

**High Altitude Observatory**

National Center for Atmospheric Research, Boulder, CO

## **TIEGCM V1.8 Model Description Draft**

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This is a draft documentation of TIEGCM1.8. Not all the code is documented so far. We will work on the documentation to 1. fill in the gaps, 2. correct errors, 3. update to version TIEGCM1.9.

Every help is very much appreciated. If you have comments or corrections please send them to [maute@ucar.edu](mailto:maute@ucar.edu).

Thank you very much.

# Contents

<b>1</b>	<b>Code Structure Overview</b>	<b>1</b>
<b>2</b>	<b>Input</b>	<b>17</b>
2.1	Solar Input . . . . .	17
2.2	Magnetospheric Input . . . . .	18
2.2.1	Parameters to define the magnetospheric inputs . . . .	18
2.2.2	The Heelis convection pattern . . . . .	21
2.2.3	The Weimer convection pattern . . . . .	24
2.2.4	High latitude auroral pattern . . . . .	24
2.3	Lower Boundary . . . . .	39
2.3.1	Migrating tides specified by Hough Modes . . . . .	40
2.3.2	Migrating and non-migrating tides specified by GSWM	41
2.3.3	Specifics about the Lower Boundary of TIMEGCM . .	42
<b>3</b>	<b>Neutral Dynamics</b>	<b>45</b>
3.1	Calculation of geopotential height . . . . .	47
3.2	Calculation vertical velocity $W$ . . . . .	50
3.3	Momentum equation /DUV.F . . . . .	52
<b>4</b>	<b>Neutral Thermodynamics</b>	<b>63</b>
4.1	Calculation of $K_T$ , $\mu$ , $C_p$ / . . . . .	64
4.2	Thermodynamic equation / . . . . .	66
<b>5</b>	<b>Chemistry</b>	<b>77</b>
5.1	Calculation of chemical reaction rates / . . . . .	78
5.1.1	Module data . . . . .	78
5.1.2	Calculation of time dependent reaction rates . . . . .	80
5.2	Calculation of electron density $N_e$ , $N^+$ , $N_2^+$ , $NO^+$ / . . . . .	83

5.3	Calculation minor species $N(^4S)$ and $NO$ , (and $HOx$ in TIMEGCM)	88
5.4	Calculation of Minor species $N(^2D), N(^4S)$ , and $NO$	100
5.4.1	calculation of $N(^2D)$	100
5.4.2	calculation of $N(^4S)$	101
5.4.3	calculation of $NO$	104
5.5	Calculation of Major species $O_2$ , and $O$ / ,	106
5.5.1	Calculation of source and sinks for $O_2$ and $O$	106
5.5.2	Calculation of major species $O_2$ and $O$ / COMP.F	108
<b>6</b>	<b>Ionospheric precesses</b>	<b>123</b>
6.1	Joule heating calculation	124
6.1.1	Joule heating calculation for ion temperature	125
6.2	Ion drag calculation /	128
6.3	Calculation of electron and ion temperature /	133
6.4	Calculation of $O^+$ number density /	145
<b>7</b>	<b>Electrodynamics</b>	<b>161</b>
7.1	Introduction	162
7.2	Steady-State Electrodynamic Equations	163
7.3	Input to the Electrodynamo	168
7.4	Apex Coordinates	170
7.5	Latitudinal modified apex grid	171
7.6	Mapping from and to the geomagnetic grid	172
7.7	High Latitude Input	176
7.7.1	Weimer	176
7.7.2	Heelis	176
7.7.3	Modification of the high latitude input	176
7.8	Field line Integration	182
7.9	Gravity and plasma pressure driven current	191
7.9.1	Gravity Driven Current	191
7.9.2	Plasma Pressure Gradient Driven Current	192
7.9.3	Field-line Integration	195
7.10	Finite Differencing	197
7.11	Solving for the electric potential	209
7.11.1	Multigrid solver <code>mudcr2</code>	209
7.11.2	Multigrid solver <code>muhcr2</code> as direct solver	211

7.11.3	Modified multigrid solver <code>mudcr2</code> . . . . .	212
7.12	Electric Field . . . . .	213
7.13	Additional features . . . . .	214
7.13.1	Magnetic perturbations . . . . .	215
7.13.2	No electrodynamo calculation . . . . .	223
7.14	Electrodynamic drift velocity calculation / . . . . .	224
<b>8</b>	<b>Numerical Algorithms</b>	<b>227</b>
8.1	. . . . .	228
8.2	. . . . .	229



# List of Figures

1.1	TIEGCM Code Structure Contents . . . . .	2
1.2	main: TIEGCM main . . . . .	3
1.3	init: model initialization . . . . .	4
1.4	advance: advance model time . . . . .	5
1.5	dynamics: dynamics and chemistry drivers . . . . .	6
1.6	aurora: aurora parameterization . . . . .	7
1.7	oplus: $O^+$ calculation . . . . .	8
1.8	dynamo: calculation of electric potential . . . . .	9
1.9	minor species composition . . . . .	10
1.10	calculation of minor species . . . . .	11
1.11	major species composition . . . . .	12
1.12	duv: calculation of neutral horizontal winds . . . . .	13
1.13	output structure . . . . .	14
1.14	filtering in TIEGCM . . . . .	15
1.15	dt: calculation of neutral temperature . . . . .	16
2.1	The ion convection pattern (northern hemisphere) for cross-tail potential of 60 KV and the IMF $B_y = 7$ nT. Many of the specification parameters are illustrated. . . . .	25
2.2	Illustration of the parameterization of the auroral oval in the TIGCM - SHOULD REPLACE WITH Roble and Ridley (1987) alfa1,2 fig. . . . .	29
7.1	Distribution of modified apex latitude points for $\lambda_0$ (crosses) and $\lambda_m^*$ (pluses) . . . . .	172
7.2	Latitudinal variation of equivalent magnetospheric conductances $\Sigma_{\phi\phi}^M(C_r)$ and $\Sigma_H^M(C_i)$ for the convection reversal boundary at $72^\circ$ . . . . .	179

7.3	Latitudinal variation of reference conductance $\Sigma^R$ for $\lambda_m^{crb} = 72^\circ$ . . . . .	181
7.4	Sketch of geometry for the field–line integration . . . . .	182
7.5	Geometry for the 9 point stencil . . . . .	202
7.6	Geometry for the 9 point stencil in the northern and southern hemisphere . . . . .	217

