257} c_{18}\right] k_{257}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{257}}{\partial T} = \left[\frac{1}{K_{231}} \frac{dK_{231}}{dT} - \frac{1}{K_{230}} \frac{dK_{230}}{dT}\right] K_{257} c_{18} c_{52} k_{257} - \left[n_{257} - \frac{b_{257}}{T}\right] \frac{X_{257}}{T}$$

Reaction 258, $LiOH + HCl \rightleftharpoons LiCl + H_2O$

$$K_{258} = \frac{K_6}{K_{227}K_{234}}$$

$$k_{258} = a_{258}T^{-n_{258}} e^{-b_{258}/T}$$

$$X_{258} = \left[K_{258}c_6c_{53} - c_2c_{55}\right]k_{258}$$

$$\frac{\partial X_{258}}{\partial c_j} = \left[-\delta_{2,j}c_{55} + \delta_{6,j}K_{258}c_{53} + \delta_{53,j}K_{258}c_6 - \delta_{55,j}c_2\right]k_{258}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{258}}{\partial T} = \left[\frac{1}{K_6}\frac{dK_6}{dT} - \frac{1}{K_{227}}\frac{dK_{227}}{dT} - \frac{1}{K_{234}}\frac{dK_{234}}{dT}\right] K_{258}c_6c_{53}k_{258}$$

$$- \left[n_{258} - \frac{b_{258}}{T}\right]\frac{X_{258}}{T}$$

Reaction 259, $LiOH + H_2 \rightleftharpoons LiH + H_2O$

$$K_{259} = \frac{K_{237}}{K_{234}}$$

$$k_{259} = a_{259}T^{-n_{259}} e^{-b_{259}/T}$$

$$X_{259} = \left[K_{259}c_8c_{53} - c_2c_{50}\right]k_{259}$$

$$\frac{\partial X_{259}}{\partial c_j} = \left[-\delta_{2,j}c_{50} + \delta_{8,j}K_{259}c_{53} - \delta_{50,j}c_2 + \delta_{53,j}K_{259}c_8\right]k_{259}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{259}}{\partial T} = \left[\frac{1}{K_{237}}\frac{dK_{237}}{dT} - \frac{1}{K_{234}}\frac{dK_{234}}{dT}\right] K_{259}c_8c_{53}k_{259}$$

$$- \left[n_{259} - \frac{b_{259}}{T}\right]\frac{X_{259}}{T}$$

Reaction 260, $LiOH + OH \rightleftharpoons LiO + H_2O$

$$K_{260} = \frac{K_{226}}{K_2}$$

$$k_{260} = a_{260} T^{-n_{260}} e^{-b_{260}/T}$$

$$X_{260} = \left[K_{260} c_{11} c_{53} - c_2 c_{51}\right] k_{260}$$

$$\frac{\partial X_{260}}{\partial c_j} = \left[-\delta_{2,j} c_{51} + \delta_{11,j} K_{260} c_{53} - \delta_{51,j} c_2 + \delta_{53,j} K_{260} c_{11}\right] k_{260}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{260}}{\partial T} = \left[\frac{1}{K_{226}} \frac{dK_{226}}{dT} - \frac{1}{K_2} \frac{dK_2}{dT}\right] K_{260} c_{11} c_{53} k_{260} - \left[n_{260} - \frac{b_{260}}{T}\right] \frac{X_{260}}{T}$$

Reaction 261, $LiOH + Cl \rightleftharpoons LiCl + OH$

$$K_{261} = \frac{K_{225}}{K_{227}}$$

$$k_{261} = a_{261} T^{-n_{261}} e^{-b_{261}/T}$$

$$X_{261} = \left[K_{261} c_{14} c_{53} - c_{11} c_{55}\right] k_{261}$$

$$\frac{\partial X_{261}}{\partial c_j} = \left[-\delta_{11,j} c_{55} + \delta_{14,j} K_{261} c_{53} + \delta_{53,j} K_{261} c_{14} - \delta_{55,j} c_{11}\right] k_{261}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{261}}{\partial T} = \left[\frac{1}{K_{225}} \frac{dK_{225}}{dT} - \frac{1}{K_{227}} \frac{dK_{227}}{dT}\right] K_{261} c_{14} c_{53} k_{261}$$

$$- \left[n_{261} - \frac{b_{261}}{T}\right] \frac{X_{261}}{T}$$

Reaction 262, $LiOH + H \rightleftharpoons LiH + OH$

$$K_{262} = \frac{K_{225}}{K_{229}}$$

$$k_{262} = a_{262} T^{-n_{262}} e^{-b_{262}/T}$$

$$X_{262} = \left[K_{262} c_{16} c_{53} - c_{11} c_{50}\right] k_{262}$$

$$\frac{\partial X_{262}}{\partial c_j} = \left[-\delta_{11,j} c_{50} + \delta_{16,j} K_{262} c_{53} - \delta_{50,j} c_{11} + \delta_{53,j} K_{262} c_{16}\right] k_{262}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{262}}{\partial T} = \left[\frac{1}{K_{225}} \frac{dK_{225}}{dT} - \frac{1}{K_{229}} \frac{dK_{229}}{dT}\right] K_{262} c_{16} c_{53} k_{262}$$

$$- \left[n_{262} - \frac{b_{262}}{T}\right] \frac{X_{262}}{T}$$

Reaction 263, $LiOH + H \rightleftharpoons LiO + H_2$

$$K_{263} = \frac{K_{226}}{K_8}$$

$$k_{263} = a_{263} T^{-n_{263}} e^{-b_{263}/T}$$

$$X_{263} = \left[K_{263} c_{16} c_{53} - c_8 c_{51}\right] k_{263}$$

$$\frac{\partial X_{263}}{\partial c_j} = \left[-\delta_{8,j} c_{51} + \delta_{16,j} K_{263} c_{53} - \delta_{51,j} c_8 + \delta_{53,j} K_{263} c_{16}\right] k_{263}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{263}}{\partial T} = \left[\frac{1}{K_{226}} \frac{dK_{226}}{dT} - \frac{1}{K_8} \frac{dK_8}{dT}\right] K_{263} c_{16} c_{53} k_{263}$$

$$- \left[n_{263} - \frac{b_{263}}{T}\right] \frac{X_{263}}{T}$$

Reaction 264, $LiOH + O \rightleftharpoons LiO + OH$

$$K_{264} = \frac{K_{226}}{K_{11}}$$

$$k_{264} = a_{264} T^{-n_{264}} e^{-b_{264}/T}$$

$$X_{264} = \left[K_{264} c_{18} c_{53} - c_{11} c_{51}\right] k_{264}$$

$$\frac{\partial X_{264}}{\partial c_j} = \left[-\delta_{11,j} c_{51} + \delta_{18,j} K_{264} c_{53} - \delta_{51,j} c_{11} + \delta_{53,j} K_{264} c_{18}\right] k_{264}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{264}}{\partial T} = \left[\frac{1}{K_{226}} \frac{dK_{226}}{dT} - \frac{1}{K_{11}} \frac{dK_{11}}{dT}\right] K_{264} c_{18} c_{53} k_{264}$$

$$- \left[n_{264} - \frac{b_{264}}{T}\right] \frac{X_{264}}{T}$$

Reaction 265, $LiOH + LiCl \rightleftharpoons Li_2O + HCl$

$$K_{265} = \frac{K_{227} K_{242}}{K_6}$$

$$k_{265} = a_{265} T^{-n_{265}} e^{-b_{265}/T}$$

$$X_{265} = \left[K_{265} c_{53} c_{55} - c_6 c_{52}\right] k_{265}$$

$$\frac{\partial X_{265}}{\partial c_j} = \left[-\delta_{6,j} c_{52} - \delta_{52,j} c_6 + \delta_{53,j} K_{265} c_{55} + \delta_{55,j} K_{265} c_{53}\right] k_{265}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{265}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} + \frac{1}{K_{242}} \frac{dK_{242}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{265} c_{53} c_{54} k_{265}$$

$$- \left[n_{265} - \frac{b_{265}}{T}\right] \frac{X_{265}}{T}$$

Reaction 266, $LiF + H_2O \rightleftharpoons LiOH + HF$

$$K_{266} = \frac{K_{228}K_{234}}{K_7}$$

$$k_{266} = a_{266}T^{-n_{266}} e^{-b_{266}/T}$$

$$X_{266} = \left[K_{266}c_2c_{54} - c_7c_{53}\right]k_{266}$$

$$\frac{\partial X_{266}}{\partial c_j} = \left[\delta_{2,j}K_{266}c_{54} - \delta_{7,j}c_{53} - \delta_{53,j}c_7 + \delta_{54,j}K_{266}c_2\right]k_{266}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{266}}{\partial T} = \left[\frac{1}{K_{228}}\frac{dK_{228}}{dT} + \frac{1}{K_{234}}\frac{dK_{234}}{dT} - \frac{1}{K_7}\frac{dK_7}{dT}\right]K_{266}c_2c_{54}k_{266}$$

$$- \left[n_{266} - \frac{b_{266}}{T}\right]\frac{X_{266}}{T}$$

Reaction 267, $LiF + HF \rightleftharpoons LiH + F_2$

$$K_{267} = \frac{K_{228}K_{236}}{K_5}$$

$$k_{267} = a_{267}T^{-n_{267}} e^{-b_{267}/T}$$

$$X_{267} = \left[K_{267}c_7c_{54} - c_5c_{50}\right]k_{267}$$

$$\frac{\partial X_{267}}{\partial c_j} = \left[-\delta_{5,j}c_{50} + \delta_{7,j}K_{267}c_{54} - \delta_{50,j}c_5 + \delta_{54,j}K_{267}c_7\right]k_{267}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{267}}{\partial T} = \left[\frac{1}{K_{228}}\frac{dK_{228}}{dT} + \frac{1}{K_{236}}\frac{dK_{236}}{dT} - \frac{1}{K_5}\frac{dK_5}{dT}\right]K_{267}c_7c_{54}k_{267}$$

$$- \left[n_{267} - \frac{b_{267}}{T}\right]\frac{X_{267}}{T}$$

Reaction 268, $LiF + H_2 \rightleftharpoons LiH + HF$

$$K_{268} = \frac{K_{228}K_{237}}{K_7}$$

$$k_{268} = a_{268}T^{-n_{268}} e^{-b_{268}/T}$$

$$X_{268} = \left[K_{268}c_8c_{54} - c_7c_{50}\right]k_{268}$$

$$\frac{\partial X_{268}}{\partial c_j} = \left[-\delta_{7,j}c_{50} + \delta_{8,j}K_{268}c_{54} - \delta_{50,j}c_7 + \delta_{54,j}K_{268}c_8\right]k_{268}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{268}}{\partial T} = \left[\frac{1}{K_{228}}\frac{dK_{228}}{dT} + \frac{1}{K_{237}}\frac{dK_{237}}{dT} - \frac{1}{K_7}\frac{dK_7}{dT}\right]K_{268}c_8c_{54}k_{268}$$

$$- \left[n_{268} - \frac{b_{268}}{T}\right]\frac{X_{268}}{T}$$

Reaction 269, $LiF + OH \rightleftharpoons LiOH + F$

$$K_{269} = \frac{K_{228}}{K_{225}}$$

$$k_{269} = a_{269}T^{-n_{269}} e^{-b_{269}/T}$$

$$X_{269} = \left[K_{269}c_{11}c_{54} - c_{15}c_{53}\right]k_{269}$$

$$\frac{\partial X_{269}}{\partial c_j} = \left[\delta_{11,j}K_{269}c_{54} - \delta_{15,j}c_{53} - \delta_{53,j}c_{15} + \delta_{54,j}K_{269}c_{11}\right]k_{269}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{269}}{\partial T} = \left[\frac{1}{K_{228}}\frac{dK_{228}}{dT} - \frac{1}{K_{225}}\frac{dK_{225}}{dT}\right]K_{269}c_{11}c_{54}k_{269}$$

$$- \left[n_{269} - \frac{b_{269}}{T}\right]\frac{X_{269}}{T}$$

Reaction 270, $LiF + OH \rightleftharpoons LiO + HF$

$$K_{270} = \frac{K_{228}K_{239}}{K_7}$$

$$k_{270} = a_{270}T^{-n_{270}} e^{-b_{270}/T}$$

$$X_{270} = \left[K_{270}c_{11}c_{54} - c_7c_{51}\right] k_{270}$$

$$\frac{\partial X_{270}}{\partial c_j} = \left[-\delta_{7,j}c_{51} + \delta_{11,j}K_{270}c_{54} - \delta_{51,j}c_7 + \delta_{54,j}K_{270}c_{11}\right] k_{270}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{270}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} + \frac{1}{K_{239}} \frac{dK_{239}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{270}c_{11}c_{54}k_{270}$$

$$- \left[n_{270} - \frac{b_{270}}{T}\right] \frac{X_{270}}{T}$$

Reaction 271, $LiF + Cl \rightleftharpoons LiCl + F$

$$K_{271} = \frac{K_{228}}{K_{227}}$$

$$k_{271} = a_{271}T^{-n_{271}} e^{-b_{271}/T}$$

$$X_{271} = \left[K_{271}c_{14}c_{54} - c_{15}c_{55}\right] k_{271}$$

$$\frac{\partial X_{271}}{\partial c_j} = \left[\delta_{14,j}K_{271}c_{54} - \delta_{15,j}c_{55} + \delta_{54,j}K_{271}c_{14} - \delta_{55,j}c_{15}\right] k_{271}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{271}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} - \frac{1}{K_{227}} \frac{dK_{227}}{dT}\right] K_{271}c_{14}c_{54}k_{271}$$

$$- \left[n_{271} - \frac{b_{271}}{T}\right] \frac{X_{271}}{T}$$

Reaction 272, $LiF + F \rightleftharpoons Li + F_2$

$$K_{272} = \frac{K_{228}}{K_5}$$

$$k_{272} = a_{272} T^{-n_{272}} e^{-b_{272}/T}$$

$$X_{272} = \left[K_{272} c_{15} c_{54} - c_5 c_{49}\right] k_{272}$$

$$\frac{\partial X_{272}}{\partial c_j} = \left[-\delta_{5,j} c_{49} + \delta_{15,j} K_{272} c_{54} - \delta_{49,j} c_5 + \delta_{54,j} K_{272} c_{15}\right] k_{272}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{272}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} - \frac{1}{K_5} \frac{dK_5}{dT}\right] K_{272} c_{15} c_{54} k_{272} - \left[n_{272} - \frac{b_{272}}{T}\right] \frac{X_{272}}{T}$$

Reaction 273, $LiF + H \rightleftharpoons Li + HF$

$$K_{273} = \frac{K_{228}}{K_7}$$

$$k_{273} = a_{273} T^{-n_{273}} e^{-b_{273}/T}$$

$$X_{273} = \left[K_{273} c_{16} c_{54} - c_7 c_{49}\right] k_{273}$$

$$\frac{\partial X_{273}}{\partial c_j} = \left[-\delta_{7,j} c_{49} + \delta_{16,j} K_{273} c_{54} - \delta_{49,j} c_7 + \delta_{54,j} K_{273} c_{16}\right] k_{273}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{273}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} - \frac{1}{K_7} \frac{dK_7}{dT}\right] K_{273} c_{16} c_{54} k_{273} - \left[n_{273} - \frac{b_{273}}{T}\right] \frac{X_{273}}{T}$$

Reaction 274, $LiF + H \rightleftharpoons LiH + F$

$$K_{274} = \frac{K_{228}}{K_{229}}$$

$$k_{274} = a_{274} T^{-n_{274}} e^{-b_{274}/T}$$

$$X_{274} = \left[K_{274} c_{16} c_{54} - c_{15} c_{50}\right] k_{274}$$

$$\frac{\partial X_{274}}{\partial c_j} = \left[-\delta_{15,j} c_{50} + \delta_{16,j} K_{274} c_{54} - \delta_{50,j} c_{15} + \delta_{54,j} K_{274} c_{16}\right] k_{274}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{274}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} - \frac{1}{K_{229}} \frac{dK_{229}}{dT}\right] K_{274} c_{16} c_{54} k_{274}$$

$$- \left[n_{274} - \frac{b_{274}}{T}\right] \frac{X_{274}}{T}$$

Reaction 275, $LiF + O \rightleftharpoons LiO + F$

$$K_{275} = \frac{K_{228}}{K_{230}}$$

$$k_{275} = a_{275} T^{-n_{275}} e^{-b_{275}/T}$$

$$X_{275} = \left[K_{275} c_{18} c_{54} - c_{15} c_{51}\right] k_{275}$$

$$\frac{\partial X_{275}}{\partial c_j} = \left[-\delta_{15,j} c_{51} + \delta_{18,j} K_{275} c_{54} - \delta_{51,j} c_{15} + \delta_{54,j} K_{275} c_{18}\right] k_{275}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{275}}{\partial T} = \left[\frac{1}{K_{228}} \frac{dK_{228}}{dT} - \frac{1}{K_{230}} \frac{dK_{230}}{dT}\right] K_{275} c_{18} c_{54} k_{275}$$

$$- \left[n_{275} - \frac{b_{275}}{T}\right] \frac{X_{275}}{T}$$

Reaction 276, $LiCl + HCl \rightleftharpoons LiH + Cl_2$

$$K_{276} = \frac{K_{227}}{K_4 K_{243}}$$

$$k_{276} = a_{276} T^{-n_{276}} e^{-b_{276}/T}$$

$$X_{276} = \left[K_{276} c_6 c_{55} - c_4 c_{50}\right] k_{276}$$

$$\frac{\partial X_{276}}{\partial c_j} = \left[-\delta_{4,j} c_{50} + \delta_{6,j} K_{276} c_{55} - \delta_{50,j} c_4 + \delta_{55,j} K_{276} c_6\right] k_{276}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{276}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT} - \frac{1}{K_{243}} \frac{dK_{243}}{dT}\right] K_{276} c_6 c_{55} k_{276}$$

$$- \left[n_{276} - \frac{b_{276}}{T}\right] \frac{X_{276}}{T}$$

Reaction 277, $LiCl + HF \rightleftharpoons LiF + HCl$

$$K_{277} = \frac{K_{227}}{K_6 K_{272}}$$

$$k_{277} = a_{277} T^{-n_{277}} e^{-b_{277}/T}$$

$$X_{277} = \left[K_{277} c_7 c_{55} - c_6 c_{54}\right] k_{277}$$

$$\frac{\partial X_{277}}{\partial c_j} = \left[-\delta_{6,j} c_{54} + \delta_{7,j} K_{277} c_{55} - \delta_{54,j} c_6 + \delta_{55,j} K_{277} c_7\right] k_{277}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{277}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT} - \frac{1}{K_{272}} \frac{dK_{272}}{dT}\right] K_{277} c_7 c_{55} k_{277}$$

$$- \left[n_{277} - \frac{b_{277}}{T}\right] \frac{X_{277}}{T}$$

Reaction 278, $LiCl + H_2 \rightleftharpoons LiH + HCl$

$$K_{278} = \frac{K_{227}K_{237}}{K_6}$$

$$k_{278} = a_{278}T^{-n_{278}} e^{-b_{278}/T}$$

$$X_{278} = \left[K_{278}c_8c_{55} - c_6c_{50}\right]k_{278}$$

$$\frac{\partial X_{278}}{\partial c_j} = \left[-\delta_{6,j}c_{50} + \delta_{8,j}K_{278}c_{55} - \delta_{50,j}c_6 + \delta_{55,j}K_{278}c_8\right]k_{278}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{278}}{\partial T} = \left[\frac{1}{K_{227}}\frac{dK_{227}}{dT} + \frac{1}{K_{237}}\frac{dK_{237}}{dT} - \frac{1}{K_6}\frac{dK_6}{dT}\right]K_{278}c_8c_{55}k_{278}$$

$$- \left[n_{278} - \frac{b_{278}}{T}\right]\frac{X_{278}}{T}$$

Reaction 279, $LiCl + OH \rightleftharpoons LiO + HCl$

$$K_{279} = \frac{K_{227}K_{239}}{K_6}$$

$$k_{279} = a_{279}T^{-n_{279}} e^{-b_{279}/T}$$

$$X_{279} = \left[K_{279}c_{11}c_{55} - c_6c_{51}\right]k_{279}$$

$$\frac{\partial X_{279}}{\partial c_j} = \left[-\delta_{6,j}c_{51} + \delta_{11,j}K_{279}c_{55} - \delta_{51,j}c_6 + \delta_{55,j}K_{279}c_{11}\right]k_{279}$$

$j = 1, 2, \cdots, 57$

$$\frac{\partial X_{279}}{\partial T} = \left[\frac{1}{K_{227}}\frac{dK_{227}}{dT} + \frac{1}{K_{239}}\frac{dK_{239}}{dT} - \frac{1}{K_6}\frac{dK_6}{dT}\right]K_{279}c_{11}c_{55}k_{279}$$

$$- \left[n_{279} - \frac{b_{279}}{T}\right]\frac{X_{279}}{T}$$

Reaction 280, $LiCl + Cl \rightleftharpoons Li + Cl_2$

$$K_{280} = \frac{K_{227}}{K_4}$$

$$k_{280} = a_{280} T^{-n_{280}} e^{-b_{280}/T}$$

$$X_{280} = \left[K_{280} c_{14} c_{55} - c_4 c_{49}\right] k_{280}$$

$$\frac{\partial X_{280}}{\partial c_j} = \left[-\delta_{4,j} c_{49} + \delta_{14,j} K_{280} c_{55} - \delta_{49,j} c_4 + \delta_{55,j} K_{280} c_{14}\right] k_{280}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{280}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_4} \frac{dK_4}{dT}\right] K_{280} c_{14} c_{55} k_{280} - \left[n_{280} - \frac{b_{280}}{T}\right] \frac{X_{280}}{T}$$

Reaction 281, $LiCl + H \rightleftharpoons Li + HCl$

$$K_{281} = \frac{K_{227}}{K_6}$$

$$k_{281} = a_{281} T^{-n_{281}} e^{-b_{281}/T}$$

$$X_{281} = \left[K_{281} c_{16} c_{55} - c_6 c_{49}\right] k_{281}$$

$$\frac{\partial X_{281}}{\partial c_j} = \left[-\delta_{6,j} c_{49} + \delta_{16,j} K_{281} c_{55} - \delta_{49,j} c_6 + \delta_{55,j} K_{281} c_{16}\right] k_{281}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{281}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_6} \frac{dK_6}{dT}\right] K_{281} c_{16} c_{55} k_{281}$$

$$- \left[n_{281} - \frac{b_{281}}{T}\right] \frac{X_{281}}{T}$$

Reaction 282, $LiCl + H \rightleftharpoons LiH + Cl$

$$K_{282} = \frac{K_{227}}{K_{229}}$$

$$k_{282} = a_{282} T^{-n_{282}} e^{-b_{282}/T}$$

$$X_{282} = \left[K_{282} c_{16} c_{55} - c_{14} c_{50}\right] k_{282}$$

$$\frac{\partial X_{282}}{\partial c_j} = \left[-\delta_{14,j} c_{50} + \delta_{16,j} K_{282} c_{55} - \delta_{50,j} c_{14} + \delta_{55,j} K_{282} c_{16}\right] k_{282}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{282}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_{229}} \frac{dK_{229}}{dT}\right] K_{282} c_{16} c_{55} k_{282}$$

$$- \left[n_{282} - \frac{b_{282}}{T}\right] \frac{X_{282}}{T}$$

Reaction 283, $LiCl + O \rightleftharpoons LiO + Cl$

$$K_{283} = \frac{K_{227}}{K_{230}}$$

$$k_{283} = a_{283} T^{-n_{283}} e^{-b_{283}/T}$$

$$X_{283} = \left[K_{283} c_{18} c_{55} - c_{14} c_{51}\right] k_{283}$$

$$\frac{\partial X_{283}}{\partial c_j} = \left[-\delta_{14,j} c_{51} + \delta_{18,j} K_{283} c_{55} - \delta_{51,j} c_{14} + \delta_{55,j} K_{283} c_{18}\right] k_{283}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{283}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_{230}} \frac{dK_{230}}{dT}\right] K_{283} c_{18} c_{55} k_{283}$$

$$- \left[n_{283} - \frac{b_{283}}{T}\right] \frac{X_{283}}{T}$$

Reaction 284, $LiCl + LiO \rightleftharpoons Li_2O + Cl$

$$K_{284} = \frac{K_{227}}{K_{231}}$$

$$k_{284} = a_{284} T^{-n_{284}} e^{-b_{284}/T}$$

$$X_{284} = \left[K_{284} c_{51} c_{55} - c_{14} c_{52}\right] k_{284}$$

$$\frac{\partial X_{284}}{\partial c_j} = \left[-\delta_{14,j} c_{52} + \delta_{51,j} K_{284} c_{55} - \delta_{52,j} c_{14} + \delta_{55,j} K_{284} c_{51}\right] k_{284}$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial X_{284}}{\partial T} = \left[\frac{1}{K_{227}} \frac{dK_{227}}{dT} - \frac{1}{K_{231}} \frac{dK_{231}}{dT}\right] K_{284} c_{51} c_{55} k_{284} - \left[n_{284} - \frac{b_{284}}{T}\right] \frac{X_{284}}{T}$$

4.2.2 Calculation of f_i and $\beta_{i,j}$ for the Chemical Relaxation Equations

For the species of interest, f_i and $\beta_{i,j}$ for the chemical relaxation equations are calculated from the following relationships:

For CO_2

$$\overline{K}_1 = \frac{44.011\rho r^*}{V}$$

$$f_1 = -\overline{K}_1 \left[X_1 + X_{13} + X_{14} - X_{18} - X_{21} + X_{50} - X_{111} + X_{165} - X_{166} + X_{203} - X_{245}\right]$$

$$\beta_{1,j} = -\overline{K}_1 \left[\frac{\partial X_1}{\partial c_j} + \frac{\partial X_{13}}{\partial c_j} + \frac{\partial X_{14}}{\partial c_j} - \frac{\partial X_{18}}{\partial c_j} - \frac{\partial X_{21}}{\partial c_j} + \frac{\partial X_{50}}{\partial c_j} - \frac{\partial X_{111}}{\partial c_j} \frac{\partial X_{165}}{\partial c_j} - \frac{\partial X_{166}}{\partial c_j} + \frac{\partial X_{203}}{\partial c_j} - \frac{\partial X_{244}}{\partial c_j}\right], \quad j = 1, 2, \cdots, 57$$

$$\beta_{1,73} = -\frac{1}{V} f_1$$

$$\beta_{1,74} = \frac{1}{\rho} f_1 - \overline{K}_1 \frac{\partial X_1}{\partial \rho}$$

$$\beta_{1,75} = -\overline{K}_1 \left[\frac{\partial X_1}{\partial T} + \frac{\partial X_{13}}{\partial T} + \frac{\partial X_{14}}{\partial T} - \frac{\partial X_{18}}{\partial T} - \frac{\partial X_{21}}{\partial T} + \frac{\partial X_{50}}{\partial T} - \frac{\partial X_{111}}{\partial T} + \frac{\partial X_{165}}{\partial T} - \frac{\partial X_{166}}{\partial T} + \frac{\partial X_{203}}{\partial T} - \frac{\partial X_{245}}{\partial T}\right]$$

For H_2O

$$\overline{K}_2 = \frac{18.016\rho r^*}{V}$$

$$f_2 = -\overline{K}_2 \left[X_2 + X_{15} + X_{16} + X_{17} - X_{31} + X_{110} + X_{120} - X_{130} + X_{134} + X_{138} - X_{147} + X_{165} + X_{203} + X_{234} + X_{235} + X_{253} - X_{258} - X_{259} - X_{260} + X_{266}\right]$$

$$\beta_{2,j} = -\overline{K}_2 \left[\frac{\partial X_2}{\partial c_j} + \frac{\partial X_{15}}{\partial c_j} + \frac{\partial X_{16}}{\partial c_j} + \frac{\partial X_{17}}{\partial c_j} - \frac{\partial X_{31}}{\partial c_j} + \frac{\partial X_{110}}{\partial c_j} + \frac{\partial X_{120}}{\partial c_j} \right.$$

$$- \frac{\partial X_{130}}{\partial c_j} + \frac{\partial X_{134}}{\partial c_j} + \frac{\partial X_{138}}{\partial c_j} - \frac{\partial X_{147}}{\partial c_j} + \frac{\partial X_{165}}{\partial c_j} + \frac{\partial X_{203}}{\partial c_j}$$

$$+ \frac{\partial X_{234}}{\partial c_j} + \frac{\partial X_{235}}{\partial c_j} + \frac{\partial X_{253}}{\partial c_j} - \frac{\partial X_{258}}{\partial c_j} - \frac{\partial X_{259}}{\partial c_j} - \frac{\partial X_{260}}{\partial c_j}$$

$$\left. + \frac{\partial X_{266}}{\partial c_j} \right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{2,73} = -\frac{1}{V} f_2$$

$$\beta_{2,74} = \frac{1}{\rho} f_2 - \overline{K}_2 \frac{\partial X_2}{\partial \rho}$$

$$\beta_{2,75} = -\overline{K}_2 \left[\frac{\partial X_2}{\partial T} + \frac{\partial X_{15}}{\partial T} + \frac{\partial X_{16}}{\partial T} + \frac{\partial X_{17}}{\partial T} - \frac{\partial X_{31}}{\partial T} + \frac{\partial X_{110}}{\partial T} + \frac{\partial X_{120}}{\partial T} \right.$$

$$- \frac{\partial X_{130}}{\partial T} + \frac{\partial X_{134}}{\partial T} + \frac{\partial X_{138}}{\partial T} - \frac{\partial X_{147}}{\partial T} + \frac{\partial X_{165}}{\partial T} + \frac{\partial X_{203}}{\partial T}$$

$$+ \frac{\partial X_{234}}{\partial T} + \frac{\partial X_{235}}{\partial T} + \frac{\partial X_{253}}{\partial T} - \frac{\partial X_{258}}{\partial T} - \frac{\partial X_{259}}{\partial T} - \frac{\partial X_{260}}{\partial T}$$

$$\left. + \frac{\partial X_{266}}{\partial T} \right]$$

For CO

$$\overline{K}_3 = \frac{28.011 \rho r^*}{V}$$

$$f_3 = \overline{K}_3 \left[X_1 - X_3 + X_{13} + X_{14} - 2X_{18} - X_{19} - X_{20} - X_{21} - X_{22} \right.$$

$$+ X_{50} - X_{51} - X_{64} - X_{76} - X_{111} + X_{114} + X_{165} - X_{166}$$

$$\left. - X_{167} + X_{172} + X_{203} - X_{204} - X_{236} - X_{245} \right]$$

$$\beta_{3,j} = \overline{K}_3 \left[\frac{\partial X_1}{\partial c_j} - \frac{\partial X_3}{\partial c_j} + \frac{\partial X_{13}}{\partial c_j} + \frac{\partial X_{14}}{\partial c_j} - 2\frac{\partial X_{18}}{\partial c_j} - \frac{\partial X_{19}}{\partial c_j} - \frac{\partial X_{20}}{\partial c_j} - \frac{\partial X_{21}}{\partial c_j} \right.$$

$$- \frac{\partial X_{22}}{\partial c_j} + \frac{\partial X_{50}}{\partial c_j} - \frac{\partial X_{51}}{\partial c_j} - \frac{\partial X_{64}}{\partial c_j} - \frac{\partial X_{76}}{\partial c_j} - \frac{\partial X_{111}}{\partial c_j} + \frac{\partial X_{114}}{\partial c_j}$$

$$+ \frac{\partial X_{165}}{\partial c_j} - \frac{\partial X_{166}}{\partial c_j} - \frac{\partial X_{167}}{\partial c_j} + \frac{\partial X_{172}}{\partial c_j} + \frac{\partial X_{203}}{\partial c_j} - \frac{\partial X_{204}}{\partial c_j}$$

$$\left. - \frac{\partial X_{236}}{\partial c_j} - \frac{\partial X_{245}}{\partial c_j} \right] , \quad j = 1, 2, \cdots, 57$$

$$\beta_{3,73} = -\frac{1}{V} f_3$$

$$\beta_{3,74} = \frac{1}{\rho} f_3 + \overline{K}_3 \left[\frac{\partial X_1}{\partial \rho} - \frac{\partial X_3}{\partial \rho} \right]$$

$$\beta_{3,75} = \overline{K}_3 \left[\frac{\partial X_1}{\partial T} - \frac{\partial X_3}{\partial T} + \frac{\partial X_{13}}{\partial T} + \frac{\partial X_{14}}{\partial T} - 2\frac{\partial X_{18}}{\partial T} - \frac{\partial X_{19}}{\partial T} - \frac{\partial X_{20}}{\partial T} - \frac{\partial X_{21}}{\partial T} \right.$$

$$- \frac{\partial X_{22}}{\partial T} + \frac{\partial X_{50}}{\partial T} - \frac{\partial X_{51}}{\partial T} - \frac{\partial X_{64}}{\partial T} - \frac{\partial X_{76}}{\partial T} - \frac{\partial X_{111}}{\partial T} + \frac{\partial X_{114}}{\partial T}$$

$$+ \frac{\partial X_{165}}{\partial T} - \frac{\partial X_{166}}{\partial T} - \frac{\partial X_{167}}{\partial T} + \frac{\partial X_{172}}{\partial T} + \frac{\partial X_{203}}{\partial T} - \frac{\partial X_{204}}{\partial T}$$

$$\left. - \frac{\partial X_{236}}{\partial T} - \frac{\partial X_{245}}{\partial T} \right]$$