# List of Tables

2.1	Input fields to module <code>heelis</code> . All these variables but <code>sunlons</code> and <code>crit</code> are specified in module <code>AURORA.F</code> . . . . .	34
2.2	Output fields of module <code>heelis.F</code> . . . . .	35
2.3	Input fields to module <code>weimer</code> . . . . .	35
2.4	Output fields of module <code>weimer.F</code> . . . . .	36
2.5	Input fields to module <code>aurora</code> . . . . .	37
2.6	Output fields of module <code>aurora.F</code> . . . . .	38
3.1	Input fields to subroutine <code>addiag</code> . . . . .	47
3.2	Output fields of subroutine <code>addiag</code> . . . . .	47
3.3	Module data of subroutine <code>addiag</code> . . . . .	48
3.4	Input fields to subroutine <code>swdot</code> . . . . .	50
3.5	Output fields of subroutine <code>swdot</code> . . . . .	50
3.6	Input fields to subroutine <code>duv</code> . . . . .	61
3.7	Output fields of subroutine <code>duv</code> . . . . .	62
3.8	Input fields to subroutine <code>glp</code> . . . . .	62
3.9	Output fields of subroutine <code>glp</code> i.e. subroutine <code>dldp</code> . . .	62
3.10	Parameters of subroutine <code>glp</code> i.e. subroutine <code>dldp</code> . . . . .	62
4.1	Input fields to subroutine <code>cpktkm</code> . . . . .	64
4.2	Output fields of subroutine <code>cpktkm</code> . . . . .	64
4.3	Input fields to subroutine <code>dt</code> . . . . .	66
4.4	Output fields of subroutine <code>dt</code> . . . . .	67
4.5	Module data of subroutine <code>dt</code> . . . . .	67
5.1	Input fields to subroutine <code>elden</code> . . . . .	83
5.2	Output fields of subroutine <code>elden</code> . . . . .	84
5.3	Module data of subroutine <code>elden</code> . . . . .	84



5.4	Input fields to subroutine <code>minor</code> . . . . .	88
5.5	Output fields of subroutine <code>minor</code> . . . . .	89
5.6	Module data of subroutine <code>minor</code> . . . . .	89
5.7	Input fields to subroutine <code>comp_n2d</code> . . . . .	100
5.8	Output fields of subroutine <code>comp_n2d</code> . . . . .	100
5.9	Input fields to subroutine <code>comp_n4s</code> . . . . .	102
5.10	Input fields to subroutine <code>comp_no</code> . . . . .	104
5.11	Input fields to subroutine <code>comp_o2o</code> . . . . .	106
5.12	Output fields of subroutine <code>comp_o2o</code> . . . . .	106
5.13	Module data used in subroutine <code>comp_o2o</code> . . . . .	119
5.14	Input fields to subroutine <code>comp</code> . . . . .	120
5.15	Output fields of subroutine <code>comp</code> . . . . .	120
5.16	Module data used in subroutine <code>comp</code> . . . . .	121
6.1	Input fields to subroutine <code>qjoule_ti</code> . . . . .	126
6.2	Output fields of subroutine <code>qjoule_ti</code> . . . . .	126
6.3	Global parameters used in subroutine <code>qjoule_ti</code> . . . . .	127
6.4	Input fields to subroutine <code>lamdas</code> . . . . .	128
6.5	Output fields of subroutine <code>lamdas</code> . . . . .	129
6.6	Local parameters used in subroutine <code>lamdas</code> . . . . .	129
6.7	Input fields to subroutine <code>setei</code> . . . . .	133
6.8	Output fields of subroutine <code>settei</code> . . . . .	134
6.9	Module data of subroutine <code>settei</code> . . . . .	134
6.10	Input fields to subroutine <code>oplus</code> . . . . .	159
6.11	Output fields of subroutine <code>oplus</code> . . . . .	160
6.12	Module data of subroutine <code>oplus</code> . . . . .	160
7.1	Input fields to subroutine <code>prep-dynamo</code> . . . . .	168
7.2	Apex quantities calculated in subroutine <code>apxparm</code> and used for the calculation of the electric potential . . . . .	171
7.3	Mapped fields in subroutine <code>transf</code> . . . . .	173
7.4	Field line integrated quantities in subroutine <code>fieldline_integrals</code>	186
7.5	Quantities after the transformation at the end of subroutine <code>transf</code> . . . . .	190
7.6	Contributions from conductance terms to nine point stencil using central differencing for all terms (see subroutine <code>cnm</code> and subroutine <code>cnmmod</code> ) . . . . .	204

7.7	Modification to stencil due to upwinding with positive flux $f_l > 0$ in <code>subroutine cnm</code> and <code>subroutine cnmmod</code> . . . . .	205
7.8	Modification to stencil due to upwinding with negative flux $f_l < 0$ in <code>subroutine cnm</code> and <code>subroutine cnmmod</code> . . . . .	206
7.9	Modification to stencil at the equator (see <code>subroutine cnm</code> or <code>subroutine cnmmod</code> ) . . . . .	207
7.10	Coefficient matrix name and dimensions at the different grid levels . . . . .	208
7.11	Input fields to <code>subroutine ionvel</code> . . . . .	224
7.12	Output fields of <code>subroutine ionvel</code> . . . . .	224

# Index

dynamo.F, 17  
qrj.F, 7  
AURORA.F, 16  
  
ADDIAG.F, 22  
AURORA.F, 7  
aurora\_cusp, 15  
aurora\_heat, 15  
  
CHEMRATES.F, 52  
comp.F, 80  
COMP\_N2D.F, 74  
COMP\_N4S.F, 74  
COMP\_NO.F, 74  
COMP\_O2O.F, 80  
CPKTKM.F, 40  
  
DIVRG.F, 25  
DT.F, 42  
DUV.F, 27  
  
ELDEN.F, 57  
  
Fourier Filter, 203  
  
HEELIS.F, 4  
  
IONVEL.F, 198  
  
LAMDAS.F, 102  
  
MINOR.F, 62  
  
OPLUS.F, 119  
  
SETTEL.F, 107  
settei.F, 15  
Shapiro Filter, 202  
SWDOT.F, 25  
  
WEIMER.F, 7

## Notation

### Variables

$\mathbf{B}$	geomagnetic field
$B$	geomagnetic field strength
$\mathbf{B}_0$	Earth main magnetic field
$B_x, B_y, B_z$	geomagnetic main field components (north, east, downward)
$\mathbf{b}_0$	unit vector along $\mathbf{B}_0$
$B_{e3}$	geomagnetic field strength in $\mathbf{e}_3$ direction [nT]
$c$	coefficient of the finite difference stencil
$\mathbf{E}$	electric field
$E_{d1}, E_{d2}$	electric field component in $\mathbf{d}_1, \mathbf{d}_2$ direction
$H$	scale height
$h$	height
$h_0$	reference height
$h_A$	apex height
$I_m$	inclination angle of dipolar geomagnetic field line at $h_0$ on a spherical Earth
$\mathbf{J}$	current density
$\mathbf{J}_{  }$	field aligned current density
$\mathbf{J}_M$	magnetospheric current density
$\mathbf{J}$	current density
$J_{mr}$	radial component of current density
$J_{Mr}$	radial component of current density for both hemispheres added together
$\mathbf{K}^M$	magnetospheric height integrated current density
$K_{m\phi}^M$	magnetospheric eastward height-integrated current density
$K_{m\lambda}^M$	magnetospheric down-/equatorward height-integrated current density
$K_{m\phi}$	eastward height-integrated current density
$K_{m\lambda}$	down-/equatorward height-integrated current density
$K_{m\phi}^D$	wind driven eastward height-integrated current density
$K_{m\lambda}^D$	wind driven down-/equatorward height-integrated current density
$\overline{m}$	mean molecular mass
$m_i$	atomic weight of specie i
$N_i$	density of specie i
$n_i$	number density of specie i
$N_e$	electron density
$p$	atmospheric pressure
$p_p$	plasma pressure
$\ln(p_0/p)$	log pressure levels

$R$	radius from Earth center to height $h$
$R_0$	radius from Earth center to height $h_0$
$T_e$	electron temperature
$T_i$	ion temperature
$T_n$	neutral temperature
$u_n, v_n, w_n$	neutral zonal, meridional and vertical wind
$W$	dimensionless vertical wind
$z$	geopotential height
$\Phi$	electric potential
$\Phi_R$	reference electric potential
$\rho_{ion}$	ion density
$\Sigma_{\phi\phi}$	magnetic eastward conductance
$\Sigma_{\lambda\lambda}$	magnetic equator-/downward conductance
$\Sigma_{\phi\lambda}, \Sigma_{\lambda\phi}$	mixed term conductances
$\Sigma_{\phi\phi}^M, \Sigma_H^M$	equivalent magnetospheric conductances
$\sigma_P, \sigma_H$	Pedersen and Hall conductivities
$\nabla$	gradient
$\sigma_P, \sigma_H$	Pedersen and Hall conductivities
$\mathbf{u}$	neutral wind
$\Phi$	electric potential
$\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3$	magnetic eastward, magnetic down-/equatorward vectors, along the field line
$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$	magnetic eastward, magnetic down-/equatorward vectors, along the field line
$D =  \mathbf{d}_1 \times \mathbf{d}_2 $	quantity of Earth geomagnetic coordinate system
$F$	quantity of dipole field
$i$	longitudinal index
$j$	latitudinal index
$k$	height index
$(\cdot)_i, (\cdot)_j, (\cdot)_k$	quantity at $\phi(i), \lambda(j), h(k)$ ,
$nlon$	number of discrete geographic longitude grid points
$nmlon$	number of discrete geomagnetic longitude grid points
$nlat$	number of discrete geographic latitude grid points
$nmlat$	number of discrete geomagnetic latitude grid points
$s_L, s_U$	lower and upper boundary for field line integration
$wgt$	weight for linear interpolation
$\phi, \lambda$	longitude, latitude

$\phi_g, \lambda_g$	geographic longitude, latitude
$\lambda_A$	apex latitude
$\lambda_m$	modified apex latitude
$\lambda_m^*$	irregular modified apex latitude grid distribution
$\lambda_0$	equally spaced latitudinal grid distribution in $\lambda_m^*$
$\lambda_m^{crb}$	modified apex latitude of convection reversal boundary
$\phi_m$	modified apex longitude
$(\cdot)_0$	refers to reference height
$(\cdot)(0)$	refers to equally spaced latitudinal grid $\lambda_0$
$(\cdot)_A$	quantity at apex of field-line
$(\cdot)_g$	refers to geographic direction
$(\cdot)'$	half pressure level $(\cdot) + \frac{1}{2}$
$(\cdot)_{d1}, (\cdot)_{d2}, (\cdot)_{d3}$	magnetic eastward, down-/equatorward, field-line direction of quantity $(\cdot)$
$(\cdot)_{e1}, (\cdot)_{e2}, (\cdot)_{e3}$	magnetic eastward, down-/equatorward, field-line direction of quantity $(\cdot)$
$(\cdot)_{eq}$	value at the geomagnetic equator
$(\cdot)_{fl}$	value on the geomagnetic field line
$(\cdot)_{m\phi}, (\cdot)_{m\lambda}$	modified apex eastward and down-/equatorward direction of quantity $(\cdot)$
$(\cdot)_{pole}$	values at the geomagnetic poles
$(\cdot)^D$	dynamo part
$(\cdot)^{p,g}$	refers to plasma pressure and gravity contribution
$(\cdot)^T$	both hemispheres added together
$\frac{d(\cdot)}{dt}$	total time rate of change
$\frac{\partial(\cdot)}{\partial}$	partial derivative
$lhs, rhs$	left and right hand side of electrodynamo equation
$T_n$	neutral temperature
$T_i$	ion temperature
$T_e$	electron temperature
$\lambda^{mag}$	ion drag tensor in geomagnetic direction
$\lambda^{geo}$	ion drag tensor in geographic direction
$\lambda_1, \lambda_2$	ion drag coefficient component in geomagnetic direction
$\sigma_H$	Hall conductivity
$\sigma_P$	Pedersen conductivity
$\Psi_{O_2}, \Psi_O, \Psi_{N_2}$	mass mixing ratio of $O_2, O, N_2$
$N_i$	number density of i
$\overline{m}$	mean molecular mass
$\overline{m}_n$	mean molecular mass of neutrals

$\overline{m}_{ion}$	mean molecular mass of ions
$\Omega$	gyro frequency
$D$	declination of geomagnetic field
$I$	inclination of geomagnetic field
$nlev$	number of discrete height levels
$nlev0$	height level index of bottom
$nlev1$	height level index of top
$\rho$	mass density
$\nu$	collision frequency
$e$	electron charge
$Q_J$	energy rate per unit mass of Joule heating
$Q_J^{T_n}$	Joule heating of neutral temperature
$\mathbf{J}$	current
$\mathbf{J}_\perp$	current perpendicular to $\mathbf{B}$
$\mathbf{E}$	electric field
$\mathbf{E}'$	electric field in the frame of neutral wind
$\mathbf{v}_{ExB}$	$\mathbf{E} \times \mathbf{B}$ drift velocity
$\mathbf{v}_n$	neutral wind vector
$\mathbf{v}_{n\perp}$	neutral wind vector $\perp$ to $\mathbf{B}$
$u_n, v_n$	zonal and meridional neutral wind components
$E_{m\phi}, E_{m\lambda}, E_z$	geomagnetic east-, north- and upward electric field
$E_x, E_y, E_z$	electric field in geographic east-, north-, upward direction on geographic grid
$\mathbf{E}_{geo}$	electric field in geographic direction
$\mathbf{E}_{mag}$	electric field in geomagnetic direction
$v_{ExB,x},$	electromagnetic drift velocity
$v_{ExB,y}, v_{ExB,z}$	(geographic east-, north-, upward)
$\phi_m, \lambda_m$	geomagnetic coordinates
$\phi_g, \lambda_g$	geographic coordinates
$\lambda_0$	equally spaced latitudinal grid points in $\lambda_m^*$
$\lambda_m^*$	irregular spaced latitudinal grid points
$\mathbf{J}_{mag}$	Jacobian $\frac{\partial s_{mag}}{\partial s_{geo}}$
$j_{11}, j_{12}, j_{21}, j_{22}$	Components of the Jacobian matrix $\mathbf{J}_{mag}$
$s_{mag}, s_{geo}$	generic magnetic and geographic coordinate systems
$k_{bot}, k_{top}$	height index for bottom and top of model
$\mathbf{f}_1, \mathbf{f}_2$	apex base vectors
$t_n$	time at time step $n$
$t_{n+1}$	time at time step $n + 1$