For Cl_2

$$\overline{K}_4 = \frac{70.914 \rho r^*}{V}$$

$$f_4 = -\overline{K}_4 \left[X_4 - X_{23} - X_{24} - X_{68} - X_{72} - X_{75} - X_{78} - X_{136} - X_{188} \right.$$

$$\left. - X_{192} - X_{193} - X_{196} - X_{276} - X_{280} \right]$$

$$\beta_{4,j} = -\overline{K}_4 \left[\frac{\partial X_4}{\partial c_j} - \frac{\partial X_{23}}{\partial c_j} - \frac{\partial X_{24}}{\partial c_j} - \frac{\partial X_{68}}{\partial c_j} - \frac{\partial X_{72}}{\partial c_j} - \frac{\partial X_{75}}{\partial c_j} - \frac{\partial X_{78}}{\partial c_j} - \frac{\partial X_{136}}{\partial c_j} \right.$$

$$\left. - \frac{\partial X_{188}}{\partial c_j} - \frac{\partial X_{192}}{\partial c_j} - \frac{\partial X_{193}}{\partial c_j} - \frac{\partial X_{196}}{\partial c_j} - \frac{\partial X_{276}}{\partial c_j} - \frac{\partial X_{280}}{\partial c_j} \right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{4,73} = -\frac{1}{V} f_4$$

$$\beta_{4,74} = \frac{1}{\rho} f_4 - \overline{K}_4 \frac{\partial X_4}{\partial \rho}$$

$$\beta_{4,75} - -\overline{K}_4 \left[\frac{\partial X_4}{\partial T} - \frac{\partial X_{23}}{\partial T} - \frac{\partial X_{24}}{\partial T} - \frac{\partial X_{68}}{\partial T} - \frac{\partial X_{72}}{\partial T} - \frac{\partial X_{75}}{\partial T} - \frac{\partial X_{78}}{\partial T} \right.$$

$$- \frac{\partial X_{136}}{\partial T} - \frac{\partial X_{188}}{\partial T} - \frac{\partial X_{192}}{\partial T} - \frac{\partial X_{193}}{\partial T} - \frac{\partial X_{196}}{\partial T}$$

$$\left. - \frac{\partial X_{276}}{\partial T} - \frac{\partial X_{280}}{\partial T} \right]$$

For F_2

$$\overline{K}_5 = \frac{38.000 \rho r^*}{V}$$

$$f_5 = -\overline{K}_5 \left[X_5 - X_{27} - X_{29} - X_{88} - X_{91} - X_{95} - X_{143} - X_{208} \right.$$

$$\left. - X_{213} - X_{214} - X_{220} - X_{267} - X_{272} \right]$$

$$\beta_{5,j} = -\overline{K}_5 \left[\frac{\partial X_5}{\partial c_j} - \frac{\partial X_{27}}{\partial c_j} - \frac{\partial X_{29}}{\partial c_j} - \frac{\partial X_{88}}{\partial c_j} - \frac{\partial X_{91}}{\partial c_j} - \frac{\partial X_{95}}{\partial c_j} - \frac{\partial X_{143}}{\partial c_j} \right.$$

$$\left. - \frac{\partial X_{208}}{\partial c_j} - \frac{\partial X_{213}}{\partial c_j} - \frac{\partial X_{214}}{\partial c_j} - \frac{\partial X_{220}}{\partial c_j} - \frac{\partial X_{267}}{\partial c_j} - \frac{\partial X_{272}}{\partial c_j} \right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{5,73} = -\frac{1}{V} f_5$$

$$\beta_{5,74} = \frac{1}{\rho} f_5 - \overline{K}_5 \frac{\partial X_5}{\partial \rho}$$

$$\beta_{5,75} = -\overline{K}_5 \left[\frac{\partial X_5}{\partial T} - \frac{\partial X_{27}}{\partial T} - \frac{\partial X_{29}}{\partial T} - \frac{\partial X_{88}}{\partial T} - \frac{\partial X_{91}}{\partial T} - \frac{\partial X_{95}}{\partial T} - \frac{\partial X_{143}}{\partial T} - \frac{\partial X_{208}}{\partial T} - \frac{\partial X_{213}}{\partial T} - \frac{\partial X_{214}}{\partial T} - \frac{\partial X_{220}}{\partial T} - \frac{\partial X_{267}}{\partial T} - \frac{\partial X_{272}}{\partial T} \right]$$

For HCl

$$\overline{K}_6 = \frac{36.465 \rho r^*}{V}$$

$$f_6 = -\overline{K}_6 \left[X_6 - X_{15} + X_{23} + 2X_{24} + X_{25} - X_{26} - X_{32} + X_{65} - X_{67} - X_{69} + X_{77} - X_{80} + X_{84} + X_{92} + X_{112} + X_{121} - X_{128} - X_{134} + X_{135} - X_{137} + X_{139} + X_{168} - X_{189} + X_{194} - X_{195} - X_{198} + X_{205} + X_{217} - X_{244} + X_{246} + X_{258} - X_{265} + X_{276} - X_{277} - X_{278} - X_{279} - X_{281} \right]$$

$$\beta_{6,j} = -\overline{K}_6 \left[\frac{\partial X_6}{\partial c_j} - \frac{\partial X_{15}}{\partial c_j} + \frac{\partial X_{23}}{\partial c_j} + 2\frac{\partial X_{24}}{\partial c_j} + \frac{\partial X_{25}}{\partial c_j} - \frac{\partial X_{26}}{\partial c_j} - \frac{\partial X_{32}}{\partial c_j} + \frac{\partial X_{65}}{\partial c_j} - \frac{\partial X_{67}}{\partial c_j} - \frac{\partial X_{69}}{\partial c_j} + \frac{\partial X_{77}}{\partial c_j} - \frac{\partial X_{80}}{\partial c_j} + \frac{\partial X_{84}}{\partial c_j} + \frac{\partial X_{92}}{\partial c_j} + \frac{\partial X_{112}}{\partial c_j} + \frac{\partial X_{121}}{\partial c_j} - \frac{\partial X_{128}}{\partial c_j} - \frac{\partial X_{134}}{\partial c_j} + \frac{\partial X_{135}}{\partial c_j} - \frac{\partial X_{137}}{\partial c_j} + \frac{\partial X_{139}}{\partial c_j} + \frac{\partial X_{168}}{\partial c_j} - \frac{\partial X_{189}}{\partial c_j} + \frac{\partial X_{194}}{\partial c_j} - \frac{\partial X_{195}}{\partial c_j} - \frac{\partial X_{198}}{\partial c_j} + \frac{\partial X_{205}}{\partial c_j} + \frac{\partial X_{217}}{\partial c_j} - \frac{\partial X_{244}}{\partial c_j} + \frac{\partial X_{246}}{\partial c_j} + \frac{\partial X_{258}}{\partial c_j} - \frac{\partial X_{265}}{\partial c_j} + \frac{\partial X_{276}}{\partial c_j} - \frac{\partial X_{277}}{\partial c_j} - \frac{\partial X_{278}}{\partial c_j} - \frac{\partial X_{279}}{\partial c_j} - \frac{\partial X_{281}}{\partial c_j} \right], \quad j = 1, 2, \cdots, 57$$

$$\beta_{6,73} = -\frac{1}{V} f_6$$

$$\beta_{6,74} = \frac{1}{\rho} f_6 - \overline{K}_6 \frac{\partial X_6}{\partial \rho}$$

$$\beta_{6,75} = -\overline{K}_6 \left[\frac{\partial X_6}{\partial T} - \frac{\partial X_{15}}{\partial T} + \frac{\partial X_{23}}{\partial T} + 2\frac{\partial X_{24}}{\partial T} + \frac{\partial X_{25}}{\partial T} - \frac{\partial X_{26}}{\partial T} - \frac{\partial X_{32}}{\partial T} \right.$$

$$+ \frac{\partial X_{65}}{\partial T} - \frac{\partial X_{67}}{\partial T} - \frac{\partial X_{69}}{\partial T} + \frac{\partial X_{77}}{\partial T} - \frac{\partial X_{80}}{\partial T} + \frac{\partial X_{84}}{\partial T} + \frac{\partial X_{92}}{\partial T}$$

$$+ \frac{\partial X_{112}}{\partial T} + \frac{\partial X_{121}}{\partial T} - \frac{\partial X_{128}}{\partial T} - \frac{\partial X_{134}}{\partial T} + \frac{\partial X_{135}}{\partial T} - \frac{\partial X_{137}}{\partial T}$$

$$+ \frac{\partial X_{139}}{\partial T} + \frac{\partial X_{168}}{\partial T} - \frac{\partial X_{189}}{\partial T} + \frac{\partial X_{194}}{\partial T} - \frac{\partial X_{195}}{\partial T} - \frac{\partial X_{198}}{\partial T}$$

$$+ \frac{\partial X_{205}}{\partial T} + \frac{\partial X_{217}}{\partial T} - \frac{\partial X_{244}}{\partial T} + \frac{\partial X_{246}}{\partial T} + \frac{\partial X_{258}}{\partial T} - \frac{\partial X_{265}}{\partial T}$$

$$\left. + \frac{\partial X_{276}}{\partial T} - \frac{\partial X_{277}}{\partial T} - \frac{\partial X_{278}}{\partial T} - \frac{\partial X_{279}}{\partial T} - \frac{\partial X_{281}}{\partial T} \right]$$

For HF

$$\overline{K}_7 = \frac{20.008 \rho r^*}{V}$$

$$f_7 = -\overline{K}_7 \left[X_7 + X_{26} + X_{27} + X_{28}\; 2X_{29} + X_{30} + X_{31} + X_{57} - X_{84} \right.$$

$$+ X_{85} - X_{89} - X_{92} + X_{93} - X_{97} + X_{113} + X_{122} + X_{169}$$

$$+ X_{183} - X_{205} + X_{206} - X_{209} - X_{215} - X_{217} + X_{218}$$

$$- X_{222} + X_{237} + X_{247} + X_{254} - X_{266} + X_{267} - X_{268}$$

$$\left. - X_{270} - X_{273} + X_{277} \right]$$

$$\beta_{7,j} = -\overline{K}_7 \left[\frac{\partial X_7}{\partial c_j} + \frac{\partial X_{26}}{\partial c_j} + \frac{\partial X_{27}}{\partial c_j} + \frac{\partial X_{28}}{\partial c_j} + 2\frac{\partial X_{29}}{\partial c_j} + \frac{\partial X_{30}}{\partial c_j} + \frac{\partial X_{31}}{\partial c_j} + \frac{\partial X_{57}}{\partial c_j} \right.$$

$$- \frac{\partial X_{84}}{\partial c_j} + \frac{\partial X_{85}}{\partial c_j} - \frac{\partial X_{89}}{\partial c_j} - \frac{\partial X_{92}}{\partial c_j} + \frac{\partial X_{93}}{\partial c_j} - \frac{\partial X_{97}}{\partial c_j} + \frac{\partial X_{113}}{\partial c_j}$$

$$+ \frac{\partial X_{122}}{\partial c_j} + \frac{\partial X_{169}}{\partial c_j} + \frac{\partial X_{183}}{\partial c_j} - \frac{\partial X_{205}}{\partial c_j} + \frac{\partial X_{206}}{\partial c_j} - \frac{\partial X_{209}}{\partial c_j}$$

$$- \frac{\partial X_{215}}{\partial c_j} - \frac{\partial X_{217}}{\partial c_j} + \frac{\partial X_{218}}{\partial c_j} - \frac{\partial X_{222}}{\partial c_j} + \frac{\partial X_{237}}{\partial c_j} + \frac{\partial X_{247}}{\partial c_j}$$

$$+ \frac{\partial X_{254}}{\partial c_j} - \frac{\partial X_{266}}{\partial c_j} + \frac{\partial X_{267}}{\partial c_j} - \frac{\partial X_{268}}{\partial c_j} - \frac{\partial X_{270}}{\partial c_j} - \frac{\partial X_{273}}{\partial c_j}$$

$$\left. + \frac{\partial X_{277}}{\partial c_j} \right] \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{7,73} = -\frac{1}{V} f_7$$

$$\beta_{7,74} = \frac{1}{\rho} f_7 - \overline{K}_7 \frac{\partial X_7}{\partial \rho}$$

$$\beta_{7,75} = -\overline{K}_7 \left[\frac{\partial X_7}{\partial T} + \frac{\partial X_{26}}{\partial T} + \frac{\partial X_{27}}{\partial T} + \frac{\partial X_{28}}{\partial T} + 2\frac{\partial X_{29}}{\partial T} + \frac{\partial X_{30}}{\partial T} + \frac{\partial X_{31}}{\partial T} \right.$$

$$+ \frac{\partial X_{57}}{\partial T} - \frac{\partial X_{84}}{\partial T} + \frac{\partial X_{85}}{\partial T} - \frac{\partial X_{89}}{\partial T} - \frac{\partial X_{92}}{\partial T} + \frac{\partial X_{93}}{\partial T} - \frac{\partial X_{97}}{\partial T}$$

$$+ \frac{\partial X_{113}}{\partial T} + \frac{\partial X_{122}}{\partial T} + \frac{\partial X_{169}}{\partial T} + \frac{\partial X_{183}}{\partial T} - \frac{\partial X_{205}}{\partial T} + \frac{\partial X_{206}}{\partial T}$$

$$- \frac{\partial X_{209}}{\partial T} - \frac{\partial X_{215}}{\partial T} - \frac{\partial X_{217}}{\partial T} + \frac{\partial X_{218}}{\partial T} - \frac{\partial X_{222}}{\partial T} + \frac{\partial X_{237}}{\partial T}$$

$$+ \frac{\partial X_{247}}{\partial T} + \frac{\partial X_{254}}{\partial T} - \frac{\partial X_{266}}{\partial T} + \frac{\partial X_{267}}{\partial T} - \frac{\partial X_{268}}{\partial T} - \frac{\partial X_{270}}{\partial T}$$

$$\left. - \frac{\partial X_{273}}{\partial T} + \frac{\partial X_{277}}{\partial T} \right]$$

For H_2

$$\overline{K}_8 = \frac{2.016 \rho r^*}{V}$$

$$f_8 = -\overline{K}_8 \left[X_8 - X_{16} - X_{24} - X_{28} - X_{29} + X_{32} + X_{33} + X_{34} - X_{131} + X_{238} + X_{248} + X_{255} + X_{259} - X_{263} + X_{268} + X_{278} \right]$$

$$\beta_{8,j} = -\overline{K}_8 \left[\frac{\partial X_8}{\partial c_j} - \frac{\partial X_{16}}{\partial c_j} - \frac{\partial X_{24}}{\partial c_j} - \frac{\partial X_{28}}{\partial c_j} - \frac{\partial X_{29}}{\partial c_j} + \frac{\partial X_{32}}{\partial c_j} + \frac{\partial X_{33}}{\partial c_j} + \frac{\partial X_{34}}{\partial c_j} - \frac{\partial X_{131}}{\partial c_j} + \frac{\partial X_{238}}{\partial c_j} + \frac{\partial X_{248}}{\partial c_j} + \frac{\partial X_{255}}{\partial c_j} + \frac{\partial X_{259}}{\partial c_j} - \frac{\partial X_{263}}{\partial c_j} + \frac{\partial X_{268}}{\partial c_j} + \frac{\partial X_{278}}{\partial c_j} \right] , \quad j = 1, 2, \cdots, 57$$

$$\beta_{8,73} = -\frac{1}{V} f_8$$

$$\beta_{8,74} = \frac{1}{\rho} f_8 - \overline{K}_8 \frac{\partial X_8}{\partial \rho}$$

$$\beta_{8,75} = -\overline{K}_8 \left[\frac{\partial X_8}{\partial T} - \frac{\partial X_{16}}{\partial T} - \frac{\partial X_{24}}{\partial T} - \frac{\partial X_{28}}{\partial T} - \frac{\partial X_{29}}{\partial T} + \frac{\partial X_{32}}{\partial T} + \frac{\partial X_{33}}{\partial T} + \frac{\partial X_{34}}{\partial T} - \frac{\partial X_{131}}{\partial T} + \frac{\partial X_{238}}{\partial T} + \frac{\partial X_{248}}{\partial T} + \frac{\partial X_{255}}{\partial T} + \frac{\partial X_{259}}{\partial T} - \frac{\partial X_{263}}{\partial T} + \frac{\partial X_{268}}{\partial T} + \frac{\partial X_{278}}{\partial T} \right]$$

For N_2

$$\overline{K}_9 = \frac{28.016\rho r^*}{V}$$

$$f_9 = -\overline{K}_9 \left[X_9 + X_{35} + X_{36} + X_{160} - X_{163}\right]$$

$$\beta_{9,j} = -\overline{K}_9 \left[\frac{\partial X_9}{\partial c_j} + \frac{\partial X_{35}}{\partial c_j} + \frac{\partial X_{36}}{\partial c_j} + \frac{\partial X_{160}}{\partial c_j} - \frac{\partial X_{163}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{9,73} = -\frac{1}{V} f_9$$

$$\beta_{9,74} = \frac{1}{\rho} f_9 - \overline{K}_9 \frac{\partial X_9}{\partial \rho}$$

$$\beta_{9,75} = -\overline{K}_9 \left[\frac{\partial X_9}{\partial T} + \frac{\partial X_{35}}{\partial T} + \frac{\partial X_{36}}{\partial T} + \frac{\partial X_{160}}{\partial T} - \frac{\partial X_{163}}{\partial T}\right]$$

For NO

$$\overline{K}_{10} = \frac{30.008\rho r^*}{V}$$

$$f_{10} = -\overline{K}_{10} \left[X_{10} - X_{20} + X_{21} - X_{35} - 2X_{36} + X_{37} + X_{38} + X_{52} + X_{66} + X_{86} - X_{117} + X_{161} + X_{162} + X_{163} + X_{170} + X_{171} - X_{200} - X_{250}\right]$$

$$\beta_{10,j} = -\overline{K}_{10} \left[\frac{\partial X_{10}}{\partial c_j} - \frac{\partial X_{20}}{\partial c_j} + \frac{\partial X_{21}}{\partial c_j} - \frac{\partial X_{35}}{\partial c_j} - 2\frac{\partial X_{36}}{\partial c_j} + \frac{\partial X_{37}}{\partial c_j} + \frac{\partial X_{38}}{\partial c_j} + \frac{\partial X_{52}}{\partial c_j} + \frac{\partial X_{66}}{\partial c_j} + \frac{\partial X_{86}}{\partial c_j} - \frac{\partial X_{117}}{\partial c_j} + \frac{\partial X_{161}}{\partial c_j} + \frac{\partial X_{162}}{\partial c_j} + \frac{\partial X_{163}}{\partial c_j} + \frac{\partial X_{170}}{\partial c_j} + \frac{\partial X_{171}}{\partial c_j} - \frac{\partial X_{200}}{\partial c_j} - \frac{\partial X_{250}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{10,73} = -\frac{1}{V} f_{10}$$

$$\beta_{10,74} = \frac{1}{\rho} f_{10} - \overline{K}_{10} \frac{\partial X_{10}}{\partial \rho}$$

$$\beta_{10,75} = -\overline{K}_{10} \left[\frac{\partial X_{10}}{\partial T} - \frac{\partial X_{20}}{\partial T} + \frac{\partial X_{21}}{\partial T} - \frac{\partial X_{35}}{\partial T} - 2\frac{\partial X_{36}}{\partial T} + \frac{\partial X_{37}}{\partial T} + \frac{\partial X_{38}}{\partial T} \right.$$
$$+ \frac{\partial X_{52}}{\partial T} + \frac{\partial X_{66}}{\partial T} + \frac{\partial X_{86}}{\partial T} - \frac{\partial X_{117}}{\partial T} + \frac{\partial X_{161}}{\partial T} + \frac{\partial X_{162}}{\partial T}$$
$$\left. + \frac{\partial X_{163}}{\partial T} + \frac{\partial X_{170}}{\partial T} + \frac{\partial X_{171}}{\partial T} - \frac{\partial X_{200}}{\partial T} - \frac{\partial X_{250}}{\partial T} \right]$$

For OH

$$\overline{K}_{11} = \frac{17.008\rho r^*}{V}$$

$$f_{11} = \overline{K}_{11} \left[X_2 - X_{11} + X_{13} + X_{15} + X_{16} + 2X_{17} + X_{19} + X_{25} + X_{30} \right.$$
$$- X_{31} + X_{33} + 2X_{34} + X_{37} + X_{39} + X_{57} + X_{59} - X_{67}$$
$$+ X_{77} + X_{81} + X_{93} + X_{98} + X_{102} + X_{108} + X_{110} + X_{112}$$
$$+ X_{116} + X_{123} + X_{129} + X_{132} - X_{140} - X_{141} + X_{168}$$
$$+ X_{169} + X_{175} + X_{183} + X_{185} + X_{194} - X_{195} + X_{199}$$
$$+ X_{218} + X_{223} + X_{225} + X_{234} - X_{239} - X_{240} + X_{248}$$
$$- X_{249} + X_{251} - X_{260} + X_{261} + X_{262} + X_{264} - X_{269}$$
$$\left. - X_{270} - X_{279} \right]$$

$$\beta_{11,j} = \overline{K}_{11}\left[\frac{\partial X_2}{\partial c_j} - \frac{\partial X_{11}}{\partial c_j} + \frac{\partial X_{13}}{\partial c_j} + \frac{\partial X_{15}}{\partial c_j} + \frac{\partial X_{16}}{\partial c_j} + 2\frac{\partial X_{17}}{\partial c_j} + \frac{\partial X_{19}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{25}}{\partial c_j} + \frac{\partial X_{30}}{\partial c_j} - \frac{\partial X_{31}}{\partial c_j} + \frac{\partial X_{33}}{\partial c_j} + 2\frac{\partial X_{34}}{\partial c_j} + \frac{\partial X_{37}}{\partial c_j} + \frac{\partial X_{39}}{\partial c_j}$$

$$+ \frac{\partial X_{57}}{\partial c_j} + \frac{\partial X_{59}}{\partial c_j} - \frac{\partial X_{67}}{\partial c_j} + \frac{\partial X_{77}}{\partial c_j} + \frac{\partial X_{81}}{\partial c_j} + \frac{\partial X_{93}}{\partial c_j} + \frac{\partial X_{98}}{\partial c_j}$$

$$+ \frac{\partial X_{102}}{\partial c_j} + \frac{\partial X_{108}}{\partial c_j} + \frac{\partial X_{110}}{\partial c_j} + \frac{\partial X_{112}}{\partial c_j} + \frac{\partial X_{116}}{\partial c_j} - \frac{\partial X_{123}}{\partial c_j}$$

$$+ \frac{\partial X_{129}}{\partial c_j} + \frac{\partial X_{132}}{\partial c_j} - \frac{\partial X_{140}}{\partial c_j} - \frac{\partial X_{141}}{\partial c_j} + \frac{\partial X_{168}}{\partial c_j} + \frac{\partial X_{169}}{\partial c_j}$$

$$+ \frac{\partial X_{175}}{\partial c_j} + \frac{\partial X_{183}}{\partial c_j} + \frac{\partial X_{185}}{\partial c_j} + \frac{\partial X_{194}}{\partial c_j} - \frac{\partial X_{195}}{\partial c_j} + \frac{\partial X_{199}}{\partial c_j}$$

$$+ \frac{\partial X_{218}}{\partial c_j} + \frac{\partial X_{223}}{\partial c_j} + \frac{\partial X_{225}}{\partial c_j} + \frac{\partial X_{234}}{\partial c_j} - \frac{\partial X_{239}}{\partial c_j} - \frac{\partial X_{240}}{\partial c_j}$$

$$+ \frac{\partial X_{248}}{\partial c_j} - \frac{\partial X_{249}}{\partial c_j} + \frac{\partial X_{251}}{\partial c_j} - \frac{\partial X_{260}}{\partial c_j} + \frac{\partial X_{261}}{\partial c_j} + \frac{\partial X_{262}}{\partial c_j}$$

$$\left. + \frac{\partial X_{264}}{\partial c_j} - \frac{\partial X_{269}}{\partial c_j} - \frac{\partial X_{270}}{\partial c_j} - \frac{\partial X_{279}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{11,73} = -\frac{1}{V} f_{11}$$

$$\beta_{11,74} = \frac{1}{\rho} f_{11} + \overline{K}_{11}\left[\frac{\partial X_2}{\partial \rho} - \frac{\partial X_{11}}{\partial \rho} + \frac{\partial X_{102}}{\partial \rho} + \frac{\partial X_{108}}{\partial \rho} + \frac{\partial X_{225}}{\partial \rho}\right]$$

$$\beta_{11,75} = \overline{K}_{11}\left[\frac{\partial X_2}{\partial T} - \frac{\partial X_{11}}{\partial T} + \frac{\partial X_{13}}{\partial T} + \frac{\partial X_{15}}{\partial T} + \frac{\partial X_{16}}{\partial T} + 2\frac{\partial X_{17}}{\partial T} + \frac{\partial X_{19}}{\partial T}\right.$$

$$+ \frac{\partial X_{25}}{\partial T} + \frac{\partial X_{30}}{\partial T} - \frac{\partial X_{31}}{\partial T} + \frac{\partial X_{33}}{\partial T} + 2\frac{\partial X_{34}}{\partial T} + \frac{\partial X_{37}}{\partial T} + \frac{\partial X_{39}}{\partial T}$$

$$+ \frac{\partial X_{57}}{\partial T} + \frac{\partial X_{59}}{\partial T} - \frac{\partial X_{67}}{\partial T} + \frac{\partial X_{77}}{\partial T} + \frac{\partial X_{81}}{\partial T} + \frac{\partial X_{93}}{\partial T} + \frac{\partial X_{98}}{\partial T}$$

$$+ \frac{\partial X_{102}}{\partial T} + \frac{\partial X_{108}}{\partial T} + \frac{\partial X_{110}}{\partial T} + \frac{\partial X_{112}}{\partial T} + \frac{\partial X_{116}}{\partial T} - \frac{\partial X_{123}}{\partial T}$$

$$+ \frac{\partial X_{129}}{\partial T} + \frac{\partial X_{132}}{\partial T} - \frac{\partial X_{140}}{\partial T} - \frac{\partial X_{141}}{\partial T} + \frac{\partial X_{168}}{\partial T} + \frac{\partial X_{169}}{\partial T}$$

$$+ \frac{\partial X_{175}}{\partial T} + \frac{\partial X_{183}}{\partial T} + \frac{\partial X_{185}}{\partial T} + \frac{\partial X_{194}}{\partial T} - \frac{\partial X_{195}}{\partial T} + \frac{\partial X_{199}}{\partial T}$$

$$+ \frac{\partial X_{218}}{\partial T} + \frac{\partial X_{223}}{\partial T} + \frac{\partial X_{225}}{\partial T} + \frac{\partial X_{234}}{\partial T} - \frac{\partial X_{239}}{\partial T} - \frac{\partial X_{240}}{\partial T}$$

$$+ \frac{\partial X_{248}}{\partial T} - \frac{\partial X_{249}}{\partial T} + \frac{\partial X_{251}}{\partial T} - \frac{\partial X_{260}}{\partial T} + \frac{\partial X_{261}}{\partial T} + \frac{\partial X_{262}}{\partial T}$$

$$\left.+ \frac{\partial X_{264}}{\partial T} - \frac{\partial X_{269}}{\partial T} - \frac{\partial X_{270}}{\partial T} - \frac{\partial X_{279}}{\partial T}\right]$$

For O_2

$$\overline{K}_{12} = \frac{32.000\rho r^*}{V}$$

$$f_{12} = -\overline{K}_{12}\left[X_{12} - X_{14} - X_{22} + X_{34} + X_{36} - X_{38} + X_{39} - X_{82} - X_{99}\right.$$

$$\left.- X_{118} - X_{170} - X_{177} - X_{186} - X_{201} + X_{241} - X_{249}\right]$$

$$\beta_{12,j} = -\overline{K}_{12}\left[\frac{\partial X_{12}}{\partial c_j} - \frac{\partial X_{14}}{\partial c_j} - \frac{\partial X_{22}}{\partial c_j} + \frac{\partial X_{34}}{\partial c_j} + \frac{\partial X_{36}}{\partial c_j} - \frac{\partial X_{38}}{\partial c_j} + \frac{\partial X_{39}}{\partial c_j}\right.$$

$$- \frac{\partial X_{82}}{\partial c_j} - \frac{\partial X_{99}}{\partial c_j} - \frac{\partial X_{118}}{\partial c_j} - \frac{\partial X_{170}}{\partial c_j} - \frac{\partial X_{177}}{\partial c_j} - \frac{\partial X_{186}}{\partial c_j}$$

$$\left. - \frac{\partial X_{201}}{\partial c_j} + \frac{\partial X_{241}}{\partial c_j} - \frac{\partial X_{249}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{12,73} = -\frac{1}{V} f_{12}$$

$$\beta_{12,74} = \frac{1}{\rho} f_{12} - \overline{K}_{12}\left[\frac{\partial X_{12}}{\partial \rho}\right]$$

$$\beta_{12,75} = -\overline{K}_{12}\left[\frac{\partial X_{12}}{\partial T} - \frac{\partial X_{14}}{\partial T} - \frac{\partial X_{22}}{\partial T} + \frac{\partial X_{34}}{\partial T} + \frac{\partial X_{36}}{\partial T} - \frac{\partial X_{38}}{\partial T} + \frac{\partial X_{39}}{\partial T}\right.$$

$$- \frac{\partial X_{82}}{\partial T} - \frac{\partial X_{99}}{\partial T} - \frac{\partial X_{118}}{\partial T} - \frac{\partial X_{170}}{\partial T} - \frac{\partial X_{177}}{\partial T} - \frac{\partial X_{186}}{\partial T}$$

$$\left. - \frac{\partial X_{201}}{\partial T} + \frac{\partial X_{241}}{\partial T} - \frac{\partial X_{249}}{\partial T}\right]$$

For C

$$\overline{K}_{13} = \frac{12.011\rho r^*}{V}$$

$$f_{13} = \overline{K}_{13}\left[X_3 + X_{18} + X_{19} + X_{20} + X_{22} + X_{51} + X_{64} - X_{114} + X_{167}\right.$$

$$\left. - X_{172} + X_{204} + X_{236}\right]$$

$$\beta_{13,j} = \overline{K}_{13}\left[\frac{\partial X_3}{\partial c_j} + \frac{\partial X_{18}}{\partial c_j} + \frac{\partial X_{19}}{\partial c_j} + \frac{\partial X_{20}}{\partial c_j} + \frac{\partial X_{22}}{\partial c_j} + \frac{\partial X_{51}}{\partial c_j} + \frac{\partial X_{64}}{\partial c_j} - \frac{\partial X_{114}}{\partial c_j}\right.$$

$$\left. + \frac{\partial X_{167}}{\partial c_j} - \frac{\partial X_{172}}{\partial c_j} + \frac{\partial X_{204}}{\partial c_j} + \frac{\partial X_{236}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{13,73} = -\frac{1}{V} f_{13}$$

$$\beta_{13,74} = \frac{1}{\rho} f_{13} + \overline{K}_{13} \frac{\partial X_3}{\partial \rho}$$

$$\beta_{13,75} = \left[\frac{\partial X_3}{\partial T} + \frac{\partial X_{18}}{\partial T} + \frac{\partial X_{19}}{\partial T} + \frac{\partial X_{20}}{\partial T} + \frac{\partial X_{22}}{\partial T} + \frac{\partial X_{51}}{\partial T} + \frac{\partial X_{64}}{\partial T} - \frac{\partial X_{114}}{\partial T}\right.$$

$$\left. + \frac{\partial X_{167}}{\partial T} - \frac{\partial X_{172}}{\partial T} + \frac{\partial X_{204}}{\partial T} + \frac{\partial X_{236}}{\partial T}\right]$$