$\Psi_i$	mass mixing ratio of specie $i$ e.g. $O_2, O, N$
$H$	scale height
$W$	dimensionless vertical velocity
$w$	vertical velocity
$N_i$	number density of species $i$ with $i = O_2, O^+, NO^+, N^+$
$N$	total number density
$\nu$	collision frequency
$\nu_{in}$	collision frequency ion-neutral
$\nu_{en}$	collision frequency electron-neutral
$\sigma_p, \sigma_h$	Pederson and Hall conductivities
$\sigma_1, \sigma_2$	conductivity in geomagnetic direction
$Z$	geopotential height
$z$	dimensionless variable $Z = -\ln \frac{p}{p_0}$ / log pressure coordinate
$p$	pressure
$p_0$	reference pressure
$\Phi$	electric potential
$\mu$	viscosity
$\mu_{ed}$	eddy viscosity
$\mu_{mol}$	molecular viscosity
$K_T$	molecular thermal conductivity
$K_E$	eddy diffusion coefficient
$k_m$	molecular viscosity
$h_d$	horizontal diffusion
$Q_{J,T}$	Joule heating of neutral temperature
$Q$	heating
$L$	loss
$C_p$	specific heat per unit mass
$\rho$	atmospheric mass density
$R$	Radius with $R = R_E + z$



## Constants

$\mathbf{g}(h_0)$	$870 \frac{cm}{s^2}$ ( <i>TIEGCM</i> )	gravitational acceleration at height $h_0$
	$945 \frac{cm}{s^2}$ ( <i>TIMEGCM</i> )	gravitational acceleration at height $h_0$
$M_i$	$1.6605 \cdot 10^{-24} g$	mass of unit atomic weight
$h_0$	$90 km(T * GCM)$	height of lower boundary for electrodynamo
$h_R$	$90 km$	reference height
$R_E$	$6.37122 \cdot 10^8 cm$	mean Earth radius
$p_0$	$5.0 \cdot 10^{-4}$	standard pressure
$k_B$	$1.38 \cdot 10^{-16} \frac{cm^2 g}{s^2 K}$	Boltzman constant
$R^*$	$8.314e7 \frac{erg}{mole K}$	gas constant
$R_{eq}$	$6.37814 \cdot 10^8$	Earth radius at the equator
$N_a$	$6.023 \times 10^{23}$	Avogadro number
$e$	$1.602 \cdot 10^{-19}$	electron charge

The model code defines these constants to the stated accuracy. We do not mean to imply that these constants are known to this accuracy nor that the low-order digits are significant to the physical approximations employed.

# Chapter 1

## Code Structure Overview

This TIEGCM code structure part is adapted from a document which can be found at the TIEGCM website <http://www.hao.ucar.edu/modeling/tgcm/> under documentation "TIEGCM Code Structure Flowchart (Documentation section of the Download page)". The version on the web has hyperlinks included.

# TIEGCM Code Structure

## Contents

• <a href="#">TIEGCM</a>	Main
• <a href="#">Init</a>	Model initialization
• <a href="#">Advance</a>	Advance model in time
• <a href="#">Dynamics</a>	Dynamics and Chemistry
• <a href="#">Aurora</a>	Aurora Parameterization
• <a href="#">Oplus</a>	O+
• <a href="#">Minor</a>	Minor Species Composition
• <a href="#">DUV</a>	Neutral Winds
• <a href="#">DT</a>	Neutral Temperature
• <a href="#">Major</a>	Major Species Composition
• <a href="#">Dynamo</a>	Electrodynamics
• <a href="#">Outhist</a>	Write to output files
• <a href="#">Filter</a>	Longitudinal filtering