For Cl

$$\overline{K}_{14} = \frac{35.457\rho r^*}{V}$$

$$f_{14} = \overline{K}_{14} \left[2X_4 + X_6 - X_{15} - X_{23} + X_{25} - X_{26} - X_{32} + X_{42} + X_{43}\right.$$

$$+ X_{44} + X_{54} - X_{62} + X_{70} - X_{75} - X_{78} - X_{79} - X_{87}$$

$$- X_{94} + X_{100} + X_{104} - X_{115} - X_{124} - X_{128} - X_{129}$$

$$- X_{136} - X_{142} + X_{151} + X_{152} + X_{153} - X_{173} - X_{184}$$

$$- X_{188} + X_{190} - X_{192} - X_{193} - X_{196} - X_{197} - X_{207}$$

$$- X_{219} + X_{227} - X_{244} + X_{246} - X_{261} - X_{271} - X_{280}$$

$$\left. + X_{282} + X_{283} + X_{284}\right]$$

$$\beta_{14,j} = \overline{K}_{14}\left[2\frac{\partial X_4}{\partial c_j} + \frac{\partial X_6}{\partial c_j} - \frac{\partial X_{15}}{\partial c_j} - \frac{\partial X_{23}}{\partial c_j} + \frac{\partial X_{25}}{\partial c_j} - \frac{\partial X_{26}}{\partial c_j} - \frac{\partial X_{32}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{42}}{\partial c_j} + \frac{\partial X_{43}}{\partial c_j} + \frac{\partial X_{44}}{\partial c_j} + \frac{\partial X_{54}}{\partial c_j} - \frac{\partial X_{62}}{\partial c_j} + \frac{\partial X_{70}}{\partial c_j} - \frac{\partial X_{75}}{\partial c_j}$$

$$- \frac{\partial X_{78}}{\partial c_j} - \frac{\partial X_{79}}{\partial c_j} - \frac{\partial X_{87}}{\partial c_j} - \frac{\partial X_{94}}{\partial c_j} + \frac{\partial X_{100}}{\partial c_j} + \frac{\partial X_{104}}{\partial c_j} - \frac{\partial X_{115}}{\partial c_j}$$

$$- \frac{\partial X_{124}}{\partial c_j} - \frac{\partial X_{128}}{\partial c_j} - \frac{\partial X_{129}}{\partial c_j} - \frac{\partial X_{136}}{\partial c_j} - \frac{\partial X_{142}}{\partial c_j} + \frac{\partial X_{151}}{\partial c_j}$$

$$+ \frac{\partial X_{152}}{\partial c_j} + \frac{\partial X_{153}}{\partial c_j} - \frac{\partial X_{173}}{\partial c_j} - \frac{\partial X_{184}}{\partial c_j} - \frac{\partial X_{188}}{\partial c_j} + \frac{\partial X_{190}}{\partial c_j}$$

$$- \frac{\partial X_{192}}{\partial c_j} - \frac{\partial X_{193}}{\partial c_j} - \frac{\partial X_{196}}{\partial c_j} - \frac{\partial X_{197}}{\partial c_j} - \frac{\partial X_{207}}{\partial c_j} - \frac{\partial X_{219}}{\partial c_j}$$

$$+ \frac{\partial X_{227}}{\partial c_j} - \frac{\partial X_{244}}{\partial c_j} + \frac{\partial X_{245}}{\partial c_j} - \frac{\partial X_{261}}{\partial c_j} - \frac{\partial X_{271}}{\partial c_j} - \frac{\partial X_{280}}{\partial c_j}$$

$$\left.+ \frac{\partial X_{282}}{\partial c_j} + \frac{\partial X_{283}}{\partial c_j} + \frac{\partial X_{284}}{\partial c_j}\right] \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{14,73} = -\frac{1}{V} f_{14}$$

$$\beta_{14,74} = \frac{1}{\rho} f_{14} + \overline{K}_{14}\left[2\frac{2X_4}{\partial \rho} + \frac{\partial X_6}{\partial \rho} + \frac{\partial X_{42}}{\partial \rho} + \frac{\partial X_{43}}{\partial \rho} + \frac{\partial X_{44}}{\partial \rho} + \frac{\partial X_{100}}{\partial \rho}\right.$$

$$\left.+ \frac{\partial X_{104}}{\partial \rho} + \frac{\partial X_{151}}{\partial \rho} + \frac{\partial X_{152}}{\partial \rho} + \frac{\partial X_{153}}{\partial \rho} + \frac{\partial X_{227}}{\partial \rho}\right]$$

$$\beta_{14,75} = \overline{K}_{14}\left[2\frac{\partial X_4}{\partial T} + \frac{\partial X_6}{\partial T} - \frac{\partial X_{15}}{\partial T} - \frac{\partial X_{23}}{\partial T} + \frac{\partial X_{25}}{\partial T} - \frac{\partial X_{26}}{\partial T} - \frac{\partial X_{32}}{\partial T} + \frac{\partial X_{42}}{\partial T}\right.$$

$$+ \frac{\partial X_{43}}{\partial T} + \frac{\partial X_{44}}{\partial T} + \frac{\partial X_{54}}{\partial T} - \frac{\partial X_{62}}{\partial T} + \frac{\partial X_{70}}{\partial T} - \frac{\partial X_{75}}{\partial T} - \frac{\partial X_{78}}{\partial T}$$

$$- \frac{\partial X_{79}}{\partial T} - \frac{\partial X_{87}}{\partial T} - \frac{\partial X_{94}}{\partial T} + \frac{\partial X_{100}}{\partial T} + \frac{\partial X_{104}}{\partial T} - \frac{\partial X_{115}}{\partial T} - \frac{\partial X_{124}}{\partial T}$$

$$- \frac{\partial X_{128}}{\partial T} - \frac{\partial X_{129}}{\partial T} - \frac{\partial X_{136}}{\partial T} - \frac{\partial X_{142}}{\partial T} + \frac{\partial X_{151}}{\partial T} + \frac{\partial X_{152}}{\partial T}$$

$$+ \frac{\partial X_{153}}{\partial T} - \frac{\partial X_{173}}{\partial T} - \frac{\partial X_{184}}{\partial T} - \frac{\partial X_{188}}{\partial T} + \frac{\partial X_{190}}{\partial T} - \frac{\partial X_{192}}{\partial T}$$

$$- \frac{\partial X_{193}}{\partial T} - \frac{\partial X_{196}}{\partial T} - \frac{\partial X_{197}}{\partial T} - \frac{\partial X_{207}}{\partial T} - \frac{\partial X_{219}}{\partial T} + \frac{\partial X_{227}}{\partial T}$$

$$- \frac{\partial X_{244}}{\partial T} + \frac{\partial X_{246}}{\partial T} - \frac{\partial X_{261}}{\partial T} - \frac{\partial X_{271}}{\partial T} - \frac{\partial X_{280}}{\partial T} + \frac{\partial X_{282}}{\partial T}$$

$$\left. + \frac{\partial X_{283}}{\partial T} + \frac{\partial X_{284}}{\partial T}\right]$$

For F

$$\overline{K}_{15} = \frac{19.000\rho r^*}{V}$$

$$f_{15} = \overline{K}_{15}\left[2X_5 + X_7 + X_{26} - X_{27} + X_{28} + X_{30} + X_{31} + X_{46} + X_{47}\right.$$

$$+ X_{48} + X_{56} - X_{58} + X_{60} + X_{87} - X_{88} - X_{91} + X_{94} - X_{95}$$

$$- X_{96} + X_{101} + X_{105} + X_{113} + X_{119} + X_{141} + X_{142}$$

$$- X_{143} + X_{145} + X_{155} + X_{156} + X_{157} + X_{158} - X_{174}$$

$$+ X_{207} - X_{208} + X_{210} - X_{213} - X_{214} + X_{219} - X_{220}$$

$$- X_{221} + X_{224} + X_{228} + X_{237} + X_{247} + X_{252} + X_{269}$$

$$\left. + X_{271} - X_{272} + X_{274} + X_{275}\right]$$

$$\beta_{15,j} = \overline{K}_{15}\left[2\frac{\partial X_5}{\partial c_j} + \frac{\partial X_7}{\partial c_j} + \frac{\partial X_{26}}{\partial c_j} - \frac{\partial X_{27}}{\partial c_j} + \frac{\partial X_{28}}{\partial c_j} + \frac{\partial X_{30}}{\partial c_j} + \frac{\partial X_{31}}{\partial c_j} + \frac{\partial X_{46}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{47}}{\partial c_j} + \frac{\partial X_{48}}{\partial c_j} + \frac{\partial X_{56}}{\partial c_j} - \frac{\partial X_{58}}{\partial c_j} + \frac{\partial X_{60}}{\partial c_j} + \frac{\partial X_{87}}{\partial c_j} - \frac{\partial X_{88}}{\partial c_j}$$

$$- \frac{\partial X_{91}}{\partial c_j} + \frac{\partial X_{94}}{\partial c_j} - \frac{\partial X_{95}}{\partial c_j} - \frac{\partial X_{96}}{\partial c_j} + \frac{\partial X_{101}}{\partial c_j} + \frac{\partial X_{105}}{\partial c_j} + \frac{\partial X_{113}}{\partial c_j}$$

$$+ \frac{\partial X_{119}}{\partial c_j} + \frac{\partial X_{141}}{\partial c_j} + \frac{\partial X_{142}}{\partial c_j} - \frac{\partial X_{143}}{\partial c_j} + \frac{\partial X_{145}}{\partial c_j} + \frac{\partial X_{155}}{\partial c_j}$$

$$+ \frac{\partial X_{156}}{\partial c_j} + \frac{\partial X_{157}}{\partial c_j} + \frac{\partial X_{158}}{\partial c_j} - \frac{\partial X_{174}}{\partial c_j} + \frac{\partial X_{207}}{\partial c_j} - \frac{\partial X_{208}}{\partial c_j}$$

$$+ \frac{\partial X_{210}}{\partial c_j} - \frac{\partial X_{213}}{\partial c_j} - \frac{\partial X_{214}}{\partial c_j} + \frac{\partial X_{219}}{\partial c_j} - \frac{\partial X_{220}}{\partial c_j} - \frac{\partial X_{221}}{\partial c_j}$$

$$+ \frac{\partial X_{224}}{\partial c_j} + \frac{\partial X_{228}}{\partial c_j} + \frac{\partial X_{237}}{\partial c_j} + \frac{\partial X_{247}}{\partial c_j} + \frac{\partial X_{252}}{\partial c_j} + \frac{\partial X_{269}}{\partial c_j}$$

$$\left.+ \frac{\partial X_{270}}{\partial c_j} - \frac{\partial X_{271}}{\partial c_j} + \frac{\partial X_{273}}{\partial c_j} + \frac{\partial X_{274}}{\partial c_j}\right] \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{15,73} = -\frac{1}{V} f_{15}$$

$$\beta_{15,74} = \frac{1}{\rho} f_{15} + \overline{K}_{15}\left[2\frac{\partial X_5}{\partial \rho} + \frac{\partial X_7}{\partial \rho} + \frac{\partial X_{46}}{\partial \rho} + \frac{\partial X_{47}}{\partial \rho} + \frac{\partial X_{48}}{\partial \rho} + \frac{\partial X_{101}}{\partial \rho}\right.$$

$$+ \frac{\partial X_{105}}{\partial \rho} + \frac{\partial X_{155}}{\partial \rho} + \frac{\partial X_{156}}{\partial \rho} + \frac{\partial X_{157}}{\partial \rho}$$

$$\left.+ \frac{\partial X_{158}}{\partial \rho} + \frac{\partial X_{228}}{\partial \rho}\right]$$

$$\beta_{15,75} = \overline{K}_{15}\left[2\frac{\partial X_5}{\partial T} + \frac{\partial X_7}{\partial T} + \frac{\partial X_{26}}{\partial T} - \frac{\partial X_{27}}{\partial T} + \frac{\partial X_{28}}{\partial T} + \frac{\partial X_{30}}{\partial T} + \frac{\partial X_{31}}{\partial T} + \frac{\partial X_{46}}{\partial T}\right.$$

$$+ \frac{\partial X_{47}}{\partial T} + \frac{\partial X_{48}}{\partial T} + \frac{\partial X_{56}}{\partial T} - \frac{\partial X_{58}}{\partial T} + \frac{\partial X_{60}}{\partial T} + \frac{\partial X_{87}}{\partial T} - \frac{\partial X_{88}}{\partial T}$$

$$- \frac{\partial X_{91}}{\partial T} + \frac{\partial X_{94}}{\partial T} - \frac{\partial X_{95}}{\partial T} - \frac{\partial X_{96}}{\partial T} + \frac{\partial X_{101}}{\partial T} + \frac{\partial X_{105}}{\partial T} + \frac{\partial X_{113}}{\partial T}$$

$$+ \frac{\partial X_{119}}{\partial T} + \frac{\partial X_{141}}{\partial T} + \frac{\partial X_{142}}{\partial T} - \frac{\partial X_{143}}{\partial T} + \frac{\partial X_{145}}{\partial T} + \frac{\partial X_{155}}{\partial T}$$

$$+ \frac{\partial X_{156}}{\partial T} + \frac{\partial X_{157}}{\partial T} + \frac{\partial X_{158}}{\partial T} - \frac{\partial X_{174}}{\partial T} + \frac{\partial X_{207}}{\partial T} - \frac{\partial X_{208}}{\partial T}$$

$$+ \frac{\partial X_{210}}{\partial T} - \frac{\partial X_{213}}{\partial T} - \frac{\partial X_{214}}{\partial T} + \frac{\partial X_{219}}{\partial T} - \frac{\partial X_{220}}{\partial T} - \frac{\partial X_{221}}{\partial T}$$

$$+ \frac{\partial X_{224}}{\partial T} + \frac{\partial X_{228}}{\partial T} + \frac{\partial X_{237}}{\partial T} + \frac{\partial X_{247}}{\partial T} + \frac{\partial X_{252}}{\partial T} + \frac{\partial X_{269}}{\partial T}$$

$$\left.+ \frac{\partial X_{271}}{\partial T} - \frac{\partial X_{272}}{\partial T} + \frac{\partial X_{274}}{\partial T} + \frac{\partial X_{275}}{\partial T}\right]$$

For H

$$\overline{K}_{16} = \frac{1.008\rho r^*}{V}$$

$$f_{16} = \overline{K}_{16}\left[X_2 + X_6 + X_7 + 2X_8 + X_{11} - X_{13} - X_{16} - X_{19} + X_{23} + X_{27}\right.$$

$$- X_{28} + X_{32} + X_{33} - X_{37} - X_{39} - X_{59} + X_{65} - X_{69} - X_{80}$$

$$- X_{81} + X_{85} - X_{89} - X_{97} - X_{98} + X_{103} - X_{116} - X_{125}$$

$$- X_{130} - X_{131} + X_{135} - X_{137} - X_{144} - X_{146} - X_{147} - X_{175}$$

$$- X_{185} - X_{189} - X_{198} - X_{199} + X_{206} - X_{209} - X_{215} - X_{222}$$

$$- X_{223} + X_{226} + X_{229} + X_{235} + X_{238} + X_{240} + X_{243} - X_{256}$$

$$\left.- X_{262} - X_{263} - X_{273} - X_{274} - X_{281} - X_{282}\right]$$

$$\beta_{16,j} = \overline{K}_{16}\left[\frac{\partial X_2}{\partial c_j} + \frac{\partial X_6}{\partial c_j} + \frac{\partial X_7}{\partial c_j} + 2\frac{\partial X_8}{\partial c_j} + \frac{\partial X_{11}}{\partial c_j} - \frac{\partial X_{13}}{\partial c_j} - \frac{\partial X_{16}}{\partial c_j} - \frac{\partial X_{19}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{23}}{\partial c_j} + \frac{\partial X_{27}}{\partial c_j} - \frac{\partial X_{28}}{\partial c_j} + \frac{\partial X_{32}}{\partial c_j} + \frac{\partial X_{33}}{\partial c_j} - \frac{\partial X_{37}}{\partial c_j} - \frac{\partial X_{39}}{\partial c_j}$$

$$- \frac{\partial X_{59}}{\partial c_j} + \frac{\partial X_{65}}{\partial c_j} - \frac{\partial X_{69}}{\partial c_j} - \frac{\partial X_{80}}{\partial c_j} - \frac{\partial X_{81}}{\partial c_j} + \frac{\partial X_{85}}{\partial c_j} - \frac{\partial X_{89}}{\partial c_j}$$

$$- \frac{\partial X_{97}}{\partial c_j} - \frac{\partial X_{98}}{\partial c_j} + \frac{\partial X_{103}}{\partial c_j} - \frac{\partial X_{116}}{\partial c_j} - \frac{\partial X_{125}}{\partial c_j} - \frac{\partial X_{130}}{\partial c_j} - \frac{\partial X_{131}}{\partial c_j}$$

$$+ \frac{\partial X_{135}}{\partial c_j} - \frac{\partial X_{137}}{\partial c_j} - \frac{\partial X_{144}}{\partial c_j} - \frac{\partial X_{146}}{\partial c_j} - \frac{\partial X_{147}}{\partial c_j} - \frac{\partial X_{175}}{\partial c_j} - \frac{\partial X_{185}}{\partial c_j}$$

$$- \frac{\partial X_{189}}{\partial c_j} - \frac{\partial X_{198}}{\partial c_j} - \frac{\partial X_{199}}{\partial c_j} + \frac{\partial X_{206}}{\partial c_j} - \frac{\partial X_{209}}{\partial c_j} - \frac{\partial X_{215}}{\partial c_j} - \frac{\partial X_{222}}{\partial c_j}$$

$$- \frac{\partial X_{223}}{\partial c_j} + \frac{\partial X_{226}}{\partial c_j} + \frac{\partial X_{229}}{\partial c_j} + \frac{\partial X_{235}}{\partial c_j} + \frac{\partial X_{238}}{\partial c_j} + \frac{\partial X_{240}}{\partial c_j} + \frac{\partial X_{243}}{\partial c_j}$$

$$\left.- \frac{\partial X_{256}}{\partial c_j} - \frac{\partial X_{262}}{\partial c_j} - \frac{\partial X_{263}}{\partial c_j} - \frac{\partial X_{273}}{\partial c_j} - \frac{\partial X_{274}}{\partial c_j} - \frac{\partial X_{281}}{\partial c_j} - \frac{\partial X_{282}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{16,73} = -\frac{1}{V} f_{16}$$

$$\beta_{16,74} = \frac{1}{\rho} f_{16} + \overline{K}_{16}\left[\frac{\partial X_2}{\partial \rho} + \frac{\partial X_6}{\partial \rho} + \frac{\partial X_7}{\partial \rho} + 2\frac{\partial X_8}{\partial \rho} + \frac{\partial X_{11}}{\partial \rho} + \frac{\partial X_{103}}{\partial \rho}\right.$$

$$\left.+ \frac{\partial X_{226}}{\partial \rho} + \frac{\partial X_{229}}{\partial \rho}\right]$$

$$\beta_{16,75} = \overline{K}_{16}\left[\frac{\partial X_2}{\partial T} + \frac{\partial X_6}{\partial T} + \frac{\partial X_7}{\partial T} + 2\frac{\partial X_8}{\partial T} + \frac{\partial X_{11}}{\partial T} - \frac{\partial X_{13}}{\partial T} - \frac{\partial X_{16}}{\partial T} - \frac{\partial X_{19}}{\partial T}\right.$$

$$+ \frac{\partial X_{23}}{\partial T} + \frac{\partial X_{27}}{\partial T} - \frac{\partial X_{28}}{\partial T} + \frac{\partial X_{32}}{\partial T} + \frac{\partial X_{33}}{\partial T} - \frac{\partial X_{37}}{\partial T} - \frac{\partial X_{39}}{\partial T}$$

$$- \frac{\partial X_{59}}{\partial T} + \frac{\partial X_{65}}{\partial T} - \frac{\partial X_{69}}{\partial T} - \frac{\partial X_{80}}{\partial T} - \frac{\partial X_{81}}{\partial T} + \frac{\partial X_{85}}{\partial T} - \frac{\partial X_{89}}{\partial T}$$

$$- \frac{\partial X_{97}}{\partial T} - \frac{\partial X_{98}}{\partial T} + \frac{\partial X_{103}}{\partial T} - \frac{\partial X_{116}}{\partial T} - \frac{\partial X_{125}}{\partial T} - \frac{\partial X_{130}}{\partial T} - \frac{\partial X_{131}}{\partial T}$$

$$+ \frac{\partial X_{135}}{\partial T} - \frac{\partial X_{137}}{\partial T} - \frac{\partial X_{144}}{\partial T} - \frac{\partial X_{146}}{\partial T} - \frac{\partial X_{147}}{\partial T} - \frac{\partial X_{175}}{\partial T}$$

$$- \frac{\partial X_{185}}{\partial T} - \frac{\partial X_{189}}{\partial T} - \frac{\partial X_{198}}{\partial T} - \frac{\partial X_{199}}{\partial T} + \frac{\partial X_{206}}{\partial T} - \frac{\partial X_{209}}{\partial T}$$

$$- \frac{\partial X_{215}}{\partial T} - \frac{\partial X_{222}}{\partial T} - \frac{\partial X_{223}}{\partial T} + \frac{\partial X_{226}}{\partial T} + \frac{\partial X_{229}}{\partial T} + \frac{\partial X_{235}}{\partial T}$$

$$+ \frac{\partial X_{238}}{\partial T} + \frac{\partial X_{240}}{\partial T} + \frac{\partial X_{243}}{\partial T} - \frac{\partial X_{256}}{\partial T} - \frac{\partial X_{262}}{\partial T} - \frac{\partial X_{263}}{\partial T}$$

$$\left.- \frac{\partial X_{273}}{\partial T} - \frac{\partial X_{274}}{\partial T} - \frac{\partial X_{281}}{\partial T} - \frac{\partial X_{282}}{\partial T}\right]$$

For N

$$\overline{K}_{17} = \frac{14.008\rho r^*}{V}$$

$$f_{17} = \overline{K}_{17}\left[2X_9 + X_{10} - X_{20} + X_{21} + X_{35} + X_{37} + X_{38} + X_{66} + X_{86}\right.$$

$$- X_{117} + X_{148} + X_{160} + X_{162} + X_{171} - X_{176} - X_{190}$$

$$\left.- X_{200} - X_{210} - X_{250}\right]$$

$$\beta_{17,j} = \overline{K}_{17}\left[2\frac{\partial X_9}{\partial c_j} + \frac{\partial X_{10}}{\partial c_j} - \frac{\partial X_{20}}{\partial c_j} + \frac{\partial X_{21}}{\partial c_j} + \frac{\partial X_{35}}{\partial c_j} + \frac{\partial X_{37}}{\partial c_j} + \frac{\partial X_{38}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{66}}{\partial c_j} + \frac{\partial X_{86}}{\partial c_j} - \frac{\partial X_{117}}{\partial c_j} + \frac{\partial X_{148}}{\partial c_j} + \frac{\partial X_{160}}{\partial c_j} + \frac{\partial X_{162}}{\partial c_j}$$

$$\left. + \frac{\partial X_{171}}{\partial c_j} - \frac{\partial X_{176}}{\partial c_j} - \frac{\partial X_{190}}{\partial c_j} - \frac{\partial X_{200}}{\partial c_j} - \frac{\partial X_{210}}{\partial c_j} - \frac{\partial X_{250}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{17,73} = -\frac{1}{V} f_{17}$$

$$\beta_{17,74} = \frac{1}{\rho} f_{17} + \overline{K}_{17}\left[2\frac{\partial X_9}{\partial \rho} + \frac{\partial X_{10}}{\partial \rho} + \frac{\partial X_{148}}{\partial \rho}\right]$$

$$\beta_{17,75} = \overline{K}_{17}\left[2\frac{\partial X_9}{\partial T} + \frac{\partial X_{10}}{\partial T} - \frac{\partial X_{20}}{\partial T} + \frac{\partial X_{21}}{\partial T} + \frac{\partial X_{35}}{\partial T} + \frac{\partial X_{37}}{\partial T} + \frac{\partial X_{38}}{\partial T}\right.$$

$$+ \frac{\partial X_{66}}{\partial T} + \frac{\partial X_{86}}{\partial T} - \frac{\partial X_{117}}{\partial T} + \frac{\partial X_{148}}{\partial T} + \frac{\partial X_{160}}{\partial T} + \frac{\partial X_{162}}{\partial T}$$

$$\left. + \frac{\partial X_{171}}{\partial T} - \frac{\partial X_{176}}{\partial T} - \frac{\partial X_{190}}{\partial T} - \frac{\partial X_{200}}{\partial T} - \frac{\partial X_{210}}{\partial T} - \frac{\partial X_{250}}{\partial T}\right]$$

For O

$$\overline{K}_{18} = \frac{16.000\rho r^*}{V}$$

$$f_{18} = \overline{K}_{18}\left[X_1 + X_3 + X_{10} + X_{11} + 2X_{12} - X_{14} - X_{17} - X_{22} - X_{25} - X_{30}\right.$$

$$- X_{33} - X_{35} - X_{38} + X_{39} + X_{40} + X_{45} + X_{49} + X_{53} + X_{58}$$

$$- X_{63} - X_{70} - X_{82} + X_{96} - X_{99} + X_{106} + X_{115} - X_{118}$$

$$- X_{126} - X_{132} - X_{145} + X_{149} + X_{150} + X_{154} + X_{159} + X_{161}$$

$$+ X_{173} + X_{174} + X_{176} - X_{177} + X_{184} - X_{186} + X_{197} - X_{201}$$

$$\left. + X_{221} - X_{224} + X_{230} + X_{239} + X_{241} - X_{257} - X_{264} - X_{275} - X_{283}\right]$$

$$
\begin{aligned}
\beta_{18,j} = \overline{K}_{18}\Bigg[& \frac{\partial X_1}{\partial c_j} + \frac{\partial X_3}{\partial c_j} + \frac{\partial X_{10}}{\partial c_j} + \frac{\partial X_{11}}{\partial c_j} + 2\frac{\partial X_{12}}{\partial c_j} - \frac{\partial X_{14}}{\partial c_j} - \frac{\partial X_{17}}{\partial c_j} - \frac{\partial X_{22}}{\partial c_j} \\
& - \frac{\partial X_{25}}{\partial c_j} - \frac{\partial X_{30}}{\partial c_j} - \frac{\partial X_{33}}{\partial c_j} - \frac{\partial X_{35}}{\partial c_j} - \frac{\partial X_{38}}{\partial c_j} + \frac{\partial X_{39}}{\partial c_j} + \frac{\partial X_{40}}{\partial c_j} \\
& + \frac{\partial X_{45}}{\partial c_j} + \frac{\partial X_{49}}{\partial c_j} + \frac{\partial X_{53}}{\partial c_j} + \frac{\partial X_{58}}{\partial c_j} - \frac{\partial X_{63}}{\partial c_j} - \frac{\partial X_{70}}{\partial c_j} - \frac{\partial X_{82}}{\partial c_j} \\
& + \frac{\partial X_{96}}{\partial c_j} - \frac{\partial X_{99}}{\partial c_j} + \frac{\partial X_{106}}{\partial c_j} + \frac{\partial X_{115}}{\partial c_j} - \frac{\partial X_{118}}{\partial c_j} - \frac{\partial X_{126}}{\partial c_j} - \frac{\partial X_{132}}{\partial c_j} \\
& - \frac{\partial X_{145}}{\partial c_j} + \frac{\partial X_{149}}{\partial c_j} + \frac{\partial X_{150}}{\partial c_j} + \frac{\partial X_{154}}{\partial c_j} + \frac{\partial X_{159}}{\partial c_j} + \frac{\partial X_{161}}{\partial c_j} \\
& + \frac{\partial X_{173}}{\partial c_j} + \frac{\partial X_{174}}{\partial c_j} + \frac{\partial X_{176}}{\partial c_j} - \frac{\partial X_{177}}{\partial c_j} + \frac{\partial X_{184}}{\partial c_j} - \frac{\partial X_{186}}{\partial c_j} \\
& + \frac{\partial X_{197}}{\partial c_j} - \frac{\partial X_{201}}{\partial c_j} + \frac{\partial X_{221}}{\partial c_j} - \frac{\partial X_{224}}{\partial c_j} + \frac{\partial X_{230}}{\partial c_j} + \frac{\partial X_{239}}{\partial c_j} \\
& + \frac{\partial X_{240}}{\partial c_j} - \frac{\partial X_{257}}{\partial c_j} - \frac{\partial X_{264}}{\partial c_j} - \frac{\partial X_{275}}{\partial c_j} - \frac{\partial X_{283}}{\partial c_j}\Bigg] \quad j = 1, 2, \cdots, 57
\end{aligned}
$$

$$\beta_{18,73} = -\frac{1}{V} f_{18}$$

$$
\begin{aligned}
\beta_{18,74} = \frac{1}{\rho} f_{18} + \overline{K}_{18}\Bigg[& \frac{\partial X_1}{\partial \rho} + \frac{\partial X_3}{\partial \rho} + \frac{\partial X_{10}}{\partial \rho} + \frac{\partial X_{11}}{\partial \rho} + 2\frac{\partial X_{12}}{\partial \rho} + \frac{\partial X_{40}}{\partial \rho} \\
& + \frac{\partial X_{45}}{\partial \rho} + \frac{\partial X_{49}}{\partial \rho} + \frac{\partial X_{106}}{\partial \rho} + \frac{\partial X_{149}}{\partial \rho} + \frac{\partial X_{150}}{\partial \rho} \\
& + \frac{\partial X_{154}}{\partial \rho} + \frac{\partial X_{159}}{\partial \rho} + \frac{\partial X_{230}}{\partial \rho}\Bigg]
\end{aligned}
$$

$$\beta_{18,75} = \overline{K}_{18}\left[\frac{\partial X_1}{\partial T} + \frac{\partial X_3}{\partial T} + \frac{\partial X_{10}}{\partial T} + \frac{\partial X_{11}}{\partial T} + 2\frac{\partial X_{12}}{\partial T} - \frac{\partial X_{14}}{\partial T} - \frac{\partial X_{17}}{\partial T} - \frac{\partial X_{22}}{\partial T}\right.$$

$$- \frac{\partial X_{25}}{\partial T} - \frac{\partial X_{30}}{\partial T} - \frac{\partial X_{33}}{\partial T} - \frac{\partial X_{35}}{\partial T} - \frac{\partial X_{38}}{\partial T} + \frac{\partial X_{39}}{\partial T} + \frac{\partial X_{40}}{\partial T}$$

$$+ \frac{\partial X_{45}}{\partial T} + \frac{\partial X_{49}}{\partial T} + \frac{\partial C_{53}}{\partial T} + \frac{\partial X_{58}}{\partial T} - \frac{\partial X_{63}}{\partial T} - \frac{\partial X_{70}}{\partial T} - \frac{\partial X_{82}}{\partial T}$$

$$+ \frac{\partial X_{96}}{\partial T} - \frac{\partial X_{99}}{\partial T} + \frac{\partial X_{106}}{\partial T} + \frac{\partial X_{115}}{\partial T} - \frac{\partial X_{118}}{\partial T} - \frac{\partial X_{126}}{\partial T} - \frac{\partial X_{132}}{\partial T}$$

$$- \frac{\partial X_{145}}{\partial T} + \frac{\partial X_{149}}{\partial T} + \frac{\partial X_{150}}{\partial T} + \frac{\partial X_{154}}{\partial T} + \frac{\partial X_{159}}{\partial T} + \frac{\partial X_{161}}{\partial T}$$

$$+ \frac{\partial X_{173}}{\partial T} + \frac{\partial X_{174}}{\partial T} + \frac{\partial X_{176}}{\partial T} - \frac{\partial X_{177}}{\partial T} + \frac{\partial X_{184}}{\partial T} - \frac{\partial X_{186}}{\partial T}$$

$$+ \frac{\partial X_{197}}{\partial T} - \frac{\partial X_{201}}{\partial T} + \frac{\partial X_{221}}{\partial T} - \frac{\partial X_{224}}{\partial T} + \frac{\partial X_{230}}{\partial T} + \frac{\partial X_{239}}{\partial T}$$

$$\left.+ \frac{\partial X_{241}}{\partial T} - \frac{\partial X_{257}}{\partial T} - \frac{\partial X_{264}}{\partial T} - \frac{\partial X_{275}}{\partial T} - \frac{\partial X_{283}}{\partial T}\right]$$

For Al

$$\overline{K}_{19} = \frac{26.980\rho r^*}{V}$$

$$f_{19} = \overline{K}_{19}\left[X_{40} + X_{41} + X_{42} + X_{46} - X_{50} - X_{51} - X_{52} - X_{53} - X_{54} - X_{55}\right.$$

$$\left.- X_{56} + X_{59} + X_{61} + X_{68} + X_{69} + X_{71} + X_{83} + X_{88} + X_{89}\right]$$

$$\beta_{19,j} = \overline{K}_{19}\left[\frac{\partial X_{40}}{\partial c_j} + \frac{\partial X_{41}}{\partial c_j} + \frac{\partial X_{42}}{\partial c_j} + \frac{\partial X_{46}}{\partial c_j} - \frac{\partial X_{50}}{\partial c_j} - \frac{\partial X_{51}}{\partial c_j} - \frac{\partial X_{52}}{\partial c_j}\right.$$

$$- \frac{\partial X_{53}}{\partial c_j} - \frac{\partial X_{54}}{\partial c_j} - \frac{\partial X_{55}}{\partial c_j} - \frac{\partial X_{56}}{\partial c_j} + \frac{\partial X_{59}}{\partial c_j} + \frac{\partial X_{61}}{\partial c_j} + \frac{\partial X_{68}}{\partial c_j}$$

$$\left.+ \frac{\partial X_{69}}{\partial c_j} + \frac{\partial X_{71}}{\partial c_j} + \frac{\partial X_{83}}{\partial c_j} + \frac{\partial X_{88}}{\partial c_j} + \frac{\partial X_{89}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{19,73} = -\frac{1}{V} f_{19}$$

$$\beta_{19,74} = \frac{1}{\rho} f_{19} + \overline{K}_{19}\left[\frac{\partial X_{40}}{\partial \rho} + \frac{\partial X_{41}}{\partial \rho} + \frac{\partial X_{42}}{\partial \rho} + \frac{\partial X_{46}}{\partial \rho}\right]$$

$$\beta_{19,75} = \overline{K}_{19}\left[\frac{\partial X_{40}}{\partial T} + \frac{\partial X_{41}}{\partial T} + \frac{\partial X_{42}}{\partial T} + \frac{\partial X_{46}}{\partial T} - \frac{\partial X_{50}}{\partial T} - \frac{\partial X_{51}}{\partial T} - \frac{\partial X_{52}}{\partial T}\right.$$

$$- \frac{\partial X_{53}}{\partial T} - \frac{\partial X_{54}}{\partial T} - \frac{\partial X_{55}}{\partial T} - \frac{\partial X_{56}}{\partial T} + \frac{\partial X_{59}}{\partial T} + \frac{\partial X_{61}}{\partial T} + \frac{\partial X_{68}}{\partial T}$$

$$\left. + \frac{\partial X_{69}}{\partial T} + \frac{\partial X_{71}}{\partial T} + \frac{\partial X_{83}}{\partial T} + \frac{\partial X_{88}}{\partial T} + \frac{\partial X_{89}}{\partial T}\right]$$

For AlO

$$\overline{K}_{20} = \frac{42.980\rho r^*}{V}$$

$$f_{20} = -\overline{K}_{20}\left[X_{40} - X_{41} - X_{44} - X_{48} - X_{50} - X_{51} - X_{52} - X_{53} - X_{55}\right.$$

$$+ X_{57} + X_{58} + X_{59} + X_{60} + X_{61} - X_{62} - 2X_{63} - X_{67}$$

$$\left. - X_{70} - X_{73} - X_{78} - X_{80} - X_{90} - X_{95} - X_{97}\right]$$

$$\beta_{20,j} = -\overline{K}_{20}\left[\frac{\partial X_{40}}{\partial c_j} - \frac{\partial X_{41}}{\partial c_j} - \frac{\partial X_{44}}{\partial c_j} - \frac{\partial X_{48}}{\partial c_j} - \frac{\partial X_{50}}{\partial c_j} - \frac{\partial X_{51}}{\partial c_j} - \frac{\partial X_{52}}{\partial c_j}\right.$$

$$- \frac{\partial X_{53}}{\partial c_j} - \frac{\partial X_{55}}{\partial c_j} + \frac{\partial X_{57}}{\partial c_j} + \frac{\partial X_{58}}{\partial c_j} + \frac{\partial X_{59}}{\partial c_j} + \frac{\partial X_{60}}{\partial c_j} + \frac{\partial X_{61}}{\partial c_j}$$

$$- \frac{\partial X_{62}}{\partial c_j} - 2\frac{\partial X_{63}}{\partial c_j} - \frac{\partial X_{67}}{\partial c_j} - \frac{\partial X_{70}}{\partial c_j} - \frac{\partial X_{73}}{\partial c_j} - \frac{\partial X_{78}}{\partial c_j} - \frac{\partial X_{80}}{\partial c_j}$$

$$\left. - \frac{\partial X_{90}}{\partial c_j} - \frac{\partial X_{95}}{\partial c_j} - \frac{\partial X_{97}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{20,73} = -\frac{1}{V} f_{20}$$

$$\beta_{20,74} = \frac{1}{\rho} f_{20} - \overline{K}_{20}\left[\frac{\partial X_{40}}{\partial \rho} - \frac{\partial X_{41}}{\partial \rho} - \frac{\partial X_{44}}{\partial \rho} - \frac{\partial X_{48}}{\partial \rho}\right]$$

$$\beta_{20,75} = -\overline{K}_{20}\left[\frac{\partial X_{40}}{\partial T} - \frac{\partial X_{41}}{\partial T} - \frac{\partial X_{44}}{\partial T} - \frac{\partial X_{48}}{\partial T} - \frac{\partial X_{50}}{\partial T} - \frac{\partial X_{51}}{\partial T} - \frac{\partial X_{52}}{\partial T}\right.$$

$$- \frac{\partial X_{53}}{\partial T} - \frac{\partial X_{55}}{\partial T} + \frac{\partial X_{57}}{\partial T} + \frac{\partial X_{58}}{\partial T} + \frac{\partial X_{59}}{\partial T} + \frac{\partial X_{60}}{\partial T} + \frac{\partial X_{61}}{\partial T}$$

$$- \frac{\partial X_{62}}{\partial T} - 2\frac{\partial X_{63}}{\partial T} - \frac{\partial X_{67}}{\partial T} - \frac{\partial X_{70}}{\partial T} - \frac{\partial X_{73}}{\partial T} - \frac{\partial X_{78}}{\partial T} - \frac{\partial X_{80}}{\partial T}$$

$$\left.- \frac{\partial X_{90}}{\partial T} - \frac{\partial X_{95}}{\partial T} - \frac{\partial X_{97}}{\partial T}\right]$$

For Al_2O

$$\overline{K}_{21} = \frac{69.960\rho r^*}{V}$$

$$f_{21} = -\overline{K}_{21}\left[X_{41} - X_{54} - X_{56} - X_{60} + X_{62} + X_{63} - X_{72}\right]$$

$$\beta_{21,j} = -\overline{K}_{21}\left[\frac{\partial X_{41}}{\partial c_j} - \frac{\partial X_{54}}{\partial c_j} - \frac{\partial X_{56}}{\partial c_j} - \frac{\partial X_{60}}{\partial c_j} + \frac{\partial X_{62}}{\partial c_j} + \frac{\partial X_{63}}{\partial c_j} - \frac{\partial X_{72}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{21,73} = -\frac{1}{V} f_{21}$$

$$\beta_{21,74} = \frac{1}{\rho} f_{21} - \overline{K}_{21} \frac{\partial X_{41}}{\partial \rho}$$

$$\beta_{21,75} = -\overline{K}_{21}\left[\frac{\partial X_{41}}{\partial T} - \frac{\partial X_{54}}{\partial T} - \frac{\partial X_{56}}{\partial T} - \frac{\partial X_{60}}{\partial T} + \frac{\partial X_{62}}{\partial T} + \frac{\partial X_{63}}{\partial T} - \frac{\partial X_{72}}{\partial c_j}\right]$$

For AlCl

$$\overline{K}_{22} = \frac{62.437\rho r^*}{V}$$

$$f_{22} = -\overline{K}_{22}\Big[X_{42} - X_{43} - X_{45} - X_{55} - X_{62} + X_{64} + X_{65} + X_{66} + X_{67} + X_{68} + X_{69} + X_{70} + 2X_{71} + X_{72} + X_{73} + X_{74} - X_{75} - X_{76} - X_{81} - X_{82} - X_{84} - X_{87}\Big]$$

$$\beta_{22,j} = -\overline{K}_{22}\left[\frac{\partial X_{42}}{\partial c_j} - \frac{\partial X_{43}}{\partial c_j} - \frac{\partial X_{45}}{\partial c_j} - \frac{\partial X_{55}}{\partial c_j} - \frac{\partial X_{62}}{\partial c_j} + \frac{\partial X_{64}}{\partial c_j} + \frac{\partial X_{65}}{\partial c_j} + \frac{\partial X_{66}}{\partial c_j} + \frac{\partial X_{67}}{\partial c_j} + \frac{\partial X_{68}}{\partial c_j} + \frac{\partial X_{69}}{\partial c_j} + \frac{\partial X_{70}}{\partial c_j} + 2\frac{\partial X_{71}}{\partial c_j} + \frac{\partial X_{72}}{\partial c_j} + \frac{\partial X_{73}}{\partial c_j} + \frac{\partial X_{74}}{\partial c_j} - \frac{\partial X_{75}}{\partial c_j} - \frac{\partial X_{76}}{\partial c_j} - \frac{\partial X_{81}}{\partial c_j} - \frac{\partial X_{82}}{\partial c_j} - \frac{\partial X_{84}}{\partial c_j} - \frac{\partial X_{87}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{22,73} = -\frac{1}{V} f_{22}$$

$$\beta_{22,74} = \frac{1}{\rho} f_{22} - \overline{K}_{22}\left[\frac{\partial X_{42}}{\partial \rho} - \frac{\partial X_{43}}{\partial \rho} - \frac{\partial X_{45}}{\partial \rho}\right]$$

$$\beta_{22,75} = -\overline{K}_{22}\left[\frac{\partial X_{42}}{\partial T} - \frac{\partial X_{43}}{\partial T} - \frac{\partial X_{45}}{\partial T} - \frac{\partial X_{55}}{\partial T} - \frac{\partial X_{62}}{\partial T} + \frac{\partial X_{64}}{\partial T} + \frac{\partial X_{65}}{\partial T} + \frac{\partial X_{66}}{\partial T} + \frac{\partial X_{67}}{\partial T} + \frac{\partial X_{68}}{\partial T} + \frac{\partial X_{69}}{\partial T} + \frac{\partial X_{70}}{\partial T} + 2\frac{\partial X_{71}}{\partial T} + \frac{\partial X_{72}}{\partial T} + \frac{\partial X_{73}}{\partial T} + \frac{\partial X_{74}}{\partial T} - \frac{\partial X_{75}}{\partial T} - \frac{\partial X_{76}}{\partial T} - \frac{\partial X_{81}}{\partial T} - \frac{\partial X_{82}}{\partial T} - \frac{\partial X_{84}}{\partial T} - \frac{\partial X_{87}}{\partial T}\right]$$

For $AlCl_2$

$$\overline{K}_{23} = \frac{97.894\rho r^*}{V}$$

$$f_{23} = -\overline{K}_{23}\left[X_{43} - X_{65} - X_{71} - X_{73} + X_{75} - X_{77} - X_{79}\right]$$

$$\beta_{23,j} = -\overline{K}_{23}\left[\frac{\partial X_{43}}{\partial c_j} - \frac{\partial X_{65}}{\partial c_j} - \frac{\partial X_{71}}{\partial c_j} - \frac{\partial X_{73}}{\partial c_j} + \frac{\partial X_{75}}{\partial c_j} - \frac{\partial X_{77}}{\partial c_j} - \frac{\partial X_{79}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{23,73} = -\frac{1}{V} f_{23}$$

$$\beta_{23,74} = \frac{1}{\rho} f_{23} - \overline{K}_{23} \frac{\partial X_{43}}{\partial \rho}$$

$$\beta_{23,75} = -\overline{K}_{23}\left[\frac{\partial X_{43}}{\partial T} - \frac{\partial X_{65}}{\partial T} - \frac{\partial X_{71}}{\partial T} - \frac{\partial X_{73}}{\partial T} + \frac{\partial X_{75}}{\partial T} - \frac{\partial X_{77}}{\partial T} - \frac{\partial X_{79}}{\partial T}\right]$$

For AlOCl

$$\overline{K}_{24} = \frac{78.437\rho r^*}{V}$$

$$f_{24} = -\overline{K}_{24}\left[X_{44} - X_{64} - X_{66} - X_{74} + X_{76} + X_{77} + X_{78} + X_{79} + X_{80} + X_{81} + X_{82} - X_{92} - X_{94}\right]$$

$$\beta_{24,j} = -\overline{K}_{24}\left[\frac{\partial X_{44}}{\partial c_j} - \frac{\partial X_{64}}{\partial c_j} - \frac{\partial X_{66}}{\partial c_j} - \frac{\partial X_{74}}{\partial c_j} + \frac{\partial X_{76}}{\partial c_j} + \frac{\partial X_{77}}{\partial c_j} + \frac{\partial X_{78}}{\partial c_j} + \frac{\partial X_{79}}{\partial c_j} + \frac{\partial X_{80}}{\partial c_j} + \frac{\partial X_{81}}{\partial c_j} + \frac{\partial X_{82}}{\partial c_j} - \frac{\partial X_{92}}{\partial c_j} - \frac{\partial X_{94}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{24,73} = -\frac{1}{V} f_{24}$$

$$\beta_{24,74} = \frac{1}{\rho} f_{24} - \overline{K}_{24} \frac{\partial X_{44}}{\partial \rho}$$

$$\beta_{24,75} = -\overline{K}_{24}\left[\frac{\partial X_{44}}{\partial T} - \frac{\partial X_{64}}{\partial T} - \frac{\partial X_{66}}{\partial T} - \frac{\partial X_{74}}{\partial T} + \frac{\partial X_{76}}{\partial T} + \frac{\partial X_{77}}{\partial T} + \frac{\partial X_{78}}{\partial T}\right.$$

$$\left. + \frac{\partial X_{79}}{\partial T} + \frac{\partial X_{80}}{\partial T} + \frac{\partial X_{81}}{\partial T} + \frac{\partial X_{82}}{\partial T} - \frac{\partial X_{92}}{\partial T} - \frac{\partial X_{94}}{\partial T}\right]$$

For AlF

$$\overline{K}_{25} = \frac{45.980\rho r^*}{V}$$

$$f_{25} = -\overline{K}_{25}\left[X_{46} - X_{47} - X_{49} - X_{57} - X_{58} - X_{74} + 2X_{83} + X_{84} + X_{85}\right.$$

$$\left. + X_{86} + X_{87} + X_{88} + X_{89} + X_{90} - X_{91} - X_{98} - X_{99}\right]$$

$$\beta_{25,j} = -\overline{K}_{25}\left[\frac{\partial X_{46}}{\partial c_j} - \frac{\partial X_{47}}{\partial c_j} - \frac{\partial X_{49}}{\partial c_j} - \frac{\partial X_{57}}{\partial c_j} - \frac{\partial X_{58}}{\partial c_j} - \frac{\partial X_{74}}{\partial c_j} + 2\frac{\partial X_{83}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{84}}{\partial c_j} + \frac{\partial X_{85}}{\partial c_j} + \frac{\partial X_{86}}{\partial c_j} + \frac{\partial X_{87}}{\partial c_j} + \frac{\partial X_{88}}{\partial c_j} + \frac{\partial X_{89}}{\partial c_j} + \frac{\partial X_{90}}{\partial c_j}$$

$$\left. - \frac{\partial X_{91}}{\partial c_j} - \frac{\partial X_{98}}{\partial c_j} - \frac{\partial X_{99}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{25,73} = -\frac{1}{V} f_{25}$$

$$\beta_{25,74} = \frac{1}{\rho} f_{25} - \overline{K}_{25}\left[\frac{\partial X_{46}}{\partial \rho} - \frac{\partial X_{47}}{\partial \rho} - \frac{\partial X_{49}}{\partial \rho}\right]$$

$$\beta_{25,75} = -\overline{K}_{25}\left[\frac{\partial X_{46}}{\partial T} - \frac{\partial X_{47}}{\partial T} - \frac{\partial X_{49}}{\partial T} - \frac{\partial X_{57}}{\partial T} - \frac{\partial X_{58}}{\partial T} - \frac{\partial X_{74}}{\partial T} + 2\frac{\partial X_{83}}{\partial T}\right.$$

$$+ \frac{\partial X_{84}}{\partial T} + \frac{\partial X_{85}}{\partial T} + \frac{\partial X_{86}}{\partial T} + \frac{\partial X_{87}}{\partial T} + \frac{\partial X_{88}}{\partial T} + \frac{\partial X_{89}}{\partial T} + \frac{\partial X_{90}}{\partial T}$$

$$\left. - \frac{\partial X_{91}}{\partial T} - \frac{\partial X_{98}}{\partial T} - \frac{\partial X_{99}}{\partial T}\right]$$

For AlF_2

$$\overline{K}_{26} = \frac{64.980\rho r^*}{V}$$

$$f_{26} = -\overline{K}_{26}\left[X_{47} - X_{83} - X_{85} - X_{90} + X_{91} - X_{93} - X_{96}\right]$$

$$\beta_{26,j} = -\overline{K}_{26}\left[\frac{\partial X_{47}}{\partial c_j} - \frac{\partial X_{83}}{\partial c_j} - \frac{\partial X_{85}}{\partial c_j} - \frac{\partial X_{90}}{\partial c_j} + \frac{\partial X_{91}}{\partial c_j} - \frac{\partial X_{93}}{\partial c_j} - \frac{\partial X_{96}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{26,73} = -\frac{1}{V} f_{26}$$

$$\beta_{26,74} = \frac{1}{\rho} f_{26} - \overline{K}_{26} \frac{\partial X_{47}}{\partial \rho}$$

$$\beta_{26,75} = \overline{K}_{26}\left[\frac{\partial X_{47}}{\partial T} - \frac{\partial X_{83}}{\partial T} - \frac{\partial X_{85}}{\partial T} - \frac{\partial X_{90}}{\partial T} + \frac{\partial X_{91}}{\partial T} - \frac{\partial X_{93}}{\partial T} - \frac{\partial X_{96}}{\partial T}\right]$$

For AlOF

$$\overline{K}_{27} = \frac{61.980\rho r^*}{V}$$

$$f_{27} = -\overline{K}_{27}\left[X_{48} + X_{56} - X_{61} + X_{74} - X_{86} + X_{90} + X_{92} + X_{93} + X_{94} + X_{95} + X_{96} + X_{97} + X_{98} + X_{99}\right]$$

$$\beta_{27,j} = -\overline{K}_{27}\left[\frac{\partial X_{48}}{\partial c_j} + \frac{\partial X_{56}}{\partial c_j} - \frac{\partial X_{61}}{\partial c_j} + \frac{\partial X_{74}}{\partial c_j} - \frac{\partial X_{86}}{\partial c_j} + \frac{\partial X_{90}}{\partial c_j} + \frac{\partial X_{92}}{\partial c_j} + \frac{\partial X_{93}}{\partial c_j} + \frac{\partial X_{94}}{\partial c_j} + \frac{\partial X_{95}}{\partial c_j} + \frac{\partial X_{96}}{\partial c_j} + \frac{\partial X_{97}}{\partial c_j} + \frac{\partial X_{98}}{\partial c_j} + \frac{\partial X_{99}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{27,73} = -\frac{1}{V} f_{27}$$

$$\beta_{27,74} = \frac{1}{\rho} f_{27} - \overline{K}_{27} \frac{\partial X_{48}}{\partial \rho}$$

$$\beta_{27,75} = -\overline{K}_{27}\left[\frac{\partial X_{48}}{\partial T} + \frac{\partial X_{56}}{\partial T} - \frac{\partial X_{61}}{\partial T} + \frac{\partial X_{74}}{\partial T} - \frac{\partial X_{86}}{\partial T} + \frac{\partial X_{90}}{\partial T} + \frac{\partial X_{92}}{\partial T} + \frac{\partial X_{93}}{\partial T} + \frac{\partial X_{94}}{\partial T} + \frac{\partial X_{95}}{\partial T} + \frac{\partial X_{96}}{\partial T} + \frac{\partial X_{97}}{\partial T} + \frac{\partial X_{98}}{\partial T} + \frac{\partial X_{99}}{\partial T}\right]$$

For B

$$\overline{K}_{28} = \frac{10.820\rho r^*}{V}$$

$$f_{28} = \overline{K}_{28}\left[X_{148} + X_{149} + X_{151} + X_{155} - X_{160} - X_{161} - X_{162} + X_{164} + X_{166} + X_{172} + X_{175} + X_{177} + X_{178} + X_{180} + X_{187} + X_{188} + X_{189} + X_{202} + X_{208} + X_{209} + X_{211}\right]$$

$$\beta_{28,j} = \overline{K}_{28}\left[\frac{\partial X_{148}}{\partial c_j} + \frac{\partial X_{149}}{\partial c_j} + \frac{\partial X_{151}}{\partial c_j} + \frac{\partial X_{155}}{\partial c_j} - \frac{\partial X_{160}}{\partial c_j} - \frac{\partial X_{161}}{\partial c_j} - \frac{\partial X_{162}}{\partial c_j} + \frac{\partial X_{164}}{\partial c_j} + \frac{\partial X_{166}}{\partial c_j} + \frac{\partial X_{172}}{\partial c_j} + \frac{\partial X_{175}}{\partial c_j} + \frac{\partial X_{177}}{\partial c_j} + \frac{\partial X_{178}}{\partial c_j} + \frac{\partial X_{180}}{\partial c_j} + \frac{\partial X_{187}}{\partial c_j} + \frac{\partial X_{188}}{\partial c_j} + \frac{\partial X_{189}}{\partial c_j} + \frac{\partial X_{202}}{\partial c_j} + \frac{\partial X_{208}}{\partial c_j} + \frac{\partial X_{209}}{\partial c_j} + \frac{\partial X_{211}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{28,73} = -\frac{1}{V} f_{28}$$

$$\beta_{28,74} = \frac{1}{\rho} f_{28} + \overline{K}_{28}\left[\frac{\partial X_{148}}{\partial \rho} + \frac{\partial X_{149}}{\partial \rho} + \frac{\partial X_{151}}{\partial \rho} + \frac{\partial X_{155}}{\partial \rho}\right]$$

$$\beta_{28,75} = \overline{K}_{28}\left[\frac{\partial X_{148}}{\partial T} + \frac{\partial X_{149}}{\partial T} + \frac{\partial X_{151}}{\partial T} + \frac{\partial X_{155}}{\partial T} - \frac{\partial X_{160}}{\partial T} - \frac{\partial X_{161}}{\partial T} - \frac{\partial X_{162}}{\partial T} + \frac{\partial X_{164}}{\partial T} + \frac{\partial X_{166}}{\partial T} + \frac{\partial X_{172}}{\partial T} + \frac{\partial X_{175}}{\partial T} + \frac{\partial X_{177}}{\partial T} + \frac{\partial X_{178}}{\partial T} + \frac{\partial X_{180}}{\partial T} + \frac{\partial X_{187}}{\partial T} + \frac{\partial X_{188}}{\partial T} + \frac{\partial X_{189}}{\partial T} + \frac{\partial X_{202}}{\partial T} + \frac{\partial X_{208}}{\partial T} + \frac{\partial X_{209}}{\partial T} + \frac{\partial X_{211}}{\partial T}\right]$$

For BN

$$\overline{K}_{29} = \frac{24.828\rho r^*}{V}$$

$$f_{29} = -\overline{K}_{29}\left[X_{148} - X_{160} - X_{161} + X_{163} - X_{170} - X_{176} - X_{190} - X_{210}\right]$$

$$\beta_{29,j} = -\overline{K}_{29}\left[\frac{\partial X_{148}}{\partial c_j} - \frac{\partial X_{160}}{\partial c_j} - \frac{\partial X_{161}}{\partial c_j} + \frac{\partial X_{163}}{\partial c_j} - \frac{\partial X_{170}}{\partial c_j} - \frac{\partial X_{176}}{\partial c_j} - \frac{\partial X_{190}}{\partial c_j} - \frac{\partial X_{210}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{29,73} = -\frac{1}{V} f_{29}$$

$$\beta_{29,74} = \frac{1}{\rho} f_{29} - \overline{K}_{29}\left[\frac{\partial X_{148}}{\partial \rho}\right]$$

$$\beta_{29,75} = -\overline{K}_{29}\left[\frac{\partial X_{148}}{\partial T} - \frac{\partial X_{160}}{\partial T} - \frac{\partial X_{161}}{\partial T} + \frac{\partial X_{163}}{\partial T} - \frac{\partial X_{170}}{\partial T} - \frac{\partial X_{176}}{\partial T} - \frac{\partial X_{190}}{\partial T} - \frac{\partial X_{210}}{\partial T}\right]$$

For BO

$$\overline{K}_{30} = \frac{26.820\rho r^*}{V}$$

$$f_{30} = -\overline{K}_{30}\left[X_{149} - X_{150} - X_{158} - X_{162} - X_{163} + 2X_{164} + X_{165} + X_{166} + X_{167} + X_{168} + X_{169} + X_{170} + X_{171} + X_{172} + X_{173} + X_{174} + X_{175} + X_{176} + X_{177} + X_{178} + X_{179} + X_{180} + X_{181} + X_{182} - X_{185} - X_{186} - X_{196} - X_{198} - X_{212} - X_{220} - X_{222}\right]$$

$$\beta_{30,j} = -\bar{K}_{30}\left[\frac{\partial X_{149}}{\partial c_j} - \frac{\partial X_{150}}{\partial c_j} - \frac{\partial X_{158}}{\partial c_j} - \frac{\partial X_{162}}{\partial c_j} - \frac{\partial X_{163}}{\partial c_j} + 2\frac{\partial X_{164}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{165}}{\partial c_j} + \frac{\partial X_{166}}{\partial c_j} + \frac{\partial X_{167}}{\partial c_j} + \frac{\partial X_{168}}{\partial c_j} + \frac{\partial X_{169}}{\partial c_j} + \frac{\partial X_{170}}{\partial c_j}$$

$$+ \frac{\partial X_{171}}{\partial c_j} + \frac{\partial X_{172}}{\partial c_j} + \frac{\partial X_{173}}{\partial c_j} + \frac{\partial X_{174}}{\partial c_j} + \frac{\partial X_{175}}{\partial c_j} + \frac{\partial X_{176}}{\partial c_j}$$

$$+ \frac{\partial X_{177}}{\partial c_j} + \frac{\partial X_{178}}{\partial c_j} + \frac{\partial X_{179}}{\partial c_j} + \frac{\partial X_{180}}{\partial c_j} + \frac{\partial X_{181}}{\partial c_j} + \frac{\partial X_{182}}{\partial c_j}$$

$$- \frac{\partial X_{185}}{\partial c_j} - \frac{\partial X_{186}}{\partial c_j} - \frac{\partial X_{196}}{\partial c_j} - \frac{\partial X_{198}}{\partial c_j} - \frac{\partial X_{212}}{\partial c_j} - \frac{\partial X_{220}}{\partial c_j}$$

$$\left.- \frac{\partial X_{222}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{30,73} = -\frac{1}{V} f_{30}$$

$$\beta_{30,74} = \frac{1}{\rho} f_{30} - \bar{K}_{30}\left[\frac{\partial X_{149}}{\partial \rho} - \frac{\partial X_{150}}{\partial \rho} - \frac{\partial X_{158}}{\partial \rho}\right]$$

$$\beta_{30,75} = -\bar{K}_{30}\left[\frac{\partial X_{149}}{\partial T} - \frac{\partial X_{150}}{\partial T} - \frac{\partial X_{158}}{\partial T} - \frac{\partial X_{162}}{\partial T} - \frac{\partial X_{163}}{\partial T} + 2\frac{\partial X_{164}}{\partial T}\right.$$

$$+ \frac{\partial X_{165}}{\partial T} + \frac{\partial X_{166}}{\partial T} + \frac{\partial X_{167}}{\partial T} + \frac{\partial X_{168}}{\partial T} + \frac{\partial X_{169}}{\partial T} + \frac{\partial X_{170}}{\partial T}$$

$$+ \frac{\partial X_{171}}{\partial T} + \frac{\partial X_{172}}{\partial T} + \frac{\partial X_{173}}{\partial T} + \frac{\partial X_{174}}{\partial T} + \frac{\partial X_{175}}{\partial T} + \frac{\partial X_{176}}{\partial T}$$

$$+ \frac{\partial X_{177}}{\partial T} + \frac{\partial X_{178}}{\partial T} + \frac{\partial X_{179}}{\partial T} + \frac{\partial X_{180}}{\partial T} + \frac{\partial X_{181}}{\partial T} + \frac{\partial X_{182}}{\partial T}$$

$$- \frac{\partial X_{185}}{\partial T} - \frac{\partial X_{186}}{\partial T} - \frac{\partial X_{196}}{\partial T} - \frac{\partial X_{198}}{\partial T} - \frac{\partial X_{212}}{\partial T} - \frac{\partial X_{220}}{\partial T}$$

$$\left.- \frac{\partial X_{222}}{\partial T}\right]$$

For BO_2

$$\overline{K}_{31} = \frac{42.820\rho r^*}{V}$$

$$f_{31} = -\overline{K}_{31}\left[X_{150} - X_{164} - X_{165} - X_{167} - X_{171} - X_{179} - X_{182} + X_{183} + X_{184} + X_{185} + X_{186} - X_{195} - X_{216} - X_{224}\right]$$

$$\beta_{31,j} = -\overline{K}_{31}\left[\frac{\partial X_{150}}{\partial c_j} - \frac{\partial X_{164}}{\partial c_j} - \frac{\partial X_{165}}{\partial c_j} - \frac{\partial X_{167}}{\partial c_j} - \frac{\partial X_{171}}{\partial c_j} - \frac{\partial X_{179}}{\partial c_j} - \frac{\partial X_{182}}{\partial c_j} + \frac{\partial X_{183}}{\partial c_j} + \frac{\partial X_{184}}{\partial c_j} + \frac{\partial X_{185}}{\partial c_j} + \frac{\partial X_{186}}{\partial c_j} - \frac{\partial X_{195}}{\partial c_j} - \frac{\partial X_{216}}{\partial c_j} - \frac{\partial X_{224}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{31,73} = -\frac{1}{V} f_{31}$$

$$\beta_{31,74} = \frac{1}{\rho} f_{31} - \overline{K}_{31} \frac{\partial X_{150}}{\partial \rho}$$

$$\beta_{31,75} = -\overline{K}_{31}\left[\frac{\partial X_{150}}{\partial T} - \frac{\partial X_{164}}{\partial T} - \frac{\partial X_{165}}{\partial T} - \frac{\partial X_{167}}{\partial T} - \frac{\partial X_{171}}{\partial T} - \frac{\partial X_{179}}{\partial T} - \frac{\partial X_{182}}{\partial T} + \frac{\partial X_{183}}{\partial T} + \frac{\partial X_{184}}{\partial T} + \frac{\partial X_{185}}{\partial T} + \frac{\partial X_{186}}{\partial T} - \frac{\partial X_{195}}{\partial T} - \frac{\partial X_{216}}{\partial T} - \frac{\partial X_{224}}{\partial T}\right]$$

For BCl

$$\overline{K}_{32} = \frac{46.277\rho r^*}{V}$$

$$f_{32} = -\overline{K}_{32}\left[X_{151} - X_{152} - X_{154} - X_{168} - X_{173} + X_{178} - X_{179} + 2X_{187} + X_{188} + X_{189} + X_{190} + X_{191} - X_{192} - X_{199} - X_{200} - X_{201} - X_{205} - X_{207}\right]$$

$$\beta_{32,j} = -\overline{K}_{32}\left[\frac{\partial X_{151}}{\partial c_j} - \frac{\partial X_{152}}{\partial c_j} - \frac{\partial X_{154}}{\partial c_j} - \frac{\partial X_{168}}{\partial c_j} - \frac{\partial X_{173}}{\partial c_j} + \frac{\partial X_{178}}{\partial c_j} - \frac{\partial X_{179}}{\partial c_j} + 2\frac{\partial X_{187}}{\partial c_j} + \frac{\partial X_{188}}{\partial c_j} + \frac{\partial X_{189}}{\partial c_j} + \frac{\partial X_{190}}{\partial c_j} + \frac{\partial X_{191}}{\partial c_j} - \frac{\partial X_{192}}{\partial c_j} - \frac{\partial X_{199}}{\partial c_j} - \frac{\partial X_{200}}{\partial c_j} - \frac{\partial X_{201}}{\partial c_j} - \frac{\partial X_{205}}{\partial c_j} - \frac{\partial X_{207}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{32,73} = -\frac{1}{V} f_{32}$$

$$\beta_{32,74} = \frac{1}{\rho} f_{32} - \overline{K}_{32}\left[\frac{\partial X_{148}}{\partial \rho} - \frac{\partial X_{149}}{\partial \rho} - \frac{\partial X_{151}}{\partial \rho}\right]$$

$$\beta_{32,75} = -\overline{K}_{32}\left[\frac{\partial X_{151}}{\partial T} - \frac{\partial X_{152}}{\partial T} - \frac{\partial X_{154}}{\partial T} - \frac{\partial X_{168}}{\partial T} - \frac{\partial X_{173}}{\partial T} + \frac{\partial X_{178}}{\partial T} - \frac{\partial X_{179}}{\partial T}\right.$$

$$+ 2\frac{\partial X_{187}}{\partial T} + \frac{\partial X_{188}}{\partial T} + \frac{\partial X_{189}}{\partial T} + \frac{\partial X_{190}}{\partial T} + \frac{\partial X_{191}}{\partial T} - \frac{\partial X_{192}}{\partial T}$$

$$\left. - \frac{\partial X_{199}}{\partial T} - \frac{\partial X_{200}}{\partial T} - \frac{\partial X_{201}}{\partial T} - \frac{\partial X_{205}}{\partial T} - \frac{\partial X_{207}}{\partial T}\right]$$