Figure 1.1: TIEGCM Code Structure Contents

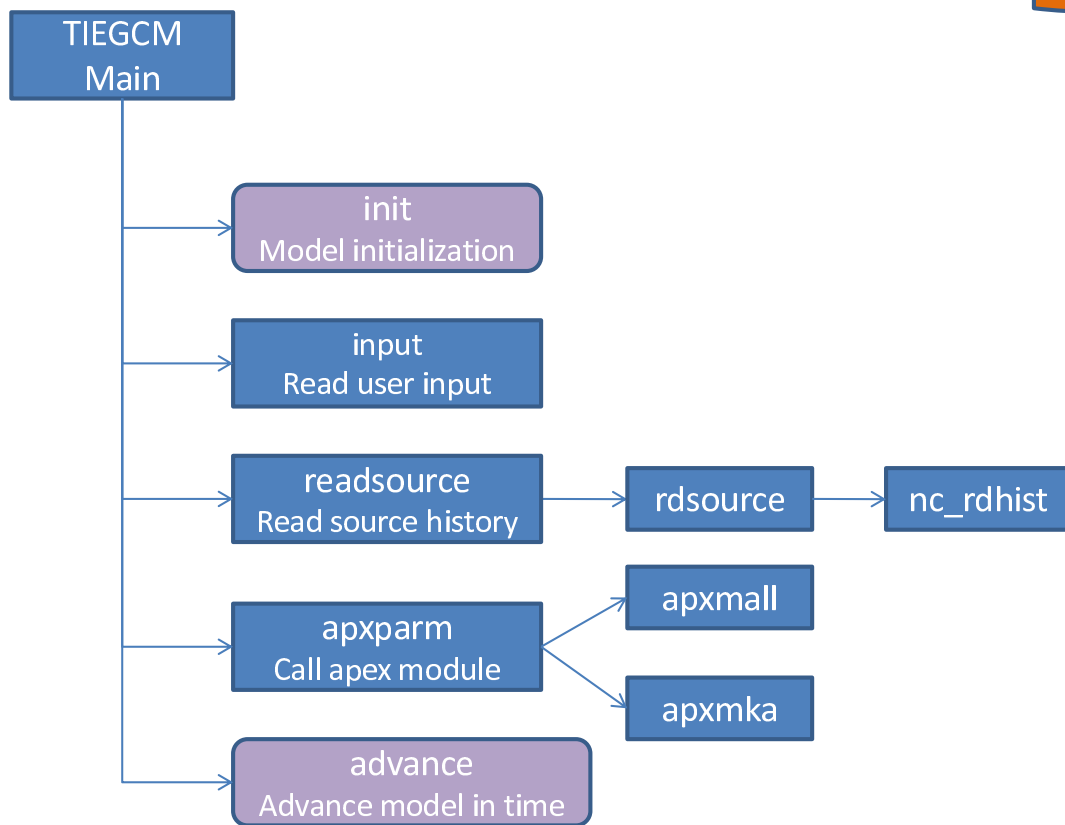
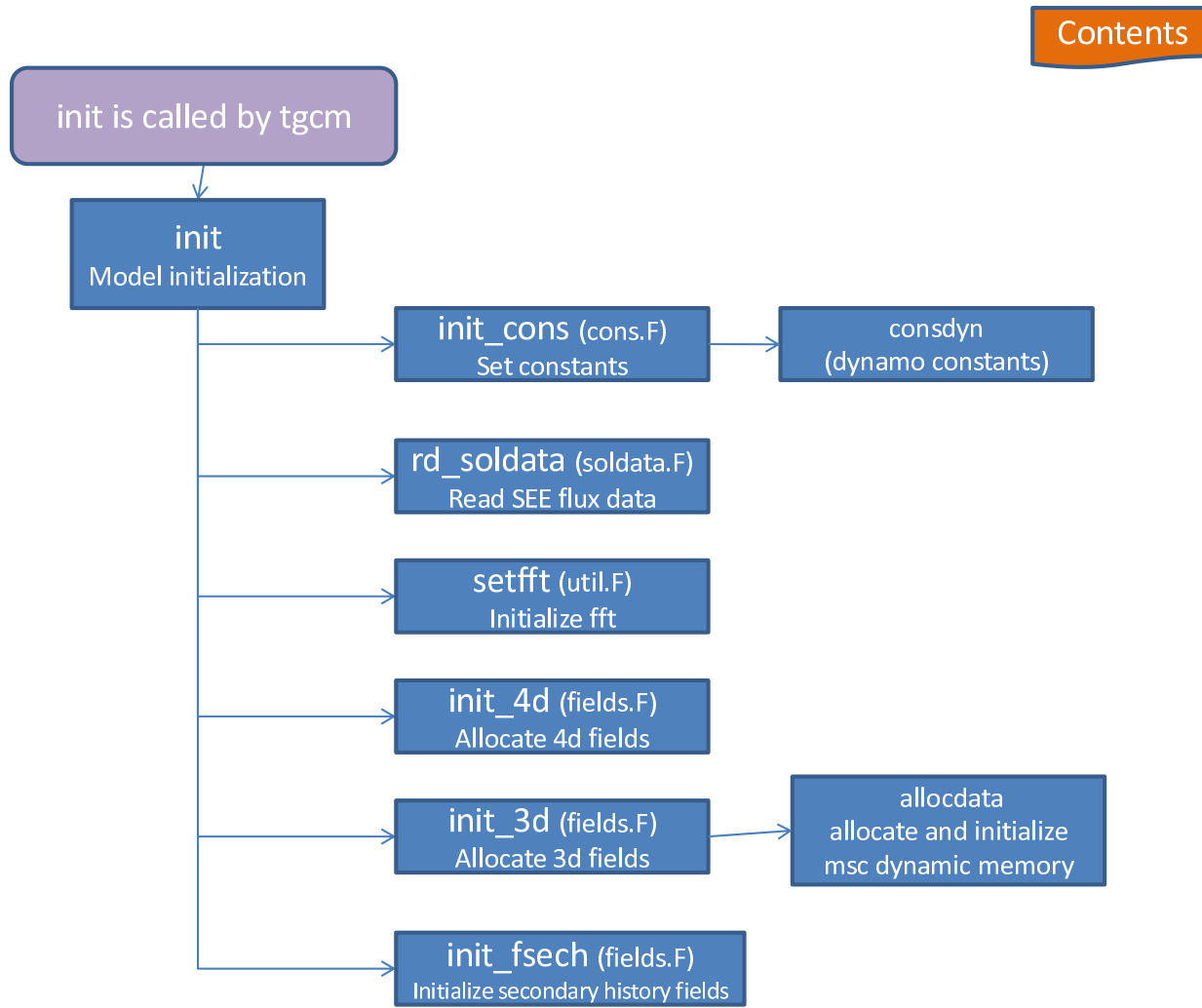