For BCl_2

$$\overline{K}_{33} = \frac{81.734\rho r^*}{V}$$

$$f_{33} = -\overline{K}_{33}\left[X_{152} - X_{153} - X_{187} + X_{192} - X_{193} - X_{194} - X_{197}\right]$$

$$\beta_{33,j} = -\overline{K}_{33}\left[\frac{\partial X_{152}}{\partial c_j} - \frac{\partial X_{153}}{\partial c_j} - \frac{\partial X_{187}}{\partial c_j} + \frac{\partial X_{192}}{\partial c_j} - \frac{\partial X_{193}}{\partial c_j} - \frac{\partial X_{194}}{\partial c_j} - \frac{\partial X_{197}}{\partial c_j}\right]$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{33,73} = -\frac{1}{V} f_{33}$$

$$\beta_{33,74} = \frac{1}{\rho} f_{33} - \overline{K}_{33}\left[\frac{\partial X_{152}}{\partial \rho} - \frac{\partial X_{153}}{\partial \rho}\right]$$

$$\beta_{33,75} = -\overline{K}_{33}\left[\frac{\partial X_{152}}{\partial T} - \frac{\partial X_{153}}{\partial T} - \frac{\partial X_{187}}{\partial T} + \frac{\partial X_{192}}{\partial T} - \frac{\partial X_{193}}{\partial T} - \frac{\partial X_{194}}{\partial T} - \frac{\partial X_{197}}{\partial T}\right]$$

For BCl_3

$$\overline{K}_{34} = \frac{117.191\rho r^*}{V}$$

$$f_{34} = -\overline{K}_{34}\left[X_{153} + X_{193}\right]$$

$$\beta_{34,j} = -\overline{K}_{34}\left[\frac{\partial X_{153}}{\partial c_j} + \frac{\partial X_{193}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{34,73} = -\frac{1}{V} f_{34}$$

$$\beta_{34,74} = \frac{1}{\rho} f_{34} - \overline{K}_{34} \frac{\partial X_{153}}{\partial \rho}$$

$$\beta_{34,75} = -\overline{K}_{34}\left[\frac{\partial X_{153}}{\partial T} + \frac{\partial X_{193}}{\partial T}\right]$$

For BOCl

$$\overline{K}_{35} = \frac{62.277\rho r^*}{V}$$

$$f_{35} = -\overline{K}_{35}\left[X_{154} - X_{178} + X_{179} - X_{184} - X_{191} + X_{194} + X_{195} + X_{196} + X_{197} + X_{198} + X_{199} + X_{200} + X_{201} - X_{217} - X_{219}\right]$$

$$\beta_{35,j} = -\overline{K}_{35}\left[\frac{\partial X_{154}}{\partial c_j} - \frac{\partial X_{178}}{\partial c_j} + \frac{\partial X_{179}}{\partial c_j} - \frac{\partial X_{184}}{\partial c_j} - \frac{\partial X_{191}}{\partial c_j} + \frac{\partial X_{194}}{\partial c_j} + \frac{\partial X_{195}}{\partial c_j} + \frac{\partial X_{196}}{\partial c_j} + \frac{\partial X_{197}}{\partial c_j} + \frac{\partial X_{198}}{\partial c_j} + \frac{\partial X_{199}}{\partial c_j} + \frac{\partial X_{200}}{\partial c_j} + \frac{\partial X_{201}}{\partial c_j} - \frac{\partial X_{217}}{\partial c_j} - \frac{\partial X_{219}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{35,73} = -\frac{1}{V} f_{35}$$

$$\beta_{35,74} = \frac{1}{\rho} f_{35} - \overline{K}_{35} \frac{\partial X_{154}}{\partial \rho}$$

$$\beta_{35,75} = -\overline{K}_{35}\left[\frac{\partial X_{154}}{\partial T} - \frac{\partial X_{178}}{\partial T} + \frac{\partial X_{179}}{\partial T} - \frac{\partial X_{184}}{\partial T} - \frac{\partial X_{191}}{\partial T} + \frac{\partial X_{194}}{\partial T} + \frac{\partial X_{195}}{\partial T} + \frac{\partial X_{196}}{\partial T} + \frac{\partial X_{197}}{\partial T} + \frac{\partial X_{198}}{\partial T} + \frac{\partial X_{199}}{\partial T} + \frac{\partial X_{200}}{\partial T} + \frac{\partial X_{201}}{\partial T} - \frac{\partial X_{217}}{\partial T} - \frac{\partial X_{219}}{\partial T}\right]$$

For BF

$$\overline{K}_{36} = \frac{29.820\rho r^*}{V}$$

$$f_{36} = -\overline{K}_{36}\left[X_{155} - X_{156} - X_{159} - X_{169} - X_{174} + X_{180} - X_{182} - X_{191} + 2X_{202} + X_{203} + X_{204} + X_{205} + X_{206} + X_{207} + X_{208} + X_{209} + X_{210} + X_{211} + X_{212} - X_{213} - X_{223}\right]$$

$$\beta_{36,j} = -\overline{K}_{36}\left[\frac{\partial X_{155}}{\partial c_j} - \frac{\partial X_{156}}{\partial c_j} - \frac{\partial X_{159}}{\partial c_j} - \frac{\partial X_{169}}{\partial c_j} - \frac{\partial X_{174}}{\partial c_j} + \frac{\partial X_{180}}{\partial c_j} - \frac{\partial X_{182}}{\partial c_j} - \frac{\partial X_{191}}{\partial c_j} + 2\frac{\partial X_{202}}{\partial c_j} + \frac{\partial X_{203}}{\partial c_j} + \frac{\partial X_{204}}{\partial c_j} + \frac{\partial X_{205}}{\partial c_j} + \frac{\partial X_{206}}{\partial c_j} + \frac{\partial X_{207}}{\partial c_j} + \frac{\partial X_{208}}{\partial c_j} + \frac{\partial X_{209}}{\partial c_j} + \frac{\partial X_{210}}{\partial c_j} + \frac{\partial X_{211}}{\partial c_j} + \frac{\partial X_{212}}{\partial c_j} - \frac{\partial X_{213}}{\partial c_j} - \frac{\partial X_{223}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{36,73} = -\frac{1}{V} f_{36}$$

$$\beta_{36,74} = \frac{1}{\rho} f_{36} - \overline{K}_{36}\left[\frac{\partial X_{155}}{\partial \rho} - \frac{\partial X_{156}}{\partial \rho} - \frac{\partial X_{159}}{\partial \rho}\right]$$

$$\beta_{36,75} = -\overline{K}_{36}\left[\frac{\partial X_{155}}{\partial T} - \frac{\partial X_{156}}{\partial T} - \frac{\partial X_{159}}{\partial T} - \frac{\partial X_{169}}{\partial T} - \frac{\partial X_{174}}{\partial T} + \frac{\partial X_{181}}{\partial T} - \frac{\partial X_{182}}{\partial T}\right.$$

$$- \frac{\partial X_{191}}{\partial T} + 2\frac{\partial X_{202}}{\partial T} + \frac{\partial X_{203}}{\partial T} + \frac{\partial X_{204}}{\partial T} + \frac{\partial X_{205}}{\partial T} + \frac{\partial X_{206}}{\partial T}$$

$$+ \frac{\partial X_{207}}{\partial T} + \frac{\partial X_{208}}{\partial T} + \frac{\partial X_{209}}{\partial T} + \frac{\partial X_{210}}{\partial T} + \frac{\partial X_{211}}{\partial T} + \frac{\partial X_{212}}{\partial T}$$

$$\left. - \frac{\partial X_{213}}{\partial T} - \frac{\partial X_{223}}{\partial T}\right]$$

For BF_2

$$\overline{K}_{37} = \frac{48.820\rho r^*}{V}$$

$$f_{37} = -\overline{K}_{37}\left[X_{156} - X_{157} - X_{181} - X_{202} - X_{206} + X_{211} - X_{212}\right.$$

$$\left. + X_{213} - X_{214} - X_{215} - X_{216} - X_{218} - X_{221}\right]$$

$$\beta_{37,j} = -\overline{K}_{37}\left[\frac{\partial X_{156}}{\partial c_j} - \frac{\partial X_{157}}{\partial c_j} - \frac{\partial X_{181}}{\partial c_j} - \frac{\partial X_{202}}{\partial c_j} - \frac{\partial X_{206}}{\partial c_j} + \frac{\partial X_{211}}{\partial c_j} - \frac{\partial X_{212}}{\partial c_j}\right.$$

$$\left. + \frac{\partial X_{213}}{\partial c_j} - \frac{\partial X_{214}}{\partial c_j} - \frac{\partial X_{215}}{\partial c_j} - \frac{\partial X_{216}}{\partial c_j} - \frac{\partial X_{218}}{\partial c_j} - \frac{\partial X_{221}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{37,73} = -\frac{1}{V} f_{37}$$

$$\beta_{37,74} = \frac{1}{\rho} f_{37} - \overline{K}_{37}\left[\frac{\partial X_{156}}{\partial \rho} - \frac{\partial X_{157}}{\partial \rho}\right]$$

$$\beta_{37,75} = -\overline{K}_{37}\left[\frac{\partial X_{156}}{\partial T} - \frac{\partial X_{157}}{\partial T} - \frac{\partial X_{181}}{\partial T} - \frac{\partial X_{202}}{\partial T} - \frac{\partial X_{206}}{\partial T} + \frac{\partial X_{211}}{\partial T}\right.$$

$$- \frac{\partial X_{212}}{\partial T} + \frac{\partial X_{213}}{\partial T} - \frac{\partial X_{214}}{\partial T} - \frac{\partial X_{215}}{\partial T} - \frac{\partial X_{216}}{\partial T} - \frac{\partial X_{218}}{\partial T}$$

$$\left. - \frac{\partial X_{221}}{\partial T}\right]$$

For BF_3

$$\overline{K}_{38} = \frac{67.820\rho r^*}{V}$$

$$f_{38} = -\overline{K}_{38}\left[X_{157} + X_{181} - X_{211} + X_{214} + X_{215}\right]$$

$$\beta_{38,j} = -\overline{K}_{38}\left[\frac{\partial X_{157}}{\partial c_j} + \frac{\partial X_{181}}{\partial c_j} - \frac{\partial X_{211}}{\partial c_j} + \frac{\partial X_{214}}{\partial c_j} + \frac{\partial X_{215}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{38,73} = -\frac{1}{V} f_{38}$$

$$\beta_{38,74} = \frac{1}{\rho} f_{38} - \overline{K}_{38} \frac{\partial X_{157}}{\partial \rho}$$

$$\beta_{38,75} = -\overline{K}_{38}\left[\frac{\partial X_{157}}{\partial T} + \frac{\partial X_{181}}{\partial T} - \frac{\partial X_{211}}{\partial T} + \frac{\partial X_{214}}{\partial T} + \frac{\partial X_{215}}{\partial T}\right]$$

For BOF

$$\overline{K}_{39} = \frac{45.820\rho r^*}{V}$$

$$f_{39} = -\overline{K}_{39}\left[X_{158} + X_{159} - X_{180} - X_{181} + X_{182} - X_{183} + X_{191} - X_{203} - X_{204} + X_{212} + 2X_{216} + X_{217} + X_{218} + X_{219} + X_{220} + X_{221} + X_{222} + X_{223} + X_{224}\right]$$

$$\beta_{39,j} = -\overline{K}_{39}\left[\frac{\partial X_{158}}{\partial c_j} + \frac{\partial X_{159}}{\partial c_j} - \frac{\partial X_{180}}{\partial c_j} - \frac{\partial X_{181}}{\partial c_j} + \frac{\partial X_{182}}{\partial c_j} - \frac{\partial X_{183}}{\partial c_j} + \frac{\partial X_{191}}{\partial c_j} - \frac{\partial X_{203}}{\partial c_j} - \frac{\partial X_{204}}{\partial c_j} + \frac{\partial X_{212}}{\partial c_j} + 2\frac{\partial X_{216}}{\partial c_j} + \frac{\partial X_{217}}{\partial c_j} + \frac{\partial X_{218}}{\partial c_j} + \frac{\partial X_{219}}{\partial c_j} + \frac{\partial X_{220}}{\partial c_j} + \frac{\partial X_{221}}{\partial c_j} + \frac{\partial X_{222}}{\partial c_j} + \frac{\partial X_{223}}{\partial c_j} + \frac{\partial X_{224}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{39,73} = -\frac{1}{V} f_{39}$$

$$\beta_{39,74} = \frac{1}{\rho} f_{39} - \overline{K}_{39}\left[\frac{\partial X_{158}}{\partial \rho} + \frac{\partial X_{159}}{\partial \rho}\right]$$

$$\beta_{39,75} = -\overline{K}_{39}\left[\frac{\partial X_{158}}{\partial T} + \frac{\partial X_{159}}{\partial T} - \frac{\partial X_{180}}{\partial T} - \frac{\partial X_{181}}{\partial T} + \frac{\partial X_{182}}{\partial T} - \frac{\partial X_{183}}{\partial T}\right.$$
$$+ \frac{\partial X_{191}}{\partial T} - \frac{\partial X_{203}}{\partial T} - \frac{\partial X_{204}}{\partial T} + \frac{\partial X_{212}}{\partial T} + 2\frac{\partial X_{216}}{\partial T} + \frac{\partial X_{217}}{\partial T}$$
$$+ \frac{\partial X_{218}}{\partial T} + \frac{\partial X_{219}}{\partial T} + \frac{\partial X_{220}}{\partial T} + \frac{\partial X_{221}}{\partial T} + \frac{\partial X_{222}}{\partial T} + \frac{\partial X_{223}}{\partial T}$$
$$\left. + \frac{\partial X_{224}}{\partial T}\right]$$

For Be

$$\overline{K}_{40} = \frac{9.013 \rho r^*}{V}$$

$$f_{40} = \overline{K}_{40}\left[X_{102} + X_{104} + X_{105} + X_{106} + X_{107} - X_{109} + X_{111} + X_{114}\right.$$
$$+ X_{116} + X_{117} + X_{118} + X_{125} + X_{127} + X_{130} + X_{133}$$
$$\left. + X_{136} + X_{137} + X_{143} + X_{144}\right]$$

$$\beta_{40,j} = \overline{K}_{40}\left[\frac{\partial X_{102}}{\partial c_j} + \frac{\partial X_{104}}{\partial c_j} + \frac{\partial X_{105}}{\partial c_j} + \frac{\partial X_{106}}{\partial c_j} + \frac{\partial X_{107}}{\partial c_j} - \frac{\partial X_{109}}{\partial c_j} + \frac{\partial X_{111}}{\partial c_j}\right.$$
$$+ \frac{\partial X_{114}}{\partial c_j} + \frac{\partial X_{116}}{\partial c_j} + \frac{\partial X_{117}}{\partial c_j} + \frac{\partial X_{118}}{\partial c_j} + \frac{\partial X_{125}}{\partial c_j} + \frac{\partial X_{127}}{\partial c_j}$$
$$\left. + \frac{\partial X_{130}}{\partial c_j} + \frac{\partial X_{133}}{\partial c_j} + \frac{\partial X_{136}}{\partial c_j} + \frac{\partial X_{137}}{\partial c_j} + \frac{\partial X_{143}}{\partial c_j} + \frac{\partial X_{144}}{\partial c_j}\right]$$

$j = 1, 2, \cdots, 57$

$$\beta_{40,73} = -\frac{1}{V} f_{40}$$

$$\beta_{40,74} = \frac{1}{\rho} f_{40} + \overline{K}_{40}\left[\frac{\partial X_{102}}{\partial \rho} + \frac{\partial X_{104}}{\partial \rho} + \frac{\partial X_{105}}{\partial \rho} + \frac{\partial X_{106}}{\partial \rho} + \frac{\partial X_{107}}{\partial \rho}\right]$$

$$\beta_{40,75} = \overline{K}_{40}\left[\frac{\partial X_{102}}{\partial T} + \frac{\partial X_{104}}{\partial T} + \frac{\partial X_{105}}{\partial T} + \frac{\partial X_{106}}{\partial T} + \frac{\partial X_{107}}{\partial T} - \frac{\partial X_{109}}{\partial T}\right.$$

$$+ \frac{\partial X_{111}}{\partial T} + \frac{\partial X_{114}}{\partial T} + \frac{\partial X_{116}}{\partial T} + \frac{\partial X_{117}}{\partial T} + \frac{\partial X_{118}}{\partial T} + \frac{\partial X_{125}}{\partial T}$$

$$+ \frac{\partial X_{127}}{\partial T} + \frac{\partial X_{130}}{\partial T} + \frac{\partial X_{133}}{\partial T} + \frac{\partial X_{136}}{\partial T} + \frac{\partial X_{137}}{\partial T} + \frac{\partial X_{143}}{\partial T}$$

$$\left. + \frac{\partial X_{144}}{\partial T}\right]$$

For BeO

$$\overline{K}_{41} = \frac{25.013 \rho r^*}{V}$$

$$f_{41} = \overline{K}_{41}\left[X_{103} - X_{106} + X_{107} - X_{110} - X_{111} - X_{112} - X_{113} - X_{114}\right.$$

$$- X_{115} - X_{116} - X_{117} - X_{118} - X_{119} + X_{123} + X_{124} + 2X_{126}$$

$$\left. + X_{128} + X_{131} + X_{132} + X_{140} + X_{145}\right]$$

$$\beta_{41,j} = \overline{K}_{41}\left[\frac{\partial X_{103}}{\partial c_j} - \frac{\partial X_{106}}{\partial c_j} + \frac{\partial X_{107}}{\partial c_j} - \frac{\partial X_{110}}{\partial c_j} - \frac{\partial X_{111}}{\partial c_j} - \frac{\partial X_{112}}{\partial c_j} - \frac{\partial X_{113}}{\partial c_j}\right.$$

$$- \frac{\partial X_{114}}{\partial c_j} - \frac{\partial X_{115}}{\partial c_j} - \frac{\partial X_{116}}{\partial c_j} - \frac{\partial X_{117}}{\partial c_j} - \frac{\partial X_{118}}{\partial c_j} - \frac{\partial X_{119}}{\partial c_j} + \frac{\partial X_{123}}{\partial c_j}$$

$$+ \frac{\partial X_{124}}{\partial c_j} + 2\frac{\partial X_{126}}{\partial c_j} + \frac{\partial X_{128}}{\partial c_j} + \frac{\partial X_{131}}{\partial c_j} + \frac{\partial X_{132}}{\partial c_j} + \frac{\partial X_{140}}{\partial c_j}$$

$$\left. + \frac{\partial X_{145}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{41,73} = -\frac{1}{V} f_{41}$$

$$\beta_{41,74} = \frac{1}{\rho} f_{41} + \overline{K}_{41}\left[\frac{\partial X_{103}}{\partial \rho} - \frac{\partial X_{106}}{\partial \rho} + \frac{\partial X_{107}}{\partial \rho}\right]$$

$$\beta_{41,75} = \overline{K}_{41}\left[\frac{\partial X_{103}}{\partial T} - \frac{\partial X_{106}}{\partial T} + \frac{\partial X_{107}}{\partial T} - \frac{\partial X_{110}}{\partial T} - \frac{\partial X_{111}}{\partial T} - \frac{\partial X_{112}}{\partial T} - \frac{\partial X_{113}}{\partial T}\right.$$

$$- \frac{\partial X_{114}}{\partial T} - \frac{\partial X_{115}}{\partial T} - \frac{\partial X_{116}}{\partial T} - \frac{\partial X_{117}}{\partial T} - \frac{\partial X_{118}}{\partial T} - \frac{\partial X_{119}}{\partial T} + \frac{\partial X_{123}}{\partial T}$$

$$- \frac{\partial X_{124}}{\partial T} + 2\frac{\partial X_{126}}{\partial T} + \frac{\partial X_{128}}{\partial T} + \frac{\partial X_{131}}{\partial T} + \frac{\partial X_{132}}{\partial T} + \frac{\partial X_{140}}{\partial T}$$

$$\left. + \frac{\partial X_{145}}{\partial T}\right]$$

For Be_2O

$$\overline{K}_{42} = \frac{34.026\rho r^*}{V}$$

$$f_{42} = -\overline{K}_{42}\left[X_{107} - X_{119} + X_{120} + X_{121} + X_{122} + X_{123} + X_{124}\right.$$

$$\left. + X_{125} + X_{126}\right]$$

$$\beta_{42,j} = -\overline{K}_{42}\left[\frac{\partial X_{107}}{\partial c_j} - \frac{\partial X_{119}}{\partial c_j} + \frac{\partial X_{120}}{\partial c_j} + \frac{\partial X_{121}}{\partial c_j} + \frac{\partial X_{122}}{\partial c_j} + \frac{\partial X_{123}}{\partial c_j}\right.$$

$$\left. + \frac{\partial X_{124}}{\partial c_j} + \frac{\partial X_{125}}{\partial c_j} + \frac{\partial X_{126}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{42,73} = -\frac{1}{V} f_{42}$$

$$\beta_{42,74} = \frac{1}{\rho} f_{42} - \overline{K}_{42}\frac{\partial X_{107}}{\partial \rho}$$

$$\beta_{42,75} = -\overline{K}_{42}\left[\frac{\partial X_{107}}{\partial T} - \frac{\partial X_{119}}{\partial T} + \frac{\partial X_{120}}{\partial T} + \frac{\partial X_{121}}{\partial T} + \frac{\partial X_{122}}{\partial T} + \frac{\partial X_{123}}{\partial T}\right.$$

$$\left. + \frac{\partial X_{124}}{\partial T} + \frac{\partial X_{125}}{\partial T} + \frac{\partial X_{126}}{\partial T}\right]$$

For BeOH

$$\overline{K}_{43} = \frac{26.021\rho r*}{V}$$

$$f_{43} = -\overline{K}_{43}\Big[X_{102} + X_{103} - X_{108} - X_{110} - X_{113} - 2X_{120} - X_{121} - X_{122} - X_{123} - X_{125} + 2X_{127} + X_{128} + X_{129} + X_{130} + X_{131} - X_{132} - X_{134} - X_{138} - X_{141} - X_{147}\Big]$$

$$\beta_{43,j} = -\overline{K}_{43}\left[\frac{\partial X_{102}}{\partial c_j} + \frac{\partial X_{103}}{\partial c_j} - \frac{\partial X_{108}}{\partial c_j} - \frac{\partial X_{110}}{\partial c_j} - \frac{\partial X_{113}}{\partial c_j} - 2\frac{\partial X_{120}}{\partial c_j} - \frac{\partial X_{121}}{\partial c_j} - \frac{\partial X_{122}}{\partial c_j} - \frac{\partial X_{123}}{\partial c_j} - \frac{\partial X_{125}}{\partial c_j} + 2\frac{\partial X_{127}}{\partial c_j} + \frac{\partial X_{128}}{\partial c_j} + \frac{\partial X_{129}}{\partial c_j} + \frac{\partial X_{130}}{\partial c_j} + \frac{\partial X_{131}}{\partial c_j} + \frac{\partial X_{132}}{\partial c_j} - \frac{\partial X_{134}}{\partial c_j} - \frac{\partial X_{138}}{\partial c_j} - \frac{\partial X_{141}}{\partial c_j} - \frac{\partial X_{147}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{43,73} = -\frac{1}{V} f_{43}$$

$$\beta_{43,74} = \frac{1}{\rho} f_{43} - \overline{K}_{43}\left[\frac{\partial X_{102}}{\partial \rho} + \frac{\partial X_{103}}{\partial \rho} - \frac{\partial X_{108}}{\partial \rho}\right]$$

$$\beta_{43,75} = -\overline{K}_{43}\left[\frac{\partial X_{102}}{\partial T} + \frac{\partial X_{103}}{\partial T} - \frac{\partial X_{108}}{\partial T} - \frac{\partial X_{110}}{\partial T} - \frac{\partial X_{113}}{\partial T} - 2\frac{\partial X_{120}}{\partial T} - \frac{\partial X_{121}}{\partial T} - \frac{\partial X_{122}}{\partial T} - \frac{\partial X_{123}}{\partial T} - \frac{\partial X_{125}}{\partial T} + 2\frac{\partial X_{127}}{\partial T} + \frac{\partial X_{128}}{\partial T} + \frac{\partial X_{129}}{\partial T} + \frac{\partial X_{130}}{\partial T} + \frac{\partial X_{131}}{\partial T} + \frac{\partial X_{132}}{\partial T} - \frac{\partial X_{134}}{\partial T} - \frac{\partial X_{138}}{\partial T} - \frac{\partial X_{141}}{\partial T} - \frac{\partial X_{147}}{\partial T}\right]$$

For BeCl

$$\overline{K}_{44} = \frac{44.470\rho r^*}{V}$$

$$f_{44} = \overline{K}_{44}\left[X_{100} - X_{104} + X_{112} + X_{115} + X_{121} + X_{124} + X_{129} - 2X_{133} - X_{134} - X_{135} - X_{136} - X_{137} + X_{139} + X_{142}\right]$$

$$\beta_{44,j} = \overline{K}_{44}\left[\frac{\partial X_{100}}{\partial c_j} - \frac{\partial X_{104}}{\partial c_j} + \frac{\partial X_{112}}{\partial c_j} + \frac{\partial X_{115}}{\partial c_j} + \frac{\partial X_{121}}{\partial c_j} + \frac{\partial X_{124}}{\partial c_j} + \frac{\partial X_{129}}{\partial c_j} - 2\frac{\partial X_{133}}{\partial c_j} - \frac{\partial X_{134}}{\partial c_j} - \frac{\partial X_{135}}{\partial c_j} - \frac{\partial X_{136}}{\partial c_j} - \frac{\partial X_{137}}{\partial c_j} + \frac{\partial X_{139}}{\partial c_j} + \frac{\partial X_{142}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{44,73} = -\frac{1}{V} f_{44}$$

$$\beta_{44,74} = \frac{1}{\rho} f_{44} + \overline{K}_{44}\left[\frac{\partial X_{100}}{\partial \rho} - \frac{\partial X_{104}}{\partial \rho}\right]$$

$$\beta_{44,75} = \overline{K}_{44}\left[\frac{\partial X_{100}}{\partial T} - \frac{\partial X_{104}}{\partial T} + \frac{\partial X_{112}}{\partial T} + \frac{\partial X_{115}}{\partial T} + \frac{\partial X_{121}}{\partial T} + \frac{\partial X_{124}}{\partial T} + \frac{\partial X_{129}}{\partial T} - 2\frac{\partial X_{131}}{\partial T} - \frac{\partial X_{134}}{\partial T} - \frac{\partial X_{135}}{\partial T} - \frac{\partial X_{136}}{\partial T} - \frac{\partial X_{137}}{\partial T} + \frac{\partial X_{139}}{\partial T} + \frac{\partial X_{142}}{\partial T}\right]$$

For $BeCl_2$

$$\overline{K}_{45} = \frac{79.927\rho r^*}{V}$$

$$f_{45} = -\overline{K}_{45}\left[X_{100} - X_{133} - X_{135}\right]$$

$$\beta_{45,j} = -\overline{K}_{45}\left[\frac{\partial X_{100}}{\partial c_j} - \frac{\partial X_{133}}{\partial c_j} - \frac{\partial X_{135}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{45,73} = -\frac{1}{V} f_{45}$$

$$\beta_{45,74} = \frac{1}{\rho} f_{45} - K_{45} \frac{\partial X_{100}}{\partial \rho}$$

$$\beta_{45,75} = -\overline{K}_{45}\left[\frac{\partial X_{100}}{\partial T} - \frac{\partial X_{131}}{\partial T} - \frac{\partial X_{135}}{\partial T}\right]$$

For BeF

$$\overline{K}_{46} = \frac{28.013\rho r*}{V}$$

$$f_{46} = \overline{K}_{46} \left[X_{101} - X_{105} + 2X_{108} - X_{118} + X_{121} - X_{136} - X_{137}\right]$$

$$- X_{138} - X_{139} - X_{140} - X_{141} - X_{142} - X_{143} + X_{144}\Big]$$

$$\beta_{46,j} = \overline{K}_{46}\left[\frac{\partial X_{101}}{\partial c_j} - \frac{\partial X_{105}}{\partial c_j} + 2\frac{\partial X_{109}}{\partial c_j} - \frac{\partial X_{119}}{\partial c_j} + \frac{\partial X_{122}}{\partial c_j} - \frac{\partial X_{138}}{\partial c_j}\right.$$

$$- \frac{\partial X_{139}}{\partial c_j} - \frac{\partial X_{140}}{\partial c_j} - \frac{\partial X_{141}}{\partial c_j} - \frac{\partial X_{142}}{\partial c_j} - \frac{\partial X_{143}}{\partial c_j} - \frac{\partial X_{144}}{\partial c_j}$$

$$\left. - \frac{\partial X_{145}}{\partial c_j} + \frac{\partial X_{146}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{46,73} = -\frac{1}{V} f_{46}$$

$$\beta_{46,74} = \frac{1}{\rho} f_{46} + \overline{K}_{46}\left[\frac{\partial X_{101}}{\partial \rho} - \frac{\partial X_{105}}{\partial \rho}\right]$$

$$\beta_{46,75} = \overline{K}_{46}\left[\frac{\partial X_{101}}{\partial T} - \frac{\partial X_{105}}{\partial T} + 2\frac{\partial X_{109}}{\partial T} - \frac{\partial X_{119}}{\partial T} + \frac{\partial X_{122}}{\partial T} - \frac{\partial X_{138}}{\partial T} - \frac{\partial X_{139}}{\partial T}\right.$$

$$\left. - \frac{\partial X_{140}}{\partial T} - \frac{\partial X_{141}}{\partial T} - \frac{\partial X_{142}}{\partial T} - \frac{\partial X_{143}}{\partial T} - \frac{\partial X_{144}}{\partial T} - \frac{\partial X_{145}}{\partial T} + \frac{\partial X_{146}}{\partial T}\right]$$

For BeF_2

$$\overline{K}_{47} = \frac{47.013\rho r^*}{V}$$

$$f_{47} = -\overline{K}_{47}\left[X_{101} + X_{109} + X_{146}\right]$$

$$\beta_{47,j} = -\overline{K}_{47}\left[\frac{\partial X_{101}}{\partial c_j} + \frac{\partial X_{109}}{\partial c_j} + \frac{\partial X_{146}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{47,73} = -\frac{1}{V} f_{47}$$

$$\beta_{47,74} = \frac{1}{\rho} f_{47} - \overline{K}_{47}\frac{\partial X_{101}}{\partial \rho}$$

$$\beta_{47,75} = -\overline{K}_{47}\left[\frac{\partial X_{101}}{\partial T} + \frac{\partial X_{109}}{\partial T} + \frac{\partial X_{146}}{\partial T}\right]$$

For BeO_2H_2

$$\overline{K}_{48} = \frac{44.836\rho r^*}{V}$$

$$f_{48} = -\overline{K}_{48}\left[X_{108} - X_{127} + X_{147}\right]$$

$$\beta_{48,j} = -\overline{K}_{48}\left[\frac{\partial X_{108}}{\partial c_j} - \frac{\partial X_{127}}{\partial c_j} + \frac{\partial X_{147}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{48,73} = -\frac{1}{V} f_{48}$$

$$\beta_{48,74} = \frac{1}{\rho} f_{48} - \overline{K}_{48}\frac{\partial X_{108}}{\partial \rho}$$

$$\beta_{48,75} = -\overline{K}_{48}\left[\frac{\partial X_{108}}{\partial T} - \frac{\partial X_{127}}{\partial T} + \frac{\partial X_{147}}{\partial T}\right]$$