Figure 1.2: main: TIEGCM main

Figure 1.3: `init`: model initialization

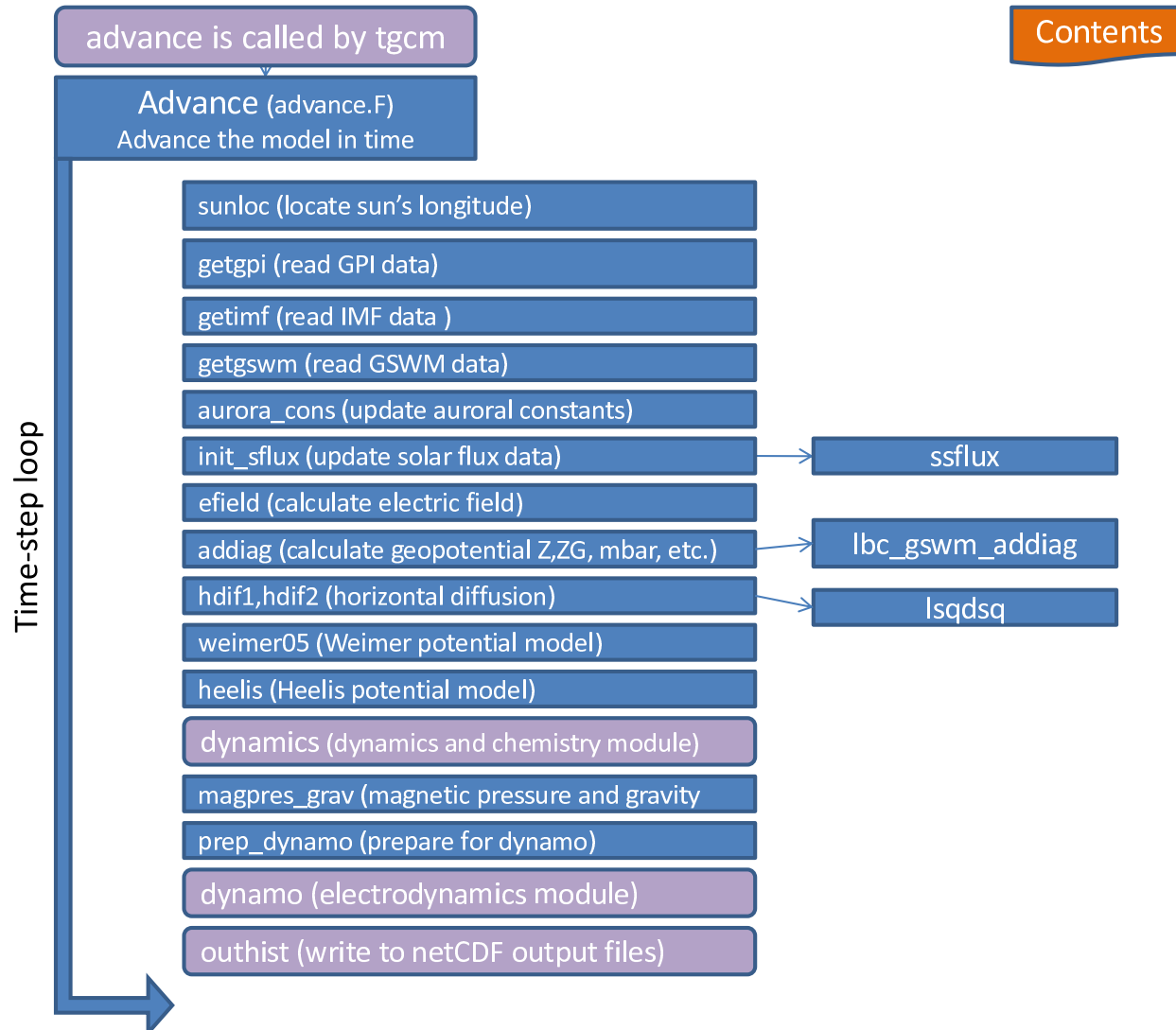


Figure 1.4: advance: advance model time