For Li

$$\overline{K}_{49} = \frac{6.940\rho r^*}{V}$$

$$f_{49} = \overline{K}_{49}\Big[X_{225} + X_{227} + X_{228} + X_{229} + X_{230} + X_{231} - X_{234} - X_{235} - X_{236} - X_{237} - X_{238} - X_{239} - X_{240} - X_{241} - X_{242} - X_{243} + X_{244} + X_{245} + X_{250} + X_{272} + X_{273} + X_{280} + X_{281}\Big]$$

$$\beta_{49,j} = \overline{K}_{49}\left[\frac{\partial X_{225}}{\partial c_j} + \frac{\partial X_{227}}{\partial c_j} + \frac{\partial X_{228}}{\partial c_j} + \frac{\partial X_{229}}{\partial c_j} + \frac{\partial X_{230}}{\partial c_j} + \frac{\partial X_{231}}{\partial c_j} - \frac{\partial X_{234}}{\partial c_j} - \frac{\partial X_{235}}{\partial c_j} - \frac{\partial X_{236}}{\partial c_j} - \frac{\partial X_{237}}{\partial c_j} - \frac{\partial X_{238}}{\partial c_j} - \frac{\partial X_{239}}{\partial c_j} - \frac{\partial X_{240}}{\partial c_j} - \frac{\partial X_{241}}{\partial c_j} - \frac{\partial X_{242}}{\partial c_j} - \frac{\partial X_{243}}{\partial c_j} + \frac{\partial X_{244}}{\partial c_j} + \frac{\partial X_{245}}{\partial c_j} + \frac{\partial X_{250}}{\partial c_j} + \frac{\partial X_{272}}{\partial c_j} + \frac{\partial X_{273}}{\partial c_j} + \frac{\partial X_{280}}{\partial c_j} + \frac{\partial X_{281}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{49,73} = -\frac{1}{V} f_{49}$$

$$\beta_{49,74} = \frac{1}{\rho} f_{49} + \overline{K}_{49}\left[\frac{\partial X_{225}}{\partial \rho} + \frac{\partial X_{227}}{\partial \rho} + \frac{\partial X_{228}}{\partial \rho} + \frac{\partial X_{229}}{\partial \rho} + \frac{\partial X_{230}}{\partial \rho} + \frac{\partial X_{231}}{\partial \rho}\right]$$

$$\beta_{49,75} = \overline{K}_{49}\left[\frac{\partial X_{225}}{\partial T} + \frac{\partial X_{227}}{\partial T} + \frac{\partial X_{228}}{\partial T} + \frac{\partial X_{229}}{\partial T} + \frac{\partial X_{230}}{\partial T} + \frac{\partial X_{231}}{\partial T} - \frac{\partial X_{234}}{\partial T} - \frac{\partial X_{235}}{\partial T} - \frac{\partial X_{236}}{\partial T} - \frac{\partial X_{237}}{\partial T} - \frac{\partial X_{238}}{\partial T} - \frac{\partial X_{239}}{\partial T} - \frac{\partial X_{240}}{\partial T} - \frac{\partial X_{241}}{\partial T} - \frac{\partial X_{242}}{\partial T} - \frac{\partial X_{243}}{\partial T} + \frac{\partial X_{244}}{\partial T} + \frac{\partial X_{245}}{\partial T} + \frac{\partial X_{250}}{\partial T} + \frac{\partial X_{272}}{\partial T} + \frac{\partial X_{273}}{\partial T} + \frac{\partial X_{280}}{\partial T} + \frac{\partial X_{281}}{\partial T}\right]$$

For LiH

$$\overline{K}_{50} = \frac{7.948\rho r^*}{V}$$

$$f_{50} = -\overline{K}_{50}\Big[X_{229} - X_{234} - X_{237} - X_{238} - X_{239} - X_{242} + X_{244} - X_{248} - X_{249} - X_{255} - X_{256} - X_{259} - X_{262} - X_{267} - X_{268} - X_{274} - X_{276} - X_{278} - X_{282}\Big]$$

$$\beta_{50,j} = -\overline{K}_{50}\left[\frac{\partial X_{229}}{\partial c_j} - \frac{\partial X_{234}}{\partial c_j} - \frac{\partial X_{237}}{\partial c_j} - \frac{\partial X_{238}}{\partial c_j} - \frac{\partial X_{239}}{\partial c_j} - \frac{\partial X_{242}}{\partial c_j} + \frac{\partial X_{244}}{\partial c_j} - \frac{\partial X_{248}}{\partial c_j} - \frac{\partial X_{249}}{\partial c_j} - \frac{\partial X_{255}}{\partial c_j} - \frac{\partial X_{256}}{\partial c_j} - \frac{\partial X_{259}}{\partial c_j} - \frac{\partial X_{262}}{\partial c_j} - \frac{\partial X_{267}}{\partial c_j} - \frac{\partial X_{268}}{\partial c_j} - \frac{\partial X_{274}}{\partial c_j} - \frac{\partial X_{276}}{\partial c_j} - \frac{\partial X_{278}}{\partial c_j} - \frac{\partial X_{282}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{50,73} = -\frac{1}{V} f_{50}$$

$$\beta_{50,74} = \frac{1}{\rho} f_{50} - \overline{K}_{50} \frac{\partial X_{229}}{\partial \rho}$$

$$\beta_{50,75} = -\overline{K}_{50}\left[\frac{\partial X_{229}}{\partial T} - \frac{\partial X_{234}}{\partial T} - \frac{\partial X_{237}}{\partial T} - \frac{\partial X_{238}}{\partial T} - \frac{\partial X_{239}}{\partial T} - \frac{\partial X_{242}}{\partial T} + \frac{\partial X_{244}}{\partial T} - \frac{\partial X_{248}}{\partial T} - \frac{\partial X_{249}}{\partial T} - \frac{\partial X_{255}}{\partial T} - \frac{\partial X_{256}}{\partial T} - \frac{\partial X_{259}}{\partial T} - \frac{\partial X_{262}}{\partial T} - \frac{\partial X_{267}}{\partial T} - \frac{\partial X_{268}}{\partial T} - \frac{\partial X_{274}}{\partial T} - \frac{\partial X_{276}}{\partial T} - \frac{\partial X_{278}}{\partial T} - \frac{\partial X_{282}}{\partial T}\right]$$

For LiO

$$\overline{K}_{51} = \frac{22.940\rho r^*}{V}$$

$$f_{51} = \overline{K}_{51}\Big[X_{226} - X_{230} + X_{231} + X_{236} + X_{240} + X_{241} + X_{242} - X_{245} - X_{246} - X_{247} - X_{248} - X_{249} - X_{250} - X_{251} - X_{252} + X_{256} + 2X_{257} + X_{260} + X_{263} + X_{264} + X_{270} + X_{275} + X_{279} + X_{283} - X_{284}\Big]$$

$$\beta_{51,j} = \overline{K}_{51}\left[\frac{\partial X_{226}}{\partial c_j} - \frac{\partial X_{230}}{\partial c_j} + \frac{\partial X_{231}}{\partial c_j} + \frac{\partial X_{236}}{\partial c_j} + \frac{\partial X_{240}}{\partial c_j} + \frac{\partial X_{241}}{\partial c_j} + \frac{\partial X_{242}}{\partial c_j} - \frac{\partial X_{245}}{\partial c_j} - \frac{\partial X_{246}}{\partial c_j} - \frac{\partial X_{247}}{\partial c_j} - \frac{\partial X_{248}}{\partial c_j} - \frac{\partial X_{249}}{\partial c_j} - \frac{\partial X_{250}}{\partial c_j} - \frac{\partial X_{251}}{\partial c_j} - \frac{\partial X_{252}}{\partial c_j} + \frac{\partial X_{256}}{\partial c_j} + 2\frac{\partial X_{257}}{\partial c_j} + \frac{\partial X_{260}}{\partial c_j} + \frac{\partial X_{263}}{\partial c_j} + \frac{\partial X_{264}}{\partial c_j} + \frac{\partial X_{270}}{\partial c_j} + \frac{\partial X_{275}}{\partial c_j} + \frac{\partial X_{279}}{\partial c_j} + \frac{\partial X_{283}}{\partial c_j} - \frac{\partial X_{284}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{51,73} = -\frac{1}{V} f_{51}$$

$$\beta_{51,74} = \frac{1}{\rho} f_{51} + \overline{K}_{51}\left[\frac{\partial X_{226}}{\partial \rho} - \frac{\partial X_{230}}{\partial \rho} + \frac{\partial X_{231}}{\partial \rho}\right]$$

$$\beta_{51,75} = \overline{K}_{51}\left[\frac{\partial X_{226}}{\partial T} - \frac{\partial X_{230}}{\partial T} + \frac{\partial X_{231}}{\partial T} + \frac{\partial X_{236}}{\partial T} + \frac{\partial X_{240}}{\partial T} + \frac{\partial X_{241}}{\partial T} + \frac{\partial X_{242}}{\partial T} - \frac{\partial X_{245}}{\partial T} - \frac{\partial X_{246}}{\partial T} - \frac{\partial X_{247}}{\partial T} - \frac{\partial X_{248}}{\partial T} - \frac{\partial X_{249}}{\partial T} - \frac{\partial X_{250}}{\partial T} - \frac{\partial X_{251}}{\partial T} - \frac{\partial X_{252}}{\partial T} + \frac{\partial X_{256}}{\partial T} + 2\frac{\partial X_{257}}{\partial T} + \frac{\partial X_{260}}{\partial T} + \frac{\partial X_{263}}{\partial T} + \frac{\partial X_{264}}{\partial T} + \frac{\partial X_{270}}{\partial T} + \frac{\partial X_{275}}{\partial T} + \frac{\partial X_{279}}{\partial T} + \frac{\partial X_{283}}{\partial T} - \frac{\partial X_{284}}{\partial T}\right]$$

For Li_2O

$$\overline{K}_{52} = \frac{29.880\rho r^*}{V}$$

$$f_{52} = -\overline{K}_{52}\Big[X_{231} - X_{243} - X_{251} - X_{252} + X_{253} + X_{254} + X_{255} + X_{256} + X_{257} - X_{265} - X_{284}\Big]$$

$$\beta_{52,j} = -\overline{K}_{52}\left[\frac{\partial X_{231}}{\partial c_j} - \frac{\partial X_{243}}{\partial c_j} - \frac{\partial X_{251}}{\partial c_j} - \frac{\partial X_{252}}{\partial c_j} + \frac{\partial X_{253}}{\partial c_j} + \frac{\partial X_{254}}{\partial c_j} + \frac{\partial X_{255}}{\partial c_j} + \frac{\partial X_{256}}{\partial c_j} + \frac{\partial X_{257}}{\partial c_j} - \frac{\partial X_{265}}{\partial c_j} - \frac{\partial X_{284}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{52,73} = -\frac{1}{V} f_{52}$$

$$\beta_{52,74} = \frac{1}{\rho} f_{52} - \overline{K}_{52}\frac{\partial X_{231}}{\partial \rho}$$

$$\beta_{52,75} = -\overline{K}_{52}\left[\frac{\partial X_{231}}{\partial T} - \frac{\partial X_{243}}{\partial T} - \frac{\partial X_{251}}{\partial T} - \frac{\partial X_{252}}{\partial T} + \frac{\partial X_{253}}{\partial T} + \frac{\partial X_{254}}{\partial T} + \frac{\partial X_{255}}{\partial T} + \frac{\partial X_{256}}{\partial T} + \frac{\partial X_{257}}{\partial T} - \frac{\partial X_{265}}{\partial T} - \frac{\partial X_{284}}{\partial T}\right]$$

For LiOH

$$\overline{K}_{53} = \frac{23.948\rho r^*}{V}$$

$$f_{53} = -\overline{K}_{53}\Big[X_{225} + X_{226} - X_{235} + X_{242} + X_{243} - X_{246} - X_{247} + X_{251} - 2X_{253} - X_{254} - X_{255} + X_{258} + X_{259} + X_{260} + X_{261} + X_{262} + X_{263} + X_{264} + X_{265} - X_{266} - X_{269}\Big]$$

$$\beta_{53,j} = -\overline{K}_{53}\left[\frac{\partial X_{225}}{\partial c_j} + \frac{\partial X_{226}}{\partial c_j} - \frac{\partial X_{235}}{\partial c_j} + \frac{\partial X_{242}}{\partial c_j} + \frac{\partial X_{243}}{\partial c_j} - \frac{\partial X_{246}}{\partial c_j}\right.$$

$$- \frac{\partial X_{247}}{\partial c_j} + \frac{\partial X_{251}}{\partial c_j} - 2\frac{\partial X_{253}}{\partial c_j} - \frac{\partial X_{254}}{\partial c_j} - \frac{\partial X_{255}}{\partial c_j} + \frac{\partial X_{258}}{\partial c_j}$$

$$+ \frac{\partial X_{259}}{\partial c_j} + \frac{\partial X_{260}}{\partial c_j} + \frac{\partial X_{261}}{\partial c_j} + \frac{\partial X_{262}}{\partial c_j} + \frac{\partial X_{263}}{\partial c_j} + \frac{\partial X_{264}}{\partial c_j}$$

$$\left. + \frac{\partial X_{265}}{\partial c_j} - \frac{\partial X_{266}}{\partial c_j} - \frac{\partial X_{269}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{53,73} = -\frac{1}{V} f_{53}$$

$$\beta_{53,74} = \frac{1}{\rho} f_{53} - \overline{K}_{53}\left[\frac{\partial X_{225}}{\partial \rho} + \frac{\partial X_{226}}{\partial \rho}\right]$$

$$\beta_{53,75} = -\overline{K}_{53}\left[\frac{\partial X_{225}}{\partial T} + \frac{\partial X_{226}}{\partial T} - \frac{\partial X_{235}}{\partial T} + \frac{\partial X_{242}}{\partial T} + \frac{\partial X_{243}}{\partial T} - \frac{\partial X_{246}}{\partial T}\right.$$

$$- \frac{\partial X_{247}}{\partial T} + \frac{\partial X_{251}}{\partial T} - 2\frac{\partial X_{253}}{\partial T} - \frac{\partial X_{254}}{\partial T} - \frac{\partial X_{255}}{\partial T} + \frac{\partial X_{258}}{\partial T}$$

$$+ \frac{\partial X_{259}}{\partial T} + \frac{\partial X_{260}}{\partial T} + \frac{\partial X_{261}}{\partial T} + \frac{\partial X_{262}}{\partial T} + \frac{\partial X_{263}}{\partial T} + \frac{\partial X_{264}}{\partial T}$$

$$\left. + \frac{\partial X_{265}}{\partial T} - \frac{\partial X_{266}}{\partial T} - \frac{\partial X_{269}}{\partial T}\right]$$

For LiF

$$\overline{K}_{54} = \frac{25.940\rho r^*}{V}$$

$$f_{54} = -\overline{K}_{54}\Big[X_{228} - 2X_{232} + X_{252} - X_{254} + X_{266} + X_{267} + X_{268}$$

$$+ X_{269} + X_{270} + X_{271} + X_{272} + X_{273} + X_{274} + X_{275}$$

$$- X_{277}\Big]$$

$$\beta_{54,j} = -\overline{K}_{54}\left[\frac{\partial X_{228}}{\partial c_j} - 2\frac{\partial X_{232}}{\partial c_j} + \frac{\partial X_{252}}{\partial c_j} - \frac{\partial X_{254}}{\partial c_j} + \frac{\partial X_{266}}{\partial c_j} + \frac{\partial X_{267}}{\partial c_j}\right.$$

$$+ \frac{\partial X_{268}}{\partial c_j} + \frac{\partial X_{269}}{\partial c_j} + \frac{\partial X_{270}}{\partial c_j} + \frac{\partial X_{271}}{\partial c_j} + \frac{\partial X_{272}}{\partial c_j} + \frac{\partial X_{273}}{\partial c_j}$$

$$\left. + \frac{\partial X_{274}}{\partial c_j} + \frac{\partial X_{275}}{\partial c_j} - \frac{\partial X_{277}}{\partial c_j}\right] \qquad j = 1, 2, \cdots, 57$$

$$\beta_{54,73} = -\frac{1}{V} f_{54}$$

$$\beta_{54,74} = \frac{1}{\rho} f_{54} - \overline{K}_{54}\left[\frac{\partial X_{228}}{\partial \rho} - 2\frac{\partial X_{232}}{\partial \rho}\right]$$

$$\beta_{54,75} = -\overline{K}_{54}\left[\frac{\partial X_{225}}{\partial T} - 2\frac{\partial X_{232}}{\partial T} + \frac{\partial X_{252}}{\partial T} - \frac{\partial X_{254}}{\partial T} + \frac{\partial X_{266}}{\partial T} + \frac{\partial X_{267}}{\partial T}\right.$$

$$+ \frac{\partial X_{268}}{\partial T} + \frac{\partial X_{269}}{\partial T} + \frac{\partial X_{270}}{\partial T} + \frac{\partial X_{271}}{\partial T} + \frac{\partial X_{272}}{\partial T} + \frac{\partial X_{273}}{\partial T}$$

$$\left. + \frac{\partial X_{274}}{\partial T} + \frac{\partial X_{275}}{\partial T} - \frac{\partial X_{277}}{\partial T}\right]$$

For LiCl

$$\overline{K}_{55} = \frac{42.397\rho r^*}{V}$$

$$f_{55} = -\overline{K}_{55}\left[X_{227} - 2X_{233} - X_{258} - X_{261} + X_{265} - X_{271} + X_{276} + X_{277} + X_{278} + X_{279} + X_{280} + X_{281} + X_{282} + X_{283} + X_{284}\right]$$

$$\beta_{55,j} = -\overline{K}_{55}\left[\frac{\partial X_{227}}{\partial c_j} - 2\frac{\partial X_{233}}{\partial c_j} - \frac{\partial X_{258}}{\partial c_j} - \frac{\partial X_{261}}{\partial c_j} + \frac{\partial X_{265}}{\partial c_j} - \frac{\partial X_{271}}{\partial c_j} + \frac{\partial X_{276}}{\partial c_j} + \frac{\partial X_{277}}{\partial c_j} + \frac{\partial X_{278}}{\partial c_j} + \frac{\partial X_{279}}{\partial c_j} + \frac{\partial X_{280}}{\partial c_j} + \frac{\partial X_{281}}{\partial c_j} + \frac{\partial X_{282}}{\partial c_j} + \frac{\partial X_{283}}{\partial c_j} + \frac{\partial X_{284}}{\partial c_j}\right] \quad j = 1, 2, \cdots, 57$$

$$\beta_{55,73} = -\frac{1}{V} f_{55}$$

$$\beta_{55,74} = \frac{1}{\rho} f_{55} - \overline{K}_{55}\left[\frac{\partial X_{227}}{\partial \rho} - 2\frac{\partial X_{233}}{\partial \rho}\right]$$

$$\beta_{55,75} = -\overline{K}_{55}\left[\frac{\partial X_{227}}{\partial T} - 2\frac{\partial X_{233}}{\partial T} - \frac{\partial X_{258}}{\partial T} - \frac{\partial X_{261}}{\partial T} + \frac{\partial X_{265}}{\partial T} - \frac{\partial X_{271}}{\partial T} + \frac{\partial X_{276}}{\partial T} + \frac{\partial X_{277}}{\partial T} + \frac{\partial X_{278}}{\partial T} + \frac{\partial X_{279}}{\partial T} + \frac{\partial X_{280}}{\partial T} + \frac{\partial X_{281}}{\partial T} + \frac{\partial X_{282}}{\partial T} + \frac{\partial X_{283}}{\partial T} + \frac{\partial X_{284}}{\partial T}\right]$$

For Li_2F_2

$$\overline{K}_{56} = \frac{51.880\rho r^*}{V}$$

$$f_{56} = -\overline{K}_{56} X_{232}$$

$$\beta_{56,j} = -\overline{K}_{56} \frac{\partial X_{232}}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{56,73} = -\frac{1}{V} f_{56}$$

$$\beta_{56,74} = \frac{1}{\rho} f_{56} - \overline{K}_{56} \frac{\partial X_{232}}{\partial \rho}$$

$$\beta_{56,75} = -\overline{K}_{56} \frac{\partial X_{232}}{\partial T}$$

For Li_2Cl_2

$$\overline{K}_{57} = \frac{84.794\rho r^*}{V}$$

$$f_{57} = -\overline{K}_{57} X_{233}$$

$$\beta_{57,j} = -\overline{K}_{57} \frac{\partial X_{233}}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{57,73} = -\frac{1}{V} f_{57}$$

$$\beta_{57,74} = \frac{1}{\rho} f_{57} - \overline{K}_{57} \frac{\partial X_{233}}{\partial \rho}$$

$$\beta_{57,75} = -\overline{K}_{57} \frac{\partial X_{233}}{\partial T}$$

4.2.3 Calculation of μ and Its Partial Derivatives

The gas viscosity and its partial derivatives are calculated from:

$$\mu = \frac{1.2469169 \times 10^{-5}}{\sqrt{R}} T^{0.6}$$

$$\frac{\partial \mu}{\partial c_j} = -\frac{1}{2} \frac{R_j}{R} \mu \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial \mu}{\partial T} = \frac{0.6}{T} \mu$$

4.2.4 Calculation of Re_i and Its Partial Derivatives

The particle Reynold's numbers and its partial derivatives are calculated from:

$$Re_i = \frac{2\rho(V - V_{pi}) r_{pi}}{\mu} \quad , \quad 1, 2, \cdots, 5$$

$$\frac{\partial Re_i}{\partial c_j} = -\frac{1}{\mu} Re_i \frac{\partial \mu}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57 \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Re_i}{\partial V_{pi}} = -\frac{Re_i}{V - V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Re_i}{\partial V} = \frac{Re_i}{V - V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Re_i}{\partial \rho} = \frac{Re_i}{\rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Re_i}{\partial T} = -\frac{Re_i}{\mu} \frac{\partial \mu}{\partial T} \quad , \quad i = 1, 2, \cdots, 5$$

4.2.5 Calculation of γ and Its Partial Derivatives

The gas ratio of specific heats and its partial derivatives are calculated from:

$$\gamma = \frac{C_P}{C_P - R}$$

$$\frac{\partial \gamma}{\partial c_j} = \left(\frac{\gamma}{C_P}\right)^2 \left(R_j C_P - R C_{pj}\right) \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial \gamma}{\partial T} = -\left(\frac{\gamma}{C_P}\right)^2 R \sum_{i=1}^{57} C_i \frac{\partial C_{pi}}{\partial T}$$

4.2.6 Calculation of Pr and Its Partial Derivatives

The gas Prandtl number and its partial derivatives are calculated from:

$$Pr = \frac{4\gamma}{9\gamma - 5}$$

$$\frac{\partial Pr}{\partial c_j} = \frac{-5}{\gamma(9\gamma - 5)} Pr \frac{\partial \gamma}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial Pr}{\partial T} = \frac{-5}{\gamma(9\gamma - 5)} Pr \frac{\partial \gamma}{\partial T}$$

4.2.7 Calculation of $Nu_i^{(o)}$ and Its partial Derivatives

The particle Nussult number and its partial derivatives are calculated from:

$$Nu_i^{(o)} = 2 + 0.37 \, Re_i^{0.6} \, Pr^{1/3}$$

$$\frac{\partial Nu_i^{(o)}}{\partial c_j} = \left(\frac{0.6}{Re_i} \frac{\partial Re_i}{\partial c_j} + \frac{1}{3Pr} \frac{\partial Pr}{\partial c_j}\right)\left[Nu_i^{(o)} - 2\right] \quad , \quad j = 1, 2, \cdots, 57 \, , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Nu_i^{(o)}}{\partial V_{pi}} = \frac{0.6\left[Nu_i^{(o)} - 2\right]}{Re_i} \frac{\partial Re_i}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Nu_i^{(o)}}{\partial V} = \frac{0.6\left[Nu_i^{(o)} - 2\right]}{Re_i} \frac{\partial Re_i}{\partial V} \quad , \quad j = 1, 2, \cdots, 5$$

$$\frac{\partial Nu_i^{(o)}}{\partial \rho} = \frac{0.6\left[Nu_i^{(o)} - 2\right]}{Re_i} \frac{\partial Re_i}{\partial \rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Nu_i^{(o)}}{\partial T} = \left(\frac{0.6}{Re_i} \frac{\partial Re_i}{\partial T} + \frac{1}{3Pr} \frac{\partial Pr}{\partial T}\right) \left[Nu_i^{(o)} - 2\right] \quad , \quad i = 1, 2, \cdots, 5$$

4.2.8 Calculation of $C_{Di}^{(o)}$ and Its Partial Derivatives

The particle drag coefficient, based on particle diameter, and its partial derivatives are calculated from:

$$C_{Di}^{(o)} = \frac{24}{Re_i} + bRe_i^n$$

$$\frac{\partial C_{Di}^{(o)}}{\partial c_j} = \frac{\partial Re_i}{\partial c_j} \left[bRe_i^n(1 + n) - C_{Di}^{(o)}\right] \frac{1}{Re_i} \quad , \quad i = 1, 2, \cdots, 5, \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial C_{Di}^{(o)}}{\partial V_{pi}} = \frac{\partial Re_i}{\partial V_{pi}} \left[bRe_i^n (1 + n) - C_{Di}^{(o)}\right] \frac{1}{Re_i} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial C_{Di}^{(o)}}{\partial V} = \frac{\partial Re_i}{\partial V} \left[bRe_i^n (1 + n) - C_{Di}^{(o)}\right] \frac{1}{Re_i} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial C_{Di}^{(o)}}{\partial \rho} = \frac{\partial Re_i}{\partial \rho} \left[bRe_i^n (1 + n) - C_{Di}^{(o)}\right] \frac{1}{Re_i} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial C_{Di}^{(o)}}{\partial T} = \frac{\partial Re_i}{\partial T} \left[bRe_i^n (1 + n) - C_{Di}^{(o)}\right] \frac{1}{Re_i} \quad , \quad i = 1, 2, \cdots, 5$$

4.2.9 Calculation of Kn_i and Its Partial Derivatives

The particle Knudsen number and its partial derivatives are calculated from:

$$Kn_i = \frac{0.63\mu}{\sqrt{RT}\,\rho r_{pi}}$$

$$\frac{\partial Kn_i}{\partial c_j} = Kn_i \left(\frac{1}{\mu}\frac{\partial \mu}{\partial c_j} - \frac{1}{2}\frac{R_j}{R} \right) \quad , \quad i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial Kn_i}{\partial \rho} = -\frac{Kn_i}{\rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial Kn_i}{\partial T} = Kn_i \left(\frac{1}{\mu}\frac{\partial \mu}{\partial T} - \frac{1}{2T} \right) \quad , \quad i = 1, 2, \cdots, 5$$

4.2.10 Calculations of f_{pi} and Its Partial Derivatives

The momentum term f_{pi} and its partial derivatives are calculated from:

$$f_{pi} = \frac{Re_i}{24} C_{Di}^{(o)} \left[\frac{(1 + 7.5\,Kn_i)(1 + 2\,Kn_i) + 1.91\,Kn_i^2}{(1 + 7.5\,Kn_i)(1 + 3\,Kn_i) + (2.29 + 5.16\,Kn_i)Kn_i^2} \right] , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial f_{pi}}{\partial c_j} = f_{pi} \left\{ \frac{1}{Re_i}\frac{\partial Re_i}{\partial c_j} + \frac{1}{C_{Di}^{(o)}}\frac{\partial C_{Di}^{(o)}}{\partial c_j} + \frac{\partial Kn_i}{\partial c_j} \cdot \right.$$

$$\left[\frac{2(1 + 7.5\,Kn_i) + 7.5(1 + 2\,Kn_i) + 3.82\,Kn_i}{(1 + 7.5\,Kn_i)(1 + 2\,Kn_i) + 1.91\,Kn_i^2} \right.$$

$$\left. \left. - \frac{3(1 + 7.5\,Kn_i) + 7.5(1 + 3\,Kn_i) + 2(2.29 + 5.16\,Kn_i)Kn_i + 5.16\,Kn_i^2}{(1 + 7.5\,Kn_i)(1 + 3\,Kn_i) + (2.29 + 5.16\,Kn_i)Kn_i^2} \right] \right\}$$

$$i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial f_{pi}}{\partial V_{pi}} = f_{pi}\left[\frac{1}{Re_i}\frac{\partial Re_i}{\partial V_{pi}} + \frac{1}{C_{Di}^{(o)}}\frac{\partial C_{Di}^{(o)}}{\partial V_{pi}}\right] , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial f_{pi}}{\partial V} = f_{pi}\left[\frac{1}{Re_i}\frac{\partial Re_i}{\partial V} + \frac{1}{C_{Di}^{(o)}}\frac{\partial C_{Di}^{(o)}}{\partial V}\right] , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial f_{pi}}{\partial \rho} = f_{pi}\left\{\frac{1}{Re_i}\frac{\partial Re_i}{\partial \rho} + \frac{1}{C_{Di}^{(o)}}\frac{\partial C_{Di}^{(o)}}{\partial \rho} + \frac{\partial Kn_i}{\partial \rho} \cdot \right.$$

$$\left[\frac{2(1 + 7.5\,Kn_i) + 7.5(1 + 2\,Kn_i) + 3.82\,Kn_i}{(1 + 7.5\,Kn_i)(1 + 2\,Kn_i) + 1.91\,Kn_i^2}\right.$$

$$\left.\left. - \frac{3(1 + 7.5\,Kn_i) + 7.5(1 + 3\,Kn_i) + 2(2.29 + 5.16\,Kn_i)Kn_i + 5.16\,Kn_i^2}{(1 + 7.5\,Kn_i)(1 + 3\,Kn_i) + (2.29 + 5.16\,Kn_i)Kn_i^2}\right]\right\}$$

$$i = 1, 2, \cdots, 5$$

$$\frac{\partial f_{pi}}{\partial T} = f_{pi}\left\{\frac{1}{Re_i}\frac{\partial Re_i}{\partial T} + \frac{1}{C_{Di}^{(o)}}\frac{\partial C_{Di}^{(o)}}{\partial T} + \frac{\partial Kn_i}{\partial T} \cdot \right.$$

$$\left[\frac{2(1 + 7.5\,Kn_i) + 7.5(1 + 2\,Kn_i) + 3.82\,Kn_i}{1 + 7.5\,Kn_i)(1 + 2\,Kn_i) + 1.91\,Kn_i^2}\right.$$

$$\left.\left. - \frac{3(1 + 7.5\,Kn_i) + 7.5(1 + 3\,Kn_i) + 2(2.29 + 5.16\,Kn_i)Kn_i + 5.16\,Kn_i^2}{(1 + 7.5\,Kn_i)(1 + 3\,Kn_i) + (2.29 + 5.16\,Kn_i)Kn_i^2}\right]\right\}$$

$$i = 1, 2, \cdots, 5$$

4.2.11 Calculation of g_{pi} and Its Partial Derivatives

The energy term g_{pi} and its partial derivatives are calculated from:

$$g_{pi} = \frac{Nu_i^{(o)}}{2\left[1 + 2.72\,\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\right]} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial g_{pi}}{\partial c_j} = g_{pi}\left(\frac{1}{Nu_i^{(o)}}\frac{\partial Nu_i^{(o)}}{\partial c_j} - 2.72\,\frac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\cdot\left\{\frac{\dfrac{1}{Nu_i^{(o)}}\dfrac{\partial Nu_i^{(o)}}{\partial c_j} + \dfrac{1}{Kn_i}\dfrac{\partial Kn_i}{\partial c_j} - \dfrac{1}{Pr}\dfrac{\partial Pr}{\partial c_j} - \dfrac{1}{2\gamma}\dfrac{\partial \gamma}{\partial c_j}}{\left[1 + 2.72\,\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\right]}\right\}\right)$$

$$i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial g_{pi}}{\partial V_{pi}} = g_{pi}\left\{\frac{1}{Nu_i^{(o)}}\frac{\partial Nu_i^{(o)}}{\partial V_{pi}} - \frac{2.72\,\dfrac{Kn_i}{\sqrt{\gamma}\,Pr}\,\dfrac{\partial Nu_i^{(o)}}{\partial V_{pi}}}{\left[1 + 2.72\,\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\right]}\right\} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial g_{pi}}{\partial V} = g_{pi}\left\{\frac{1}{Nu_i^{(o)}}\frac{\partial Nu_i^{(o)}}{\partial V} - \frac{2.72\,\dfrac{Kn_i}{\sqrt{\gamma}\,Pr}\,\dfrac{\partial Nu_i^{(o)}}{\partial V}}{\left[1 + 2.72\,\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\right]}\right\} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial g_{pi}}{\partial \rho} = g_{pi}\left\{\frac{1}{Nu_i^{(o)}}\frac{\partial Nu_i^{(o)}}{\partial \rho} - 2.72\,\frac{\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\left[\dfrac{1}{Kn_i}\dfrac{\partial Kn_i}{\partial \rho} + \dfrac{1}{Nu_i^{(o)}}\dfrac{\partial Nu_i^{(o)}}{\partial \rho}\right]}{\left[1 + 2.72\,\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\right]}\right\}$$

$i = 1, 2, \cdots, 5$

$$\frac{\partial g_{pi}}{\partial T} = g_{pi}\left\{\frac{1}{Nu_i^{(o)}}\frac{\partial Nu_i^{(o)}}{\partial T} - 2.72\,\frac{\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\left[\dfrac{1}{Nu_i^{(o)}}\dfrac{\partial Nu_i^{(o)}}{\partial T} + \dfrac{1}{Kn_i}\dfrac{\partial Kn_i}{\partial T} - \dfrac{1}{Pr}\dfrac{\partial Pr}{\partial T} - \dfrac{1}{2\gamma}\dfrac{\partial \gamma}{\partial T}\right]}{\left[1 + 2.72\,\dfrac{Kn_i\,Nu_i^{(o)}}{\sqrt{\gamma}\,Pr}\right]}\right\}$$

$i = 1, 2, \cdots, 5$

4.2.12 Calculation of f_i and $\beta_{i,j}$ for the Particle Relaxation Equations

For the particle sizes of interest f_i and $\beta_{i,j}$, for the particle relaxation equations, are calculated from the following relationships:

$$f_{i+57} = \frac{9}{2}\,\frac{\mu f_{pi}\, r^*(V - V_{pi})}{m_{pi}\, r_{pi}^2\, V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+57,\,j} = f_{i+57}\left(\frac{1}{\mu}\frac{\partial \mu}{\partial c_j} + \frac{1}{f_{pi}}\frac{\partial f_{pi}}{\partial c_j}\right) \quad , \quad i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{i+57,\,i+57} = f_{i+57}\left[\frac{1}{f_{pi}}\frac{\partial f_{pi}}{\partial V_{pi}} - \frac{V}{V_{pi}(V - V_{pi})}\right] \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+57,\,73} = f_{i+57} \left[\frac{1}{f_{pi}} \frac{\partial f_{pi}}{\partial V} + \frac{1}{(V - V_{pi})} \right] \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+57,\,74} = f_{i+57} \frac{1}{f_{pi}} \frac{\partial f_{pi}}{\partial \rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+57,\,75} = f_{i+57} \left(\frac{1}{\mu} \frac{\partial \mu}{\partial T} + \frac{1}{f_{pi}} \frac{\partial f_{pi}}{\partial T} \right) \quad , \quad i = 1, 2, \cdots, 5$$

$$f_{i+67} = \frac{3\mu g_{pi} \, r^* \, C_{Pg} \, (T_{pi} - T)}{m_{pi} r_{pi}^2 \, Pr \, V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+67,\,j} = f_{i+67} \left(\frac{1}{\mu} \frac{\partial \mu}{\partial c_j} + \frac{1}{g_{pi}} \frac{\partial g_{pi}}{\partial c_j} + \frac{C_{Pj}}{C_{Pg}} - \frac{1}{Pr} \frac{\partial Pr}{\partial c_j} \right) ,$$

$$i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{i+67,\,i+57} = f_{i+67} \left(\frac{1}{g_{pi}} \frac{\partial g_{pi}}{\partial c_j} - \frac{1}{V_{pi}} \right) \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+67,\,i+67} = f_{i+67} \frac{1}{(T_{pi} - T)} \frac{\partial T_{pi}}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

where:

$$\frac{dT_{pi}}{dh_{pi}} = \frac{1}{C_{pi}} \quad , \quad T_{pi} \neq T_{pmi}$$

$$\frac{dT_{pi}}{dh_{pi}} = 0 \quad , \quad T_{pi} = T_{pmi}$$

$$\beta_{i+67,\,73} = f_{i+67} \frac{1}{g_{pi}} \frac{\partial g_{pi}}{\partial V} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+67,74} = f_{i+67} \frac{1}{g_{pi}} \frac{\partial g_{pi}}{\partial \rho}, \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+67,75} = f_{i+67} \left[\frac{1}{\mu}\frac{\partial \mu}{\partial T} + \frac{1}{g_{pi}}\frac{\partial g_{pi}}{\partial T} + \frac{1}{C_{Pg}}\frac{\partial C_{Pg}}{\partial T} - \frac{1}{(T_{pi} - T)} - \frac{1}{Pr}\frac{\partial Pr}{\partial T} \right]$$

$$i = 1, 2, \cdots, 5$$

4.2.13 Calculation of the Pressure and Pressure Derivatives

For subsonic flows, the pressure distribution is given by the pressure table and the pressure and pressure derivatives are calculated from:

$$P = P(x_n) + \left.\frac{dP}{dx}\right|_{x_n} (x - x_n) + \frac{1}{2} \left.\frac{d^2P}{dx^2}\right|_{x_n} \left(x - x_n\right)^2$$

$$\frac{dP}{dx} = \left.\frac{dP}{dx}\right|_{x_n} + \left.\frac{d^2P}{dx^2}\right|_{x_n} (x - x_n)$$

$$\frac{d^2P}{dx^2} = \left.\frac{d^2P}{dx^2}\right|_{x_n}$$

where $(1/2)(x_{n-1} + x_n) \leq x \leq (1/2)(x_n + x_{n+1})$ and the subscript n refers to the nth entry in the pressure and pressure derivative tables.