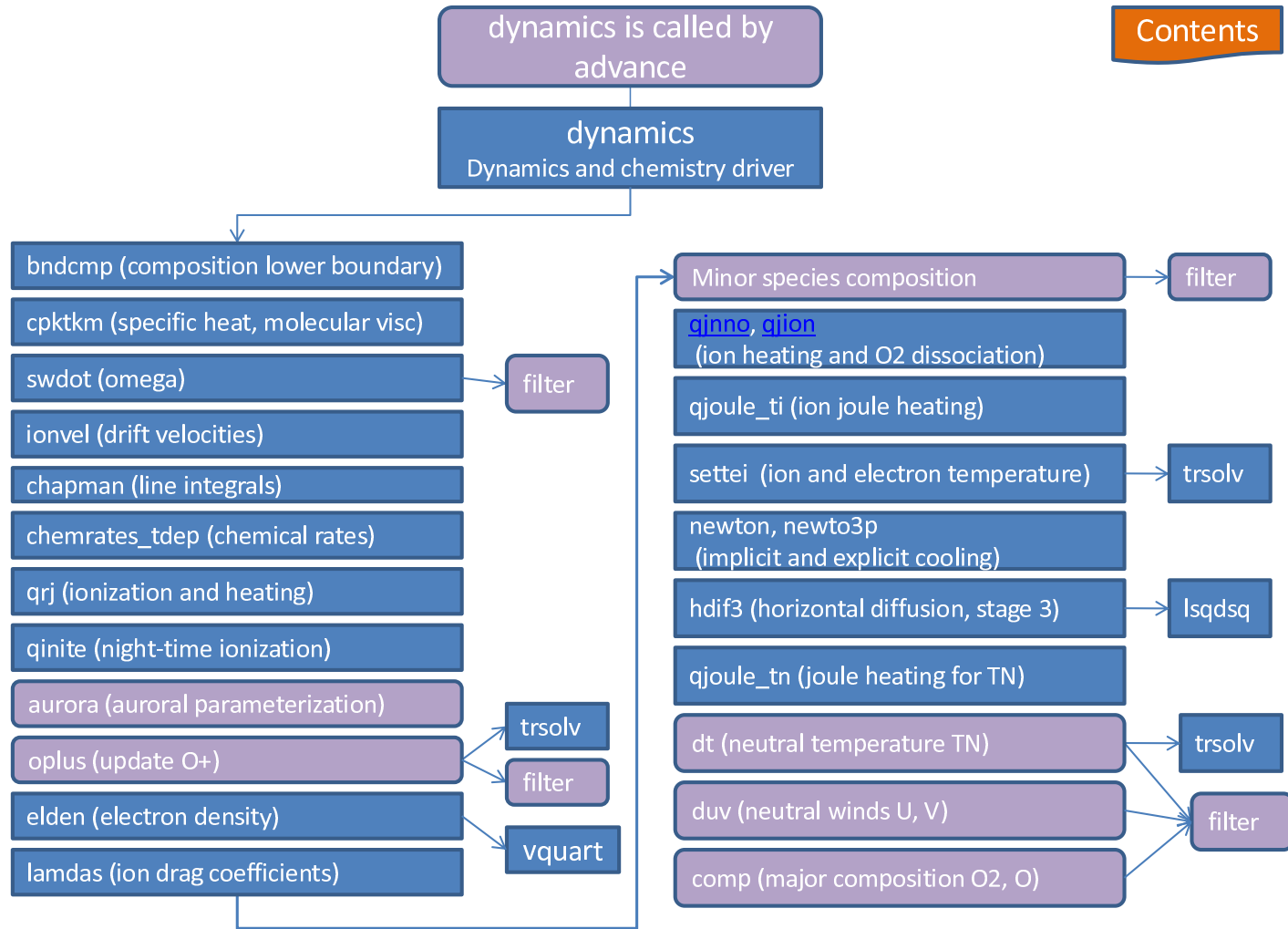


Figure 1.5: dynamics: dynamics and chemistry drivers

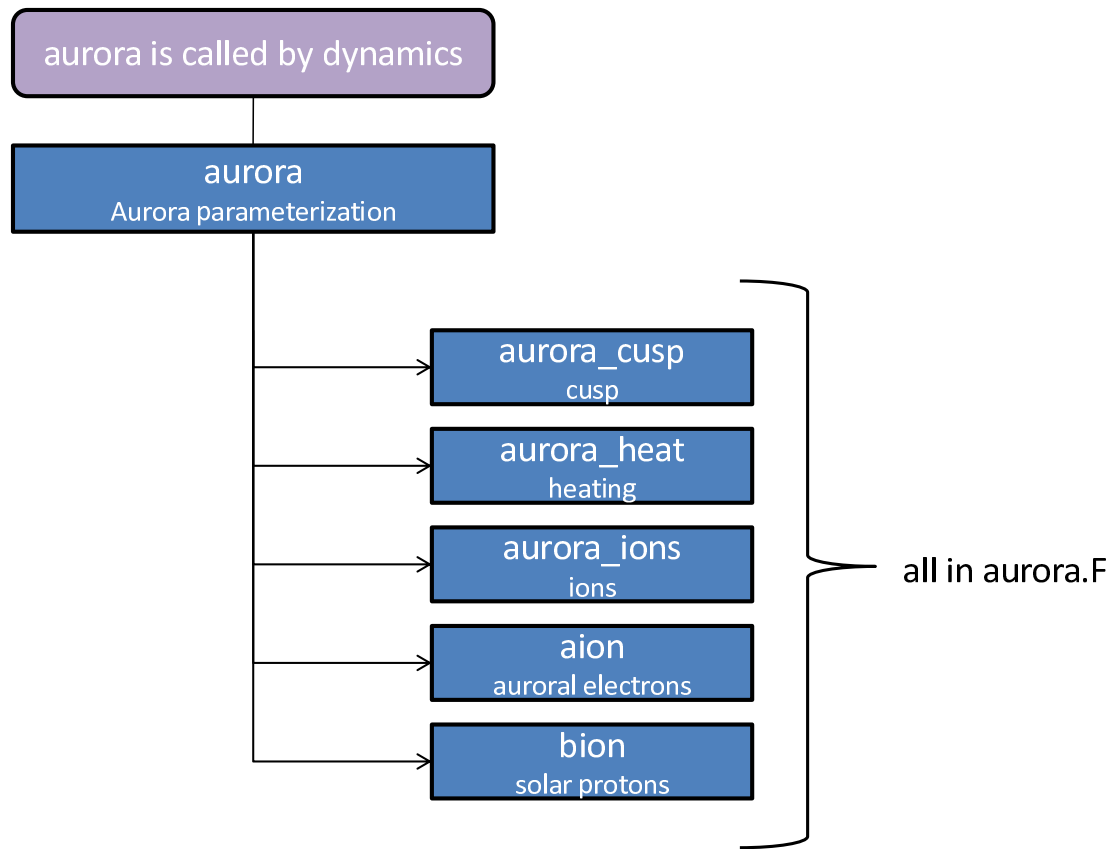
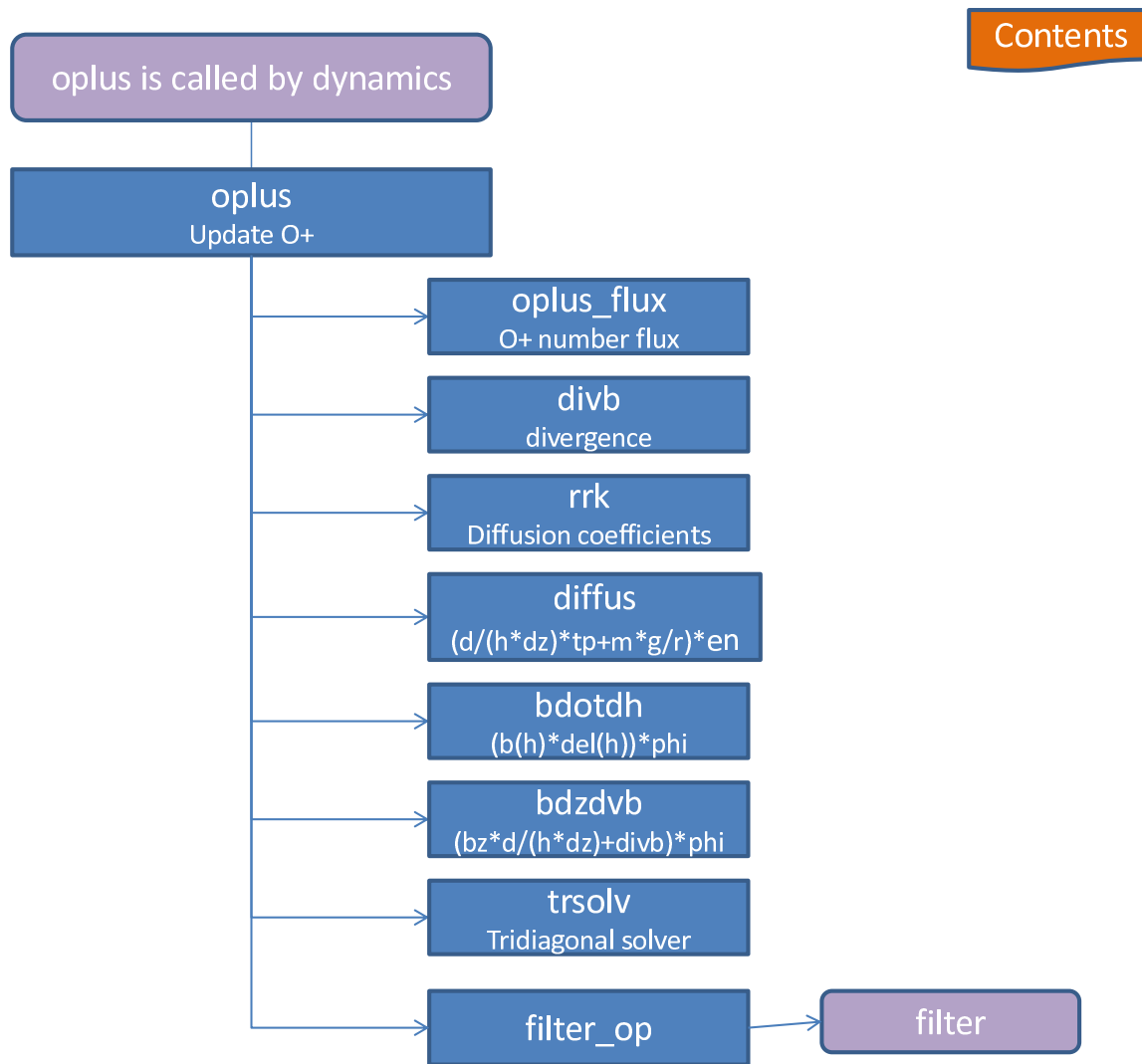