For supersonic flows, the pressure is determined by integration.

4.2.14 Calculation of the Area and Area Derivatives

For supersonic flow, the area and area derivatives are calculated from:

$$a = \left[1 + R^* - \left(R^{*2} - x^2\right)^{1/2}\right]^2$$

$$\frac{da}{dx} = \frac{2x}{\left(R^{*2} - x^2\right)^{1/2}} \left[1 + R^* - \left(R^{*2} - x^2\right)^{1/2}\right]$$

$$\frac{d^2a}{dx^2} = \left[\frac{2}{\left(R^{*2} - x^2\right)^{1/2}} + \frac{2x^2}{\left(R^* - x^2\right)^{3/2}}\right] \left[1 + R^* - \left(R^* - x^2\right)^{1/2}\right] + \frac{2x^2}{R^{*2} - x^2}$$

when $x \leq x_t$ and

$$a = \left[r_1 + (x - x_1) \tan \theta_1\right]^2$$

$$\frac{da}{dx} = 2\left[r_1 + (x - x_1) \tan \theta_1\right] \tan \theta_1$$

$$\frac{d^2a}{dx^2} = 2 \tan^2 \theta_1$$

when $x > x_t$

4.2.15 Calculation of M^2 and Its Partial Derivatives

For supersonic flows, M^2 and its partial derivatives are calculated from:

$$M^2 = \frac{V^2}{\gamma RT}$$

$$\frac{\partial M^2}{\partial c_j} = -\frac{M^2}{\gamma}\frac{\partial \gamma}{\partial c_j} - \frac{M^2}{T} R_j \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial M^2}{\partial V} = \frac{2M^2}{V}$$

$$\frac{\partial M^2}{\partial T} = -\frac{M^2}{T}$$

where only the $(\partial M^2/\partial c_j)$'s of interest are calculated.

4.2.16 Calculation of S_1, S_2, S_3 and S_4 and Their Partial Derivatives

The summation terms S_1, S_2, S_3 and S_4 and their partial derivatives are calculated from:

$$S_1 = \frac{1}{R} \sum_{i=1}^{57} f_i R_i$$

$$\frac{\partial S_1}{\partial c_j} = \frac{1}{R} \sum_{i=1}^{57} \beta_{i,j} R_i - \frac{R_j}{R} S_1 , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial S_1}{\partial V} = \frac{1}{R} \sum_{i=1}^{57} \beta_{i,73} R_i$$

$$\frac{\partial S_1}{\partial \rho} = \frac{1}{R} \sum_{i=1}^{57} \beta_{i,74} R_i$$

$$\frac{\partial S_1}{\partial T} = \frac{1}{R} \sum_{i=1}^{57} \beta_{i,75} R_i$$

$$S_2 = \frac{1}{RT} \sum_{i=1}^{57} f_i h_i$$

$$\frac{\partial S_2}{\partial c_j} = \frac{1}{RT} \sum_{i=1}^{57} \beta_{i,j} h_i - \frac{R_j}{R} S_2 , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial S_2}{\partial V} = \frac{1}{RT} \sum_{i=1}^{57} \beta_{i,73} h_i$$

$$\frac{\partial S_2}{\partial \rho} = \frac{1}{RT} \sum_{i=1}^{57} \beta_{i,73} h_i$$

$$\frac{\partial S_2}{\partial T} = \frac{1}{RT} \sum_{i=1}^{57} \beta_{i,75} h_i + \frac{1}{RT} \sum_{i=1}^{57} f_i C_{pi} - \frac{S_2}{T}$$

$$S_3 = \frac{r^*}{\rho RTV} \sum_{i=1}^{5} \rho_{pi} \left[f_{i+57} \; V_{pi}(V - V_{pi}) - f_{i+67} \; V_{pi} \right]$$

$$\frac{\partial S_3}{\partial c_j} = \frac{r^*}{\rho RTV} \sum_{i=1}^{5} \rho_{pi} \left[\beta_{i+57,j} \; V_{pi}(V - V_{pi}) - \beta_{i+67,j} \; V_{pi} \right] - \frac{R_j}{R} S_3 ,$$

$$j = 1, 2, \cdots, 57$$

$$\frac{\partial S_3}{\partial V_{pi}} = \frac{r^*}{\rho RTV}\left\{\rho_{pi}\left[\beta_{i+57,\, i+57}\, V_{pi}(V - V_{pi}) - \beta_{i+67,\, i+57}\, V_{pi} - f_{i+57}(2V_{pi} - V) - f_{i+67}\right]\right\} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial S_3}{\partial \rho_{pi}} = \frac{r^*}{\rho RTV}\left[f_{i+57} V_{pi}(V - V_{pi}) - f_{i+67}\, V_{pi}\right] \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial S_3}{\partial h_{pi}} = \frac{-r^*}{\rho RTV}\, \rho_{pi}\beta_{i+67,\, i+67}\, V_{pi} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial S_3}{\partial V} = \frac{-S_3}{V} + \frac{r^*}{\rho RTV}\sum_{i=1}^{5} \rho_{pi}\left[\beta_{i+57,\, 73}\, V_{pi}(V - V_{pi}) - \beta_{i+67,\, 73}\, V_{pi} + f_{i+57}\, V_{pi}\right]$$

$$\frac{\partial S_3}{\partial \rho} = \frac{r^*}{\rho RTV}\sum_{i=1}^{5} \rho_{pi}\left[\beta_{i+57,\, 74}\, V_{pi}\, (V - V_{pi}) - \beta_{i+67,\, 74}\, V_{pi}\right] - \frac{S_3}{\rho}$$

$$\frac{\partial S_3}{\partial T} = \frac{r^*}{\rho RTV}\sum_{i=1}^{5} \rho_{pi}\left[\beta_{i+57,\, 75}\, V_{pi}\, (V - V_{pi}) - \beta_{i+67,\, 75}\, V_{pi}\right] - \frac{S_3}{T}$$

$$S_4 = \sum_{i=1}^{5} \rho_{pi}\, f_{i+57}\, V_{pi}$$

$$\frac{\partial S_4}{\partial c_j} = \sum_{i=1}^{5} \rho_{pi}\, \beta_{i+57,\, j}\, V_{pi} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial S_4}{\partial V_{pi}} = \rho_{pi}\, (f_{i+57} + \beta_{i+57,\, i+57}\, V_{pi}) \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial S_4}{\partial \rho_{pi}} = V_{pi}\, (f_{i+57} + \rho_{pi}\beta_{i+57,\, i+62}) \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial S_4}{\partial V} = \sum_{i=1}^{5} \rho_{pi} V_{pi}\, \beta_{i+57,\, 73}$$

$$\frac{\partial S_4}{\partial \rho} = \sum_{i=1}^{5} \rho_{pi} V_{pi} \beta_{i+57,\, 74}$$

$$\frac{\partial S_4}{\partial T} = \sum_{i=1}^{5} \rho_{pi} V_{pi} \beta_{i+57,\, 75}$$

where the sums are performed only over the species of interest and only the $(\partial S_1/\partial c_j)$'s, $(\partial S_2/\partial c_j)$'s, $(\partial S_3/\partial c_j)$'s and $(\partial S_4/\partial c_j)$'s of interest are calculated.

4.2.17 Calculation of B and Its Partial Derivatives

The erergy exchange term and its partial derivatives are calculated from:

$$B = \frac{\gamma - 1}{\gamma} (S_2 - S_3)$$

$$\frac{\partial B}{\partial c_j} = \frac{\gamma - 1}{\gamma} \left(\frac{\partial S_2}{\partial c_j} - \frac{\partial S_3}{\partial c_j} \right) + \frac{1}{\gamma(\gamma - 1)} \frac{B \partial \gamma}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial B}{\partial V_{pi}} = - \frac{\gamma - 1}{\gamma} \frac{\partial S_3}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial B}{\partial \rho_{pi}} = - \frac{\gamma - 1}{\gamma} \frac{\partial S_3}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial B}{\partial h_{pi}} = - \frac{\gamma - 1}{\gamma} \frac{\partial S_3}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial B}{\partial V} = \frac{\gamma - 1}{\gamma} \left(\frac{\partial S_2}{\partial V} - \frac{\partial S_3}{\partial V} \right)$$

$$\frac{\partial B}{\partial V} = \frac{\gamma - 1}{\gamma} \left(\frac{\partial S_2}{\partial V} - \frac{\partial S_3}{\partial V} \right)$$

$$\frac{\partial B}{\partial \rho} = \frac{\gamma - 1}{\gamma} \left(\frac{\partial S_2}{\partial \rho} - \frac{\partial S_3}{\partial \rho} \right)$$

$$\frac{\partial B}{\partial T} = \frac{\gamma - 1}{\gamma} \left(\frac{\partial S_2}{\partial T} - \frac{\partial S_3}{\partial T} \right) + \frac{1}{\gamma(\gamma - 1)} B \frac{\partial \gamma}{\partial T}$$

where only the $(\partial B/\partial c_j)$'s of interest are calculated.

4.2.18 Calculation of A and Its Partial Derivatives

The diabatic heat addition term A and its partial derivatives are calculated from:

$$A = S_1 - B$$

$$\frac{\partial A}{\partial c_j} = \frac{\partial S_1}{\partial c_j} - \frac{\partial B}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial A}{\partial V_{pi}} = \frac{\partial B}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial A}{\partial \rho_{pi}} = \frac{-\partial B}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial A}{\partial h_{pi}} = \frac{-\partial B}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial A}{\partial V} = \frac{\partial S_1}{\partial V} - \frac{\partial B}{\partial V}$$

$$\frac{\partial A}{\partial \rho} = \frac{\partial S_1}{\partial \rho} - \frac{\partial B}{\partial \rho}$$

$$\frac{\partial A}{\partial T} = \frac{\partial S_1}{\partial T} - \frac{\partial B}{\partial T}$$

where only the $(\partial A/\partial c_j)$'s of interest are calculated.

4.2.19 Calculation of C and Its Partial Derivatives

The total particle drag term C and its partial derivatives are calculated from:

$$C = S_4$$

$$\frac{\partial C}{\partial c_j} = \frac{\partial S_4}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial C}{\partial V_{pi}} = \frac{\partial S_4}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial C}{\partial \rho_{pi}} = \frac{\partial S_4}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial C}{\partial V} = \frac{\partial S_4}{\partial V}$$

$$\frac{\partial C}{\partial \rho} = \frac{\partial S_4}{\partial \rho}$$

$$\frac{\partial C}{\partial T} = \frac{\partial S_4}{\partial T}$$

where only the $(\partial C/\partial c_j)$'s of interest are calculated.

4.2.20 Calculation of E and Its Partial Derivatives

The diabatic heat addition term E and its partial derivatives are calculated from:

$$E = A + \frac{C}{\rho V^2}$$

$$\frac{\partial E}{\partial c_j} = \frac{\partial A}{\partial c_j} + \frac{1}{\rho V^2}\frac{\partial C}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial E}{\partial V_{pi}} = \frac{\partial A}{\partial V_{pi}} + \frac{1}{\rho V^2}\frac{\partial C}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial E}{\partial \rho_{pi}} = \frac{\partial A}{\partial \rho_{pi}} + \frac{1}{\rho V^2}\frac{\partial C}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial E}{\partial h_{pi}} = \frac{\partial A}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial E}{\partial V} = \frac{\partial A}{\partial V} - \frac{\partial C}{\rho V^3} + \frac{1}{\rho V^2}\frac{\partial C}{\partial V}$$

$$\frac{\partial E}{\partial \rho} = \frac{\partial A}{\partial \rho} - \frac{C}{\rho^2 V^2} + \frac{1}{\rho V^2}\frac{\partial C}{\partial \rho}$$

$$\frac{\partial E}{\partial T} = \frac{\partial A}{\partial T} + \frac{1}{\rho V^2}\frac{\partial C}{\partial T}$$

where only the $(\partial E/\partial c_j)$'s of interest are calculated.

4.2.21 Calculation of F_i and Its Partial Derivatives

The supersonic particle continuity term F_i and its partial derivatives are calculated from:

$$F_i = -\frac{f_{i+57}}{V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial F_i}{\partial c_j} = -\frac{\beta_{i+57,j}}{V_{pi}} \quad , \quad i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial F_i}{\partial V_{pi}} = -\frac{1}{V_{pi}} \beta_{i+57,i+57} - \frac{F_i}{V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial F_i}{\partial V} = -\frac{1}{V_{pi}} \beta_{i+57,73} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial F_i}{\partial \rho} = -\frac{1}{V_{pi}} \beta_{i+57,74} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial F_i}{\partial T} = -\frac{1}{V_{pi}} \beta_{i+57,75} \quad , \quad i = 1, 2, \cdots, 5$$

where only the $(\partial F_i / \partial c_j)$'s of interest are calculated.

4.2.22 Calculation of D_i and Its Partial Derivatives

The subsonic particle continuity term D_i and its partial derivatives are calculated from:

$$D_i = E - F_i \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial D_i}{\partial c_j} = \frac{\partial E}{\partial c_j} - \frac{\partial F_i}{\partial c_j} \quad , \quad i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\frac{\partial D_i}{\partial V_{pi}} = \frac{\partial E}{\partial V_{pi}} - \frac{\partial F_i}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial D_i}{\partial \rho_{pi}} = \frac{\partial E}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial D_i}{\partial h_{pi}} = \frac{\partial E}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial D_i}{\partial V} = \frac{\partial E}{\partial V} - \frac{\partial F_i}{\partial V} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial D_i}{\partial \rho} = \frac{\partial E}{\partial \rho} - \frac{\partial F_i}{\partial \rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\frac{\partial D_i}{\partial T} = \frac{\partial E}{\partial T} - \frac{\partial F_i}{\partial T} \quad , \quad i = 1, 2, \cdots, 5$$

where only the $(\partial D_i / \partial c_j)$'s of interest are calculated.

4.2.23 Calculation of f_i, α_i and $\beta_{i,j}$ for the Fluid Dynamic Equations

For subsonic flow, f_i, α_i and $\beta_{i,j}$ for the fluid dynamic equations are calculated from the following relationships:

For ρ_{pi}

$$f_{i+62} = \left(\frac{1}{\gamma P} \frac{M^2 - 1}{M^2} \frac{dP}{dx} - D_i\right) \rho_{pi} \quad , \quad i = 1, 2, \cdots, 5$$

$$\alpha_{i+62} = \frac{M^2 - 1}{M^2} \frac{\rho_{pi}}{\gamma P} \left[\frac{d^2P}{dx^2} - \frac{1}{P}\left(\frac{dP}{dx}\right)^2\right] \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62, j} = \rho_{pi} \left\{\frac{1}{P} \frac{dP}{dx} \frac{1}{\gamma \left(M^2\right)^2} \left[\frac{\partial M^2}{\partial c_j} - \frac{M^2(M^2 - 1)}{\gamma} \frac{\partial \gamma}{\partial c_j}\right] - \frac{\partial D_i}{\partial c_j}\right\}$$

$$i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{i+62, i+57} = -\rho_{pi} \frac{\partial D_i}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\, i+62} = -D_i - \rho_{pi} \frac{\partial D_i}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\, i+67} = -\rho_{pi} \frac{\partial D_i}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\, 73} = \rho_{pi} \left[\frac{1}{P} \frac{dP}{dx} - \frac{1}{\gamma \left(M^2\right)^2} \frac{\partial M^2}{\partial V} - \frac{\partial D_i}{\partial V} \right] \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\, 74} = -\rho_{pi} \frac{\partial D_i}{\partial \rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\, 75} = \rho_{pi} \left\{ \frac{1}{P} \frac{dP}{dx} \frac{1}{\gamma \left(M^2\right)^2} \left[\frac{\partial M^2}{\partial T} - \frac{M^2(M^2 - 1)}{\gamma} \frac{\partial \gamma}{\partial T} \right] - \frac{\partial D_i}{\partial T} \right\} \quad , \quad i = 1, 2, \cdots, 5$$

where only the $\beta_{i+62,\, j}$'s of interest are calculated.

For V

$$f_{73} = -\frac{1}{\rho V} \left(\frac{dP}{dx} + C \right)$$

$$\alpha_{73} = -\frac{1}{\rho V} \frac{d^2P}{dx^2}$$

$$\beta_{73,\, j} = -\frac{1}{\rho V} \frac{\partial C}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{73,\, i+57} = -\frac{1}{\rho V} \frac{\partial C}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{73,\, i+62} = -\frac{1}{\rho V} \frac{\partial C}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{73,\, 73} = -\frac{f_{73}}{V} - \frac{1}{\rho V} \frac{\partial C}{\partial V}$$

$$\beta_{73,74} = -\frac{f_{73}}{\rho} - \frac{1}{\rho V}\frac{\partial C}{\partial \rho}$$

$$\beta_{73,75} = -\frac{1}{\rho V}\frac{\partial C}{\partial T}$$

where only the $\beta_{73,j}$'s of interest are calculated.

For ρ

$$f_{74} = \left(\frac{1}{\gamma P}\frac{dP}{dx} - A\right)\rho$$

$$\alpha_{74} = \frac{\rho}{\gamma P}\left[\frac{d^2P}{dx^2} - \frac{1}{P}\left(\frac{dP}{dx}\right)^2\right]$$

$$\beta_{74,j} = -\frac{\rho}{\gamma^2 P}\frac{dP}{dx}\frac{\partial \gamma}{\partial c_j} - \rho\frac{\partial A}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{74,i+57} = -\rho\frac{\partial A}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{74,i+62} = -\rho\frac{\partial A}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{74,i+67} = -\rho\frac{\partial A}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{74,73} = -\rho\frac{\partial A}{\partial V}$$

$$\beta_{74,74} = \frac{1}{\rho} f_{74} - \rho\frac{\partial A}{\partial \rho}$$

$$\beta_{74,75} = -\rho\left(\frac{\partial A}{\partial T} + \frac{1}{\gamma^2 P}\frac{dP}{dx}\frac{\partial \gamma}{\partial T}\right)$$

where only the $\beta_{74,j}$'s of interest are calculated.

For T

$$f_{75} = \left(\frac{\gamma - 1}{\gamma} \frac{1}{P} \frac{dP}{dx} - B\right) T$$

$$\alpha_{75} = \frac{\gamma - 1}{\gamma} \left[\frac{d^2P}{dx^2} - \frac{1}{P}\left(\frac{dP}{dx}\right)^2\right] \frac{T}{P}$$

$$\beta_{75,\, j} = \left(\frac{1}{\gamma^2} \frac{1}{P} \frac{dP}{dx} \frac{\partial \gamma}{\partial c_j} - \frac{\partial B}{\partial c_j}\right) T \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{75,\, i+57} = -T \frac{\partial B}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{75,\, i+62} = -T \frac{\partial B}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{75,\, i+67} = -T \frac{\partial B}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{75,\, 73} = -T \frac{\partial B}{\partial V}$$

$$\beta_{75,\, 74} = -T \frac{\partial B}{\partial \rho}$$

$$\beta_{75,\, 75} = \frac{f_{75}}{T} + \frac{1}{\gamma^2} \frac{T}{P} \frac{dP}{dx} \frac{\partial \gamma}{\partial T} - T \frac{\partial B}{\partial T}$$

where only the $\beta_{75,\, j}$'s of interest are calculated.

For supersonic flows, f_i α_i and $\beta_{i,\, j}$ for the fluid dynamic equations are calculated from the following relationships:

For ρ_{pi}

$$f_{i+62} = -\left(\frac{1}{a} \frac{da}{dx} - F_i\right) \quad , \quad i = 1, 2, \cdots, 5$$

$$\alpha_{i+62} = -\frac{1}{a} \left[\frac{d^2a}{dx^2} - \frac{1}{a}\left(\frac{da}{dx}\right)^2\right] \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\,j} = \frac{\partial F_i}{\partial c_j} \quad , \quad i = 1, 2, \cdots, 5 \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{i+62,\,i+57} = \frac{\partial F_i}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\,i+62} = \frac{\partial F_i}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\,73} = \frac{\partial F_i}{\partial V} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\,74} = \frac{\partial F_i}{\partial \rho} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{i+62,\,75} = \frac{\partial F_i}{\partial T} \quad , \quad i = 1, 2, \cdots, 5$$

where only the $\beta_{i+62,\,j}$'s of interest are calculated.

For V

$$f_{73} = \left(\frac{1}{a}\frac{da}{dx} - E\right)\frac{V}{M^2 - 1}$$

$$\alpha_{73} = \frac{1}{a}\left[\frac{d^2a}{dx^2} - \frac{1}{a}\left(\frac{da}{dx}\right)^2\right]\frac{V}{M^2 - 1}$$

$$\beta_{73,\,j} = -\frac{V}{M^2 - 1}\frac{\partial E}{\partial c_j} - \frac{f_{73}}{M^2 - 1}\frac{\partial M^2}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{73,\,i+57} = \frac{-V}{M^2 - 1}\frac{\partial E}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{73,\,i+62} = \frac{-V}{M^2 - 1}\frac{\partial E}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{73,\,i+67} = \frac{-V}{M^2 - 1}\frac{\partial E}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{73,73} = f_{73}\left(\frac{1}{V} - \frac{1}{M^2 - 1}\frac{\partial M^2}{\partial V}\right) - \frac{V}{M^2 - 1}\frac{\partial E}{\partial V}$$

$$\beta_{73,74} = \frac{-V}{M^2 - 1}\frac{\partial E}{\partial \rho}$$

$$\beta_{73,75} = \frac{-f_{73}}{M^2 - 1}\frac{\partial M^2}{\partial T} - \frac{V}{M^2 - 1}\frac{\partial E}{\partial T}$$

$$\beta_{73,76} = \frac{-V}{M^2 - 1}\frac{\partial E}{\partial P}$$

where only the $\beta_{73,j}$'s of interest are calculated.

For ρ

$$f_{74} = -\left[\left(\frac{1}{a}\frac{da}{dx} - E\right)\frac{M^2}{M^2 - 1} + A\right]\rho$$

$$\alpha_{74} = -\frac{1}{a}\left[\frac{d^2a}{dx^2} - \frac{1}{a}\left(\frac{da}{dx}\right)^2\right]\frac{\rho M^2}{M^2 - 1}$$

$$\beta_{74,j} = -\frac{\rho}{\left(M^2 - 1\right)^2}\left(E - \frac{1}{a}\frac{da}{dx}\right)\frac{\partial M^2}{\partial c_j} + \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial c_j} - \frac{\partial A}{\partial c_j}\right),$$

$$j = 1, 2, \cdots, 57$$

$$\beta_{74,i+57} = \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial V_{pi}} - \frac{\partial A}{\partial V_{pi}}\right), \quad i = 1, 2, \cdots, 5$$

$$\beta_{74,i+62} = \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial \rho_{pi}} - \frac{\partial A}{\partial \rho_{pi}}\right), \quad i = 1, 2, \cdots, 5$$

$$\beta_{74,i+67} = \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial h_{pi}} - \frac{\partial A}{\partial h_{pi}}\right), \quad i = 1, 2, \cdots, 5$$

$$\beta_{74,73} = \frac{-\rho}{\left(M^2 - 1\right)^2}\left(E - \frac{1}{a}\frac{da}{dx}\right)\frac{\partial M^2}{\partial V} + \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial V} - \frac{\partial A}{\partial V}\right)$$

$$\beta_{74,74} = \frac{f_{74}}{\rho} + \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial \rho} - \frac{\partial A}{\partial \rho}\right)$$

$$\beta_{74,75} = -\frac{\rho}{\left(M^2 - 1\right)^2}\left(E - \frac{1}{a}\frac{da}{dx}\right)\frac{\partial M^2}{\partial T} + \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial T} - \frac{\partial A}{\partial T}\right)$$

$$\beta_{74,76} = \rho\left(\frac{M^2}{M^2 - 1}\frac{\partial E}{\partial P} - \frac{\partial A}{\partial P}\right)$$

where only the $\beta_{74,j}$'s of interest are calculated.

For T

$$f_{75} = -\left[(\gamma - 1)\left(\frac{1}{a}\frac{da}{dx} - E\right)\frac{M^2}{M^2 - 1} + B\right] T$$

$$\alpha_{75} = -\frac{(\gamma - 1)}{a}\left[\frac{d^2a}{dx^2} - \frac{1}{a}\left(\frac{da}{dx}\right)^2\right]\frac{TM^2}{M^2 - 1}$$

$$\beta_{75,j} = -\frac{(\gamma - 1)T}{\left(M^2 - 1\right)^2}\left(E - \frac{1}{a}\frac{da}{dx}\right)\frac{\partial M^2}{\partial c_j} + \frac{(\gamma - 1)TM^2}{M^2 - 1}\frac{\partial E}{\partial c_j} - T\frac{\partial B}{\partial c_j}$$

$$+ \frac{TM^2}{M^2 - 1}\left(E - \frac{1}{a}\frac{da}{dx}\right)\frac{\partial \gamma}{\partial c_j}, \quad j = 1, 2, \cdots, 57$$

$$\beta_{75,i+57} = \frac{T(\gamma - 1)M^2}{M^2 - 1}\frac{\partial E}{\partial V_{pi}} - T\frac{\partial B}{\partial V_{pi}}, \quad i = 1, 2, \cdots, 5$$

$$\beta_{75,i+62} = \frac{T(\gamma - 1)M^2}{M^2 - 1}\frac{\partial E}{\partial \rho_{pi}} - T\frac{\partial B}{\partial \rho_{pi}}, \quad i = 1, 2, \cdots, 5$$

$$\beta_{75,i+67} = \frac{T(\gamma - 1)M^2}{M^2 - 1}\frac{\partial E}{\partial h_{pi}} - T\frac{\partial B}{\partial h_{pi}}, \quad i = 1, 2, \cdots, 5$$

$$\beta_{75,73} = -\frac{(\gamma - 1)T}{\left(M^2 - 1\right)^2}\left(E - \frac{1}{a}\frac{da}{dx}\right)\frac{\partial M^2}{\partial V} + \frac{(\gamma - 1)M^2T}{M^2 - 1}\frac{\partial E}{\partial V} - T\frac{\partial B}{\partial V}$$

$$\beta_{75,74} = \frac{(\gamma - 1)TM^2}{M^2 - 1} \frac{\partial E}{\partial \rho} - T \frac{\partial B}{\partial \rho}$$

$$\beta_{75,75} = \frac{f_{75}}{T} - \frac{(\gamma - 1)T}{\left(M^2 - 1\right)^2} \left(E - \frac{1}{a} \frac{da}{dx}\right) \frac{\partial M^2}{\partial T} + \frac{(\gamma - 1)M^2 T}{M^2 - 1} \frac{\partial E}{\partial T} - T \frac{\partial B}{\partial T}$$

$$+ \left(E - \frac{1}{a} \frac{da}{dx}\right) \frac{M^2 T}{M^2 - 1} \frac{\partial \gamma}{\partial T}$$

$$\beta_{75,76} = \frac{(\gamma - 1)TM^2}{M^2 - 1} \frac{\partial E}{\partial P} - T \frac{\partial B}{\partial P}$$

where only the $\beta_{75,j}$'s of interest are calculated.

For P

$$f_{76} = -\left(\frac{1}{a} \frac{da}{dx} - E\right) \frac{\gamma M^2 P}{M^2 - 1}$$

$$\alpha_{76} = -\frac{1}{a} \left[\frac{d^2 a}{dx^2} - \frac{1}{a} \left(\frac{da}{dx}\right)^2\right] \frac{\gamma M^2 P}{M^2 - 1}$$

$$\beta_{76,j} = -\frac{f_{76}}{M^2(M^2 - 1)} \frac{\partial M^2}{\partial c_j} + \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial c_j} + \frac{f_{76}}{\gamma} \frac{\partial \gamma}{\partial c_j} \quad , \quad j = 1, 2, \cdots, 57$$

$$\beta_{76,i+57} = \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial V_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{76,i+62} = \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial \rho_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{76,i+67} = \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial h_{pi}} \quad , \quad i = 1, 2, \cdots, 5$$

$$\beta_{76,73} = -\frac{f_{76}}{M^2(M^2 - 1)} \frac{\partial M^2}{\partial V} + \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial V}$$

$$\beta_{76,74} = \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial \rho}$$

$$\beta_{76,75} = - \frac{f_{76}}{M^2(M^2 - 1)} \frac{\partial M^2}{\partial T} + \frac{\gamma M^2 P}{M^2 - 1} \frac{\partial E}{\partial T} + \frac{f_{76}}{\gamma} \frac{\partial \gamma}{\partial T}$$

$$\beta_{76,76} = \frac{f_{76}}{P}$$

where only the $\beta_{76,j}$'s of interest are calculated.

4.3 INTEGRATION SUBROUTINE

Given the derivatives (f_i) and partial derivatives (α_i and $\beta_{i,j}$) of the chemical relaxation equations and the fluid dynamic equations, this subroutine integrates these equations using the second order implicit integration method described in Section 3. The subroutine also determines the integration step size required to maintain the integration accuracy within prescribed bounds. These calculations are performed in the following order:

- Values of the derivatives and partial derivatives at the present point are obtained from the Derivative Evaluation Subroutine (described in Section 4.2) using the species concentrations and fluid dynamic variables.
- Values of the species concentrations and the fluid dynamic variables at the next point in the nozzle are calculated from the corrector formulas.
- The maximum allowable integration step size which will maintain the integration accuracy within the prescribed bounds is calculated from the error formulas and the next integration step size is calculated.
- The integration then proceeds using the calculated step size.

The calculations performed in this subroutine are described in the following sections.

4.3.1 Integration Procedure

The species concentrations and the fluid dynamic variables at the forward point are calculated by solving the appropriate set of linear nonhomogeneous algebraic equations.

Initial Step

$$\left(1 - \frac{1}{2}\beta_{i,i,o}h\right) k_{i,1} - \frac{1}{2}\sum_{j=1}^{N}(1 - \delta_{i,j})\beta_{i,j,o}k_{j,1}h = \frac{1}{2}\alpha_{i,o}h$$

General Step

$$\left(1 - \frac{2}{3}\beta_{i,i,n}h\right) k_{i,n+1} - \frac{2}{3}\sum_{j=1}^{N}(1 - \delta_{i,j})\beta_{i,j,n}k_{j,n+1}h = \frac{1}{3}\left[k_{i,n} + 2(f_{i,n} + \alpha_{i,n}h)h\right]$$

Special Step

$$\left(1 - \frac{h_{n+1} + h_n}{2h_{n+1} + h_n}\beta_{i,i,n}h_{n+1}\right)k_{i,n+1} - \frac{h_{n+1} + h_n}{(2h_{n+1} + h_n)h_n}\sum_{j=1}^{N}(1 - \delta_{i,j})\beta_{i,j,n}k_{j,n+1}h_{n+1}$$

$$= \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n}\left[k_{i,n} + (f_{i,n} + \alpha_{i,n}h_{n+1})\frac{h_n}{h_{n+1}}(h_{n+1} + h_n)\right]$$

The special step calculation is used only at print stations or in halving the step size if required. If the special step calculation is used to determine the properties at a print station, the calculation is resumed using the general step calculation and the previous step size (h_n).

4.3.2 Step Size Determination

After each integration step (after the second step), the integration step size for the next step is calculated from

$$h_{n+2} = 2h_{n+1}, \quad \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}}\right|_{max} < \frac{\delta}{10}$$

$$h_{n+2} = \frac{1}{2} h_{n+1} \quad , \quad \left| \frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}} \right|_{max} > \delta$$

$$h_{n+2} = h_{n+1} \quad , \quad \frac{\delta}{10} \leq \left| \frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3k_{i,n+1} - k_{i,n}} \right|_{max} \leq \delta$$

On option, only the fluid dynamic equations are used in determining the integration step size. If the step size is halved for the third step, the integration is restarted with half the original step size.

4.4 SPECIES THERMAL FUNCTION SUBROUTINE

Given the temperature, this subroutine calculates the species free energy (F_i), enthalpy (h_i), heat capacity (C_{pi}) and the heat capacity temperature derivative (dC_{pi}/dT). For the species of interest, these quantities are calculated from

$$F_i = F_i(n\Delta T_T) + \frac{F_i(n\Delta T_T) - h_i(n\Delta T_T)}{n\Delta T_T}(T - n\Delta T_T) - \frac{1}{2}\frac{C_{pi}(n\Delta T_T)}{n\Delta T_T}\left(T - n\Delta T_T\right)^2$$

$$h_i = h_i(n\Delta T_T) + C_{pi}(n\Delta T_T)(T - n\Delta T_T) + \frac{1}{2}\left.\frac{dC_{pi}}{dT}\right|_{n\Delta T_T}\left(T - n\Delta T_T\right)^2$$

$$C_{pi} = C_{pi}(n\Delta T_T) + \left.\frac{dC_{pi}}{dT}\right|_{n\Delta T_T}(T - n\Delta T_T) + \frac{1}{2}\left.\frac{d^2C_{pi}}{dT^2}\right|_{n\Delta T_T}\left(T - n\Delta T_T\right)^2$$

$$\frac{dC_{pi}}{dT} = \left.\frac{dC_{pi}}{dT}\right|_{n\Delta T_T} + \left.\frac{d^2C_{pi}}{dT^2}\right|_{n\Delta T_T}(T - n\Delta T_T)$$

when $|T - n\Delta T_T| \leq (1/2)n\Delta T_T$. If $|T - n\Delta T_T| > (1/2)n\Delta T_T$, n is set equal to the integer nearest $T/\Delta T_T$ and new values of $F_i(n\Delta T_T)$, $h_i(n\Delta T_T)$, $C_{pi}(n\Delta T_T)$, $dC_{pi}/dT|_{n\Delta T_T}$ and $d^2C_{pi}/dT^2|_{n\Delta T_T}$ are obtained from the thermal function tables.

4.5 EQUILIBRIUM FUNCTION SUBROUTINE

Given the temperature and species thermal functions, this subroutine calculates the dissociation-recombination reaction equilibrium constants and their temperature derivatives. For the reactions of interest, these quantities are calculated from:

Reaction 1, $CO_2 + M \rightleftharpoons CO + O + M$

$$K_1 = \frac{13.9432}{T} e^{-\left[(\Delta H_1/T) + F_1 - F_3 - F_{18}\right]}$$

$$\frac{dK_1}{dT} = \left(-\frac{h_1}{R_1 T} + \frac{h_3}{R_3 T} + \frac{h_{18}}{R_{18} T} - 1\right)\frac{K_1}{T}$$

Reaction 2, $H_2O + M \rightleftharpoons OH + H + M$

$$K_2 = \frac{1.30296}{T} e^{-\left[(\Delta H_2 + T) + F_2 - F_{11} - F_{16}\right]}$$

$$\frac{dK_2}{dT} = \left(-\frac{h_2}{R_2 T} + \frac{h_{11}}{R_{11} T} + \frac{h_{16}}{R_{16} T} - 1\right)\frac{K_2}{T}$$

Reaction 3, $CO + M \rightleftharpoons C + O + M$

$$K_3 = \frac{9.39389}{T} e^{-\left[(\Delta H_3/T) + F_3 - F_{13} - F_{18}\right]}$$

$$\frac{dK_3}{dT} = \left(-\frac{h_3}{R_3 T} + \frac{h_{13}}{R_{13} T} + \frac{h_{18}}{R_{18} T} - 1\right)\frac{K_3}{T}$$

Reaction 4, $Cl_2 + M \rightleftharpoons 2Cl + M$

$$K_4 = \frac{24.2743}{T} e^{-\left[(\Delta H_4/T) + F_4 - 2F_{14}\right]}$$

$$\frac{dK_4}{dT} = \left(-\frac{h_4}{R_4 T} + 2\frac{h_{14}}{R_{14} T} - 1\right)\frac{K_4}{T}$$

Reaction 5, $F_2 + M \rightleftharpoons 2F + M$

$$K_5 = \frac{13.0076}{T} e^{-\left[(\Delta H_5/T) + F_5 - 2F_{15}\right]}$$

$$\frac{dK_5}{dT} = \left(-\frac{h_5}{R_5 T} + 2\frac{h_{15}}{R_{15} T} - 1\right)\frac{K_5}{T}$$

Reaction 6, $HCl + M \rightleftharpoons H + Cl + M$

$$K_6 = \frac{1.34203}{T} e^{-\left[(\Delta H_6/T) + F_6 - F_{14} - F_{16}\right]}$$

$$\frac{dK_6}{dT} = \left(-\frac{h_6}{R_6 T} + \frac{h_{14}}{R_{14} T} + \frac{h_{16}}{R_{16} T} - 1\right)\frac{K_6}{T}$$

Reaction 7, $HF + M \rightleftharpoons H + F + M$

$$K_7 = \frac{1.31064}{T} e^{-\left[(\Delta H_7/T) + F_7 - F_{15} - F_{16}\right]}$$

$$\frac{dK_7}{dT} = \left(-\frac{h_7}{R_7 T} + \frac{h_{15}}{R_{15} T} + \frac{h_{16}}{R_{16} T} - 1\right)\frac{K_7}{T}$$

Reaction 8, $H_2\ M \rightleftharpoons 2H + M$

$$K_8 = \frac{0.690085}{T} e^{-\left[(\Delta H_8/T) + F_8 - 2F_{16}\right]}$$

$$\frac{dK_8}{dT} = \left(-\frac{h_8}{R_8 T} + 2\frac{h_{16}}{R_{16} T} - 1\right)\frac{K_8}{T}$$

Reaction 9, $N_2 + M \rightleftharpoons 2N + M$

$$K_9 = \frac{9.59005}{T} e^{-\left[(\Delta H_9/T) + F_9 - 2F_{17}\right]}$$

$$\frac{dK_9}{dT} = \left(-\frac{h_9}{R_9 T} + 2\frac{h_{17}}{R_{17} T} - 1\right)\frac{K_9}{T}$$

Reaction 10, $NO + M \rightleftarrows N + O + M$

$$K_{10} = \frac{10.2267}{T} e^{-\left[(\Delta H_{10}/T) + F_{10} - F_{17} - F_{18}\right]}$$

$$\frac{dK_{10}}{dT} = \left(- \frac{h_{10}}{R_{10}T} + \frac{h_{17}}{R_{17}T} + \frac{h_{18}}{R_{18}T} - 1\right) \frac{K_{10}}{T}$$

Reaction 11, $OH + M \rightleftarrows O + H + M$

$$K_{11} = \frac{1.29838}{T} e^{-\left[(\Delta H_{11}/T + F_{11} - F_{16} - F_{18}\right]}$$

$$\frac{dK_{11}}{dT} = \left(- \frac{h_{11}}{R_{11}T} + \frac{h_{16}}{R_{16}T} + \frac{h_{18}}{R_{18}T} - 1\right) \frac{K_{11}}{T}$$

Reaction 12, $O_2 + M \rightleftarrows 2O + M$

$$K_{12} = \frac{10.9538}{T} e^{-\left[(\Delta H_{12}/T) + F_{12} - 2F_{18}\right]}$$

$$\frac{dK_{12}}{dT} = \left(- \frac{h_{12}}{R_{12}T} + 2\frac{h_{18}}{R_{18}T} - 1\right) \frac{K_{12}}{T}$$

Reaction 40, $AlO + M \rightleftarrows Al + O + M$

$$K_{40} = \frac{13.7522}{T} e^{-\left[(\Delta H_{40}/T) + F_{20} - F_{18} - F_{19}\right]}$$

$$\frac{dK_{40}}{dT} = \left(- \frac{h_{20}}{R_{20}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{19}}{R_{19}T} - 1\right) \frac{K_{40}}{T}$$

Reaction 41, $Al_2O + M \rightleftarrows Al + AlO + M$

$$K_{41} = \frac{22.6952}{T} e^{-\left[(\Delta H_{41}/T) + F_{21} - F_{19} - F_{20}\right]}$$

$$\frac{dK_{41}}{dT} = \left(- \frac{h_{21}}{R_{21}T} + \frac{h_{19}}{R_{19}T} + \frac{h_{20}}{R_{20}T} - 1\right) \frac{K_{41}}{T}$$

Reaction 42, $AlCl + M \rightleftharpoons Al + Cl + M$

$$K_{42} = \frac{20.9786}{T} e^{-\left[(\Delta H_{42}/T) + F_{22} - F_{14} - F_{19}\right]}$$

$$\frac{dK_{42}}{T} = \left(- \frac{h_{22}}{R_{22}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{19}}{R_{19}T} - 1\right) \frac{K_{42}}{T}$$

Reaction 43, $AlCl_2 + M \rightleftharpoons AlCl + Cl + M$

$$K_{43} = \frac{30.9644}{T} e^{-\left[(\Delta H_{43}/T) + F_{23} - F_{14} - F_{22}\right]}$$

$$\frac{dK_{43}}{dT} = \left(- \frac{h_{23}}{R_{23}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{22}}{R_{22}T} - 1\right) \frac{K_{43}}{T}$$

Reaction 44, $AlOCl + M \rightleftharpoons AlO + Cl + M$

$$K_{44} = \frac{26.6025}{T} e^{-\left[(\Delta H_{44}/T) + F_{24} - F_{14} - F_{20}\right]}$$

$$\frac{dK_{44}}{dT} = \left(- \frac{h_{24}}{R_{24}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{20}}{R_{20}T} - 1\right) \frac{K_{44}}{T}$$

Reaction 45, $AlOCl + M \rightleftharpoons AlCl + O + M$

$$K_{45} = \frac{17.4388}{T} e^{-\left[(\Delta H_{45}/T) + F_{24} - F_{18} - F_{22}\right]}$$

$$\frac{dK_{45}}{dT} = \left(- \frac{h_{24}}{R_{24}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{22}}{R_{22}T} - 1\right) \frac{K_{45}}{T}$$

Reaction 46, $AlF + M \rightleftharpoons Al + F + M$

$$K_{46} = \frac{15.2652}{T} e^{-\left[(\Delta H_{46}/T) + F_{25} - F_{15} - F_{19}\right]}$$

$$\frac{dK_{46}}{dT} = \left(- \frac{h_{25}}{R_{25}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{19}}{R_{19}T} - 1\right) \frac{K_{46}}{T}$$

Reaction 47, $AlF_2 + M \rightleftharpoons AlF + F + M$

$$K_{47} = \frac{18.4085}{T} e^{-\left[(\Delta H_{47}/T) + F_{26} - F_{15} - F_{25}\right]}$$

$$\frac{dK_{47}}{dT} = \left(- \frac{h_{26}}{R_{26}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{25}}{R_{25}T} - 1\right) \frac{K_{47}}{T}$$

Reaction 48, $AlOF + M \rightleftharpoons AlO + F + M$

$$K_{48} = \frac{18.0403}{T} e^{-\left[(\Delta H_{48}/T) + F_{27} - F_{15} - F_{20}\right]}$$

$$\frac{dK_{48}}{dT} = \left(- \frac{h_{27}}{R_{27}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{20}}{R_{20}T} - 1\right) \frac{K_{48}}{T}$$

Reaction 49, $AlOF + M \rightleftharpoons AlF + O + M$

$$K_{49} = \frac{16.2522}{T} e^{-\left[(\Delta H_{49}/T) + F_{27} - F_{18} - F_{25}\right]}$$

$$\frac{dK_{49}}{dT} = \left(- \frac{h_{27}}{R_{27}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{25}}{R_{25}T} - 1\right) \frac{K_{49}}{T}$$

Reaction 100, $BeCl_2 + M \rightleftharpoons BeCl + Cl + M$

$$K_{100} = \frac{27.0116}{T} e^{-\left[(\Delta H_{100}/T) + F_{45} - F_{14} - F_{44}\right]}$$

$$\frac{dK_{100}}{dT} = \left(- \frac{h_{45}}{R_{45}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{44}}{R_{44}T} - 1\right) \frac{K_{100}}{T}$$

Reaction 101, $BeF_2 + M \rightleftharpoons BeF + F + M$

$$K_{101} = \frac{15.5014}{T} e^{-\left[(\Delta H_{101}/T) + F_{47} - F_{15} - F_{46}\right]}$$

$$\frac{dK_{101}}{dT} = \left(- \frac{h_{47}}{R_{47}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{46}}{R_{46}T} - 1\right) \frac{K_{101}}{T}$$

Reaction 102, $BeOH + M \rightleftharpoons Be + OH + M$

$$K_{102} = \frac{8.06628}{T} e^{-\left[(\Delta H_{102}/T) + F_{43} - F_{11} - F_{40}\right]}$$

$$\frac{dK_{102}}{dT} = \left(-\frac{h_{43}}{R_{43}T} + \frac{h_{11}}{R_{11}T} + \frac{h_{40}}{R_{40}T} - 1\right)\frac{K_{102}}{T}$$

Reaction 103, $BeOH + M \rightleftharpoons BeO + H + M$

$$K_{103} = \frac{1.32671}{T} e^{-\left[(\Delta H_{103}/T) + F_{43} - F_{16} - F_{41}\right]}$$

$$\frac{dK_{103}}{dT} = \left(-\frac{h_{43}}{R_{43}T} + \frac{h_{16}}{R_{16}T} + \frac{h_{41}}{R_{41}T} - 1\right)\frac{K_{103}}{T}$$

Reaction 104, $BeCl + M \rightleftharpoons Be + Cl + M$

$$K_{104} = \frac{9.83964}{T} e^{-\left[(\Delta H_{104}/T) + F_{44} - F_{14} - F_{40}\right]}$$

$$\frac{dK_{104}}{dT} = \left(-\frac{h_{44}}{R_{44}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{40}}{R_{40}T} - 1\right)\frac{K_{104}}{T}$$

Reaction 105, $BeF + M \rightleftharpoons Be + F + M$

$$K_{105} = \frac{8.37025}{T} e^{-\left[(\Delta H_{105}/T) + F_{46} - F_{15} - F_{40}\right]}$$

$$\frac{dK_{105}}{dT} = \left(-\frac{h_{46}}{R_{46}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{40}}{R_{40}T} - 1\right)\frac{K_{105}}{T}$$

Reaction 106, $BeO + M \rightleftharpoons Be + O + M$

$$K_{106} = \frac{7.89402}{T} e^{-\left[(\Delta H_{106}/T) + F_{41} - F_{18} - F_{40}\right]}$$

$$\frac{dK_{106}}{dT} = \left(-\frac{h_{41}}{R_{41}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{40}}{R_{40}T} - 1\right)\frac{K_{106}}{T}$$

Reaction 107, $Be_2O + M \rightleftharpoons Be + BeO + M$

$$K_{107} = \frac{9.07194}{T} e^{-\left[(\Delta H_{107}/T) + F_{42} - F_{40} - F_{41}\right]}$$

$$\frac{dK_{107}}{dT} = \left(- \frac{h_{42}}{R_{42}T} + \frac{h_{40}}{R_{40}T} + \frac{h_{41}}{R_{41}T} - 1\right) \frac{K_{107}}{T}$$

Reaction 108, $BeO_2H_2 + M \rightleftharpoons BeOH + OH + M$

$$K_{108} = \frac{14.0829}{T} e^{-\left[(\Delta H_{108}/T) + F_{48} - F_{11} - F_{43}\right]}$$

$$\frac{dK_{108}}{dT} = \left(- \frac{h_{48}}{R_{48}T} + \frac{h_{11}}{R_{11}T} + \frac{h_{43}}{R_{43}T} - 1\right) \frac{K_{108}}{T}$$

Reaction 148, $BN + M \rightleftharpoons B + N + M$

$$K_{148} = \frac{8.35866}{T} e^{-\left[(\Delta H_{148}/T) + F_{29} - F_{17} - F_{28}\right]}$$

$$\frac{dK_{148}}{dT} = \left(- \frac{h_{29}}{R_{29}T} + \frac{h_{17}}{R_{17}T} + \frac{h_{28}}{R_{28}T} - 1\right) \frac{K_{148}}{T}$$

Reaction 149, $BO + M \rightleftharpoons B + O + M$

$$K_{149} = \frac{8.83820}{T} e^{-\left[(\Delta H_{149}/T) + F_{30} - F_{18} - F_{28}\right]}$$

$$\frac{dK_{149}}{dT} = \left(- \frac{h_{30}}{R_{30}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{28}}{R_{28}T} - 1\right) \frac{K_{149}}{T}$$

Reaction 150, $BO_2 + M \rightleftharpoons BO + O + M$

$$K_{150} = \frac{13.7217}{T} e^{-\left[(\Delta H_{150}/T) + F_{31} - F_{18} - F_{30}\right]}$$

$$\frac{dK_{150}}{dT} = \left(- \frac{h_{31}}{R_{31}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{30}}{R_{30}T} - 1\right) \frac{K_{150}}{T}$$

Reaction 151, $BCl + M \rightleftharpoons B + Cl + M$

$$K_{151} = \frac{11.3511}{T} e^{-\left[(\Delta H_{151}/T) + F_{32} - F_{14} - F_{28}\right]}$$

$$\frac{dK_{151}}{dT} = \left(- \frac{h_{32}}{R_{32}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{28}}{R_{28}T} - 1\right)\frac{K_{151}}{T}$$

Reaction 152, $BCl_2 + M \rightleftharpoons BCl + Cl + M$

$$K_{152} = \frac{27.4878}{T} e^{-\left[(\Delta H_{152}/T) + F_{33} - F_{14} - F_{32}\right]}$$

$$\frac{dK_{152}}{dT} = \left(- \frac{h_{33}}{R_{33}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{32}}{R_{32}T} - 1\right)\frac{K_{152}}{T}$$

Reaction 153, $BCl_3 + M \rightleftharpoons BCl_2 + Cl + M$

$$K_{153} = \frac{33.8628}{T} e^{-\left[(\Delta H_{153}/T + F_{34} - F_{14} - F_{33}\right]}$$

$$\frac{dK_{153}}{dT} = \left(- \frac{h_{34}}{R_{34}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{33}}{R_{33}T} - 1\right)\frac{K_{153}}{T}$$

Reaction 154, $BOCl + M \rightleftharpoons BCl + O + M$

$$K_{154} = \frac{16.2792}{T} e^{-\left[(\Delta H_{154}/T) + F_{35} - F_{18} - F_{32}\right]}$$

$$\frac{dK_{154}}{dT} = \left(- \frac{h_{35}}{R_{35}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{32}}{R_{32}T} - 1\right)\frac{K_{154}}{T}$$

Reaction 155, $BF + M \rightleftharpoons B + F + M$

$$K_{155} = \frac{9.43948}{T} e^{-\left[(\Delta H_{155}/T) + F_{36} - F_{15} - F_{28}\right]}$$

$$\frac{dK_{155}}{dT} = \left(- \frac{h_{36}}{R_{36}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{28}}{R_{28}T} - 1\right)\frac{K_{155}}{T}$$

Reaction 156, $BF_2 + M \rightleftharpoons BF + F + M$

$$K_{156} = \frac{15.8905}{T} e^{-\left[(\Delta H_{156}/T) + F_{37} - F_{15} - F_{36}\right]}$$

$$\frac{dK_{156}}{dT} = \left(- \frac{h_{37}}{R_{37}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{36}}{R_{36}T} - 1\right) \frac{K_{156}}{T}$$

Reaction 157, $BF_3 + M \rightleftharpoons BF_2 + F + M$

$$K_{157} = \frac{18.7270}{T} e^{-\left[(\Delta H_{157}/T) + F_{38} - F_{15} - F_{37}\right]}$$

$$\frac{dK_{157}}{dT} = \left(- \frac{h_{38}}{R_{38}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{37}}{R_{37}T} - 1\right) \frac{K_{157}}{T}$$

Reaction 158, $BOF + M \rightleftharpoons BO + F + M$

$$K_{158} = \frac{15.2276}{T} e^{-\left[(\Delta H_{158}/T) + F_{39} - F_{15} - F_{30}\right]}$$

$$\frac{dK_{158}}{dT} = \left(- \frac{h_{39}}{R_{39}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{30}}{R_{30}T} - 1\right) \frac{K_{158}}{T}$$

Reaction 159, $BOF + M \rightleftharpoons BF + O + M$

$$K_{159} = \frac{14.2577}{T} e^{-\left[(\Delta H_{159}/T) + F_{39} - F_{18} - F_{36}\right]}$$

$$\frac{dK_{159}}{dT} = \left(- \frac{h_{39}}{R_{39}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{36}}{R_{36}T} - 1\right) \frac{K_{159}}{T}$$

Reaction 225, $LiOH + M \rightleftharpoons Li + OH + M$

$$K_{225} = \frac{6.74867}{T} e^{-\left[(\Delta H_{225}/T) + F_{53} - F_{11} - F_{49}\right]}$$

$$\frac{dK_{225}}{dT} = \left(- \frac{h_{53}}{R_{53}T} + \frac{h_{11}}{R_{11}T} + \frac{h_{49}}{R_{49}T} - 1\right) \frac{K_{225}}{T}$$

Reaction 226, $LiOH + M \rightleftarrows LiO + H + M$

$$K_{226} = \frac{1.32208}{T} e^{-\left[(\Delta H_{226}/T) + F_{53} - F_{16} - F_{51}\right]}$$

$$\frac{dK_{226}}{dT} = \left(- \frac{h_{53}}{R_{53}T} + \frac{h_{16}}{R_{16}T} + \frac{h_{51}}{R_{51}T} - 1\right)\frac{K_{226}}{T}$$

Reaction 227, $LiCl + M \rightleftarrows Li + Cl + M$

$$K_{227} = \frac{7.94697}{T} e^{-\left[(\Delta H_{227}/T) + F_{55} - F_{14} - F_{49}\right]}$$

$$\frac{dK_{227}}{dT} = \left(- \frac{h_{55}}{R_{55}T} + \frac{h_{14}}{R_{14}T} + \frac{h_{49}}{R_{49}T} - 1\right)\frac{K_{227}}{T}$$

Reaction 228, $LiF + M \rightleftarrows Li + F + M$

$$K_{228} = \frac{6.96015}{T} e^{-\left[(\Delta H_{228}/T) + F_{54} - F_{15} - F_{49}\right]}$$

$$\frac{dK_{228}}{dT} = \left(- \frac{h_{54}}{R_{54}T} + \frac{h_{15}}{R_{15}T} + \frac{h_{49}}{R_{49}T} - 1\right)\frac{K_{228}}{T}$$

Reaction 229, $LiH + M \rightleftarrows Li + H + M$

$$K_{229} = \frac{1.20514}{T} e^{-\left[(\Delta H_{229}/T) + F_{50} - F_{16} - F_{49}\right]}$$

$$\frac{dK_{229}}{dT} = \left(- \frac{h_{50}}{R_{50}T} + \frac{h_{16}}{R_{16}T} + \frac{h_{49}}{R_{49}T} - 1\right)\frac{K_{229}}{T}$$

Reaction 230, $LiO + M \rightleftarrows Li + O + M$

$$K_{230} = \frac{6.62767}{T} e^{-\left[(\Delta H_{230}/T) + F_{51} - F_{18} - F_{49}\right]}$$

$$\frac{dK_{230}}{dT} = \left(- \frac{h_{51}}{R_{51}T} + \frac{h_{18}}{R_{18}T} + \frac{h_{49}}{R_{49}T} - 1\right)\frac{K_{230}}{T}$$

Reaction 231, $Li_2O + M \rightleftarrows Li + LiO + M$

$$K_{231} = \frac{7.29535}{T} e^{-\left[(\Delta H_{231}/T) + F_{52} - F_{49} - F_{51}\right]}$$

$$\frac{dK_{231}}{dT} = \left(-\frac{h_{52}}{R_{52}T} + \frac{h_{49}}{R_{49}T} + \frac{h_{51}}{R_{51}T} - 1\right)\frac{K_{231}}{T}$$

Reaction 232, $Li_2F_2 + M \rightleftarrows 2LiF + M$

$$K_{232} = \frac{17.7589}{T} e^{-\left[(\Delta H_{232}/T) + F_{56} - 2F_{54}\right]}$$

$$\frac{dK_{232}}{dT} = \left(-\frac{h_{56}}{R_{56}T} + 2\frac{h_{54}}{R_{54}T} - 1\right)\frac{K_{232}}{T}$$

Reaction 233, $Li_2Cl_2 + M \rightleftarrows 2LiCl + M$

$$K_{233} = \frac{29.0255}{T} e^{-\left[(\Delta H_{233}/T) + F_{57} - 2F_{55}\right]}$$

$$\frac{dK_{233}}{dT} = \left(-\frac{h_{57}}{R_{57}T} + 2\frac{h_{55}}{R_{55}T} - 1\right)\frac{K_{233}}{T}$$

4.6 OUTPUT SUBROUTINE

The output subroutine processes the output data, converts the data to the proper units and calculates the required output quantities. These calculations are performed in the following order.

- The pressure is converted to psia.
- The species mass fractions are converted to mole fractions.
- The performance parameters are calculated.
- The gas static enthalpy and the percentage total enthalpy change during the integration from the chamber are calculated.
- The entropy change from the chamber is calculated.
- The average expansion coefficients are calculated.

The calculations performed by this subroutine are described in the following sections.

4.6.1 Pressure Conversion

The pressure (in psia) is calculated from

$$P(\text{psia}) = \frac{P}{4633.056}$$

4.6.2 Species Concentration Conversion

The species mole fractions are calculated from

$$c_{i,m} = \frac{R_i}{R} c_i$$

4.6.3 Performance Parameter Calculation

At the throat, the characteristic exhaust velocity is calculated from

$$C^* = \frac{P_c}{\rho^* V^*}$$

The vacuum specific impulse is calculated from

$$I_{sp} = \frac{1}{32.174}\left(V + \frac{P}{\rho V}\right)$$

The vacuum thrust coefficient is calculated from

$$C_F = 32.174 \frac{I_{sp}}{c*}$$

4.6.4 Enthalpy Calculations

The gas static enthalpy is calculated from

$$h = \sum_{i=1}^{57} c_i h_i$$

where the sum is performed only over the species of interest. The percentage total enthalpy change during the integration from the chamber is calculated from

$$\Delta H_T(\%) = 100\left[1 - \frac{h + \frac{1}{2} V^2}{H_c}\right]$$

4.6.5 Entropy Change Calculation

The entropy change from the chamber is calculated from

$$\Delta S(\mathrm{Btu/lb}\ {}^{o}\mathrm{R}) = \frac{3.9952 \cdot 10^{-5}}{T} \sum_{i=1}^{18} c_i(h_i - F_i) - S_c$$

where the sum is performed only over the species of interest.

4.6.6 Average Expansion Coefficient Calculations

At the throat, the average temperature expansion coefficient is calculated from

$$N_T^* = 2\frac{T_c}{T*} - 1.$$

In the expansion cone, the average temperature expansion coefficient is calculated by iteration from

$$N_T^{(n+1)} = \frac{L^{(n)} + 1}{L^{(n)} - 1}$$

where

$$L^{(n)} = \frac{\ln\left[\dfrac{2}{N_T^{(n)} - 1}\,\epsilon^{2}\left(\dfrac{T_c}{T} - 1\right)\right]}{\ln\left[\dfrac{2}{N_T^{(n)} + 1}\,\dfrac{T_c}{T}\right]}$$

and $N_T^{(1)}$ is the last average temperature expansion coefficient calculated.

The average pressure expansion coefficient is calculated by iteration from

$$N_P^{(n+1)} = -2 \ln \frac{P}{P_c}\left[\ln\left\{\frac{2}{N_P^{(n)} - 1}\,\epsilon^{2}\left[1 - \left(\frac{P}{P_c}\right)^{N_P^{(n)} - 1/N_P^{(1)}}\right]\left(\frac{N_P^{(1)} + 1}{2}\right)^{N_P^{(n)} + 1/N_P^{(n)} - 1}\right\}\right]^{-1}$$

where $N_P^{(1)}$ is the last average temperature expansion coefficient calculated.

The average expansion gamma is calculated from

$$\overline{\gamma} = \frac{\ln \dfrac{P}{P_c}}{\ln \dfrac{\rho}{\rho_c}}$$

5. REFERENCES

1. J. O. Hirschfelder, C. F. Curtiss and R. B. Bird, Molecular Theory of Gases and Liquids, John Wiley and Sons, Inc., New York, 1954.

2. J. R. Kliegel, "Gas Particle Nozzle Flows," In Ninth International Symposium on Combustion, Academic Press, Inc., New York, 1963.

3. P. I. Gold, "Chemical Species of Importance in Nonequilibrium Performance Calculations," 5435-6005-TU000, TRW Systems, October 1965.

4. S. W. Benson and T. Fueno, "Mechanism of Atom Recombination by Consecutive Vibrational Deactivations," J. Chem. Physics 36, 1597 (1962).

5. T. F. Tyson, "An Implicit Integration Method for Chemical Kinetics," 9840-6002-RU-000, TRW Space Technology Laboratories, September 1964.