Figure 1.6: aurora: aurora parameterization



Figure 1.7: `oplus`:  $O^+$  calculation

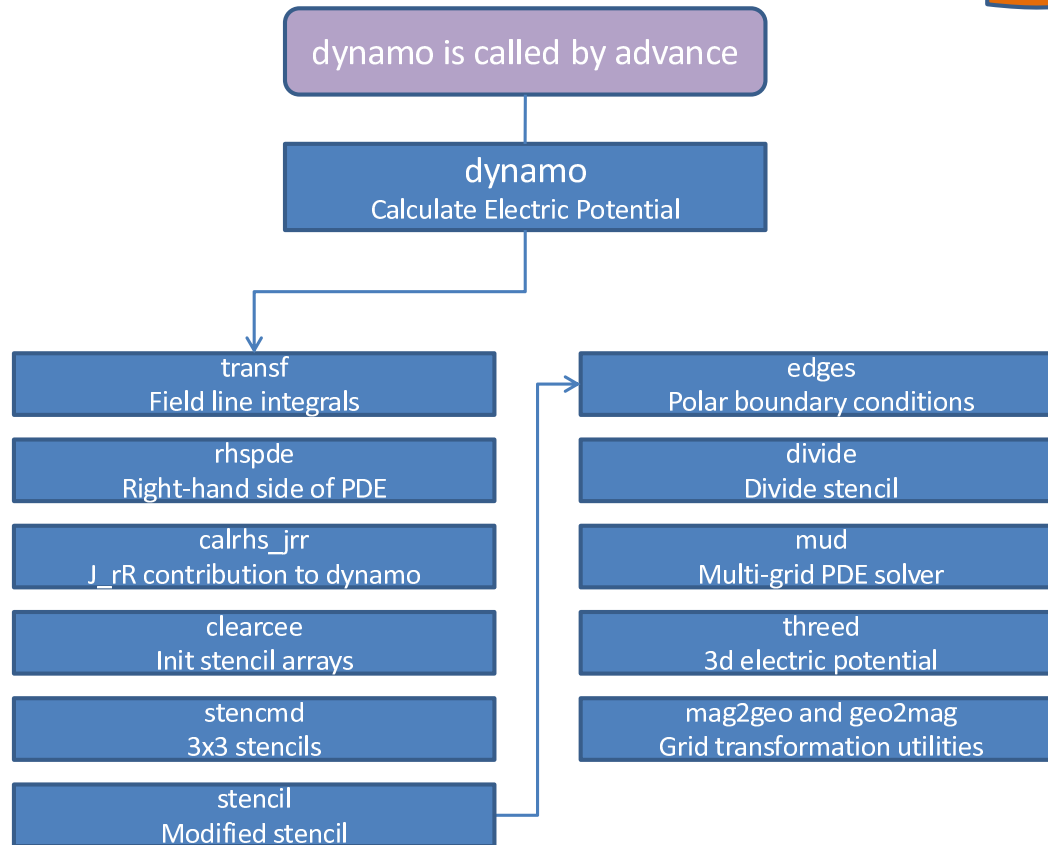


Figure 1.8: dynamo: calculation of electric potential

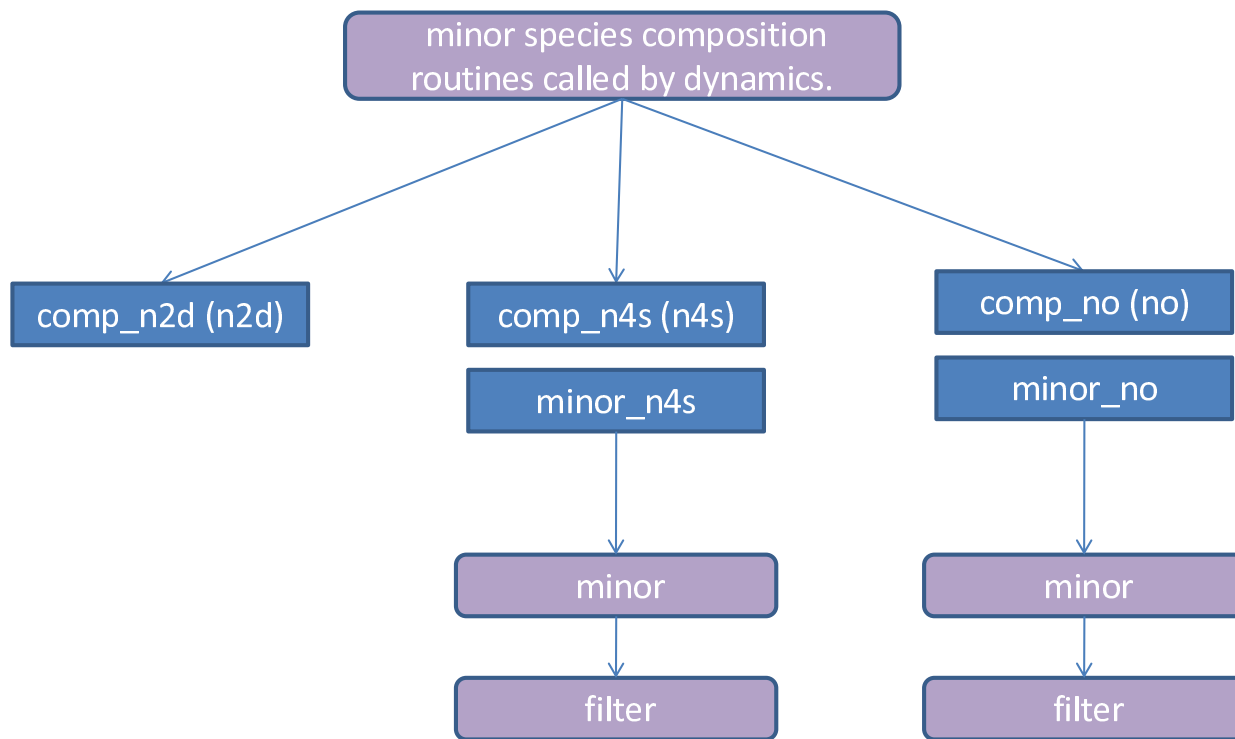
[Contents](#)

Figure 1.9: minor species composition

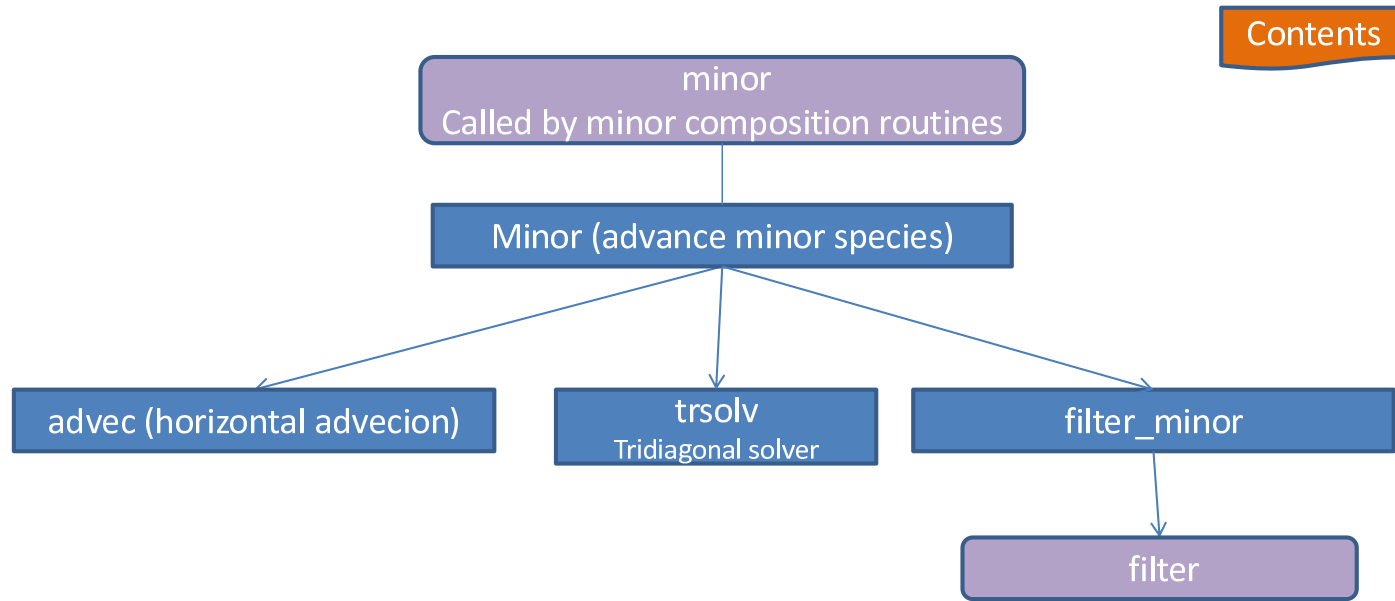


Figure 1.10: calculation of minor species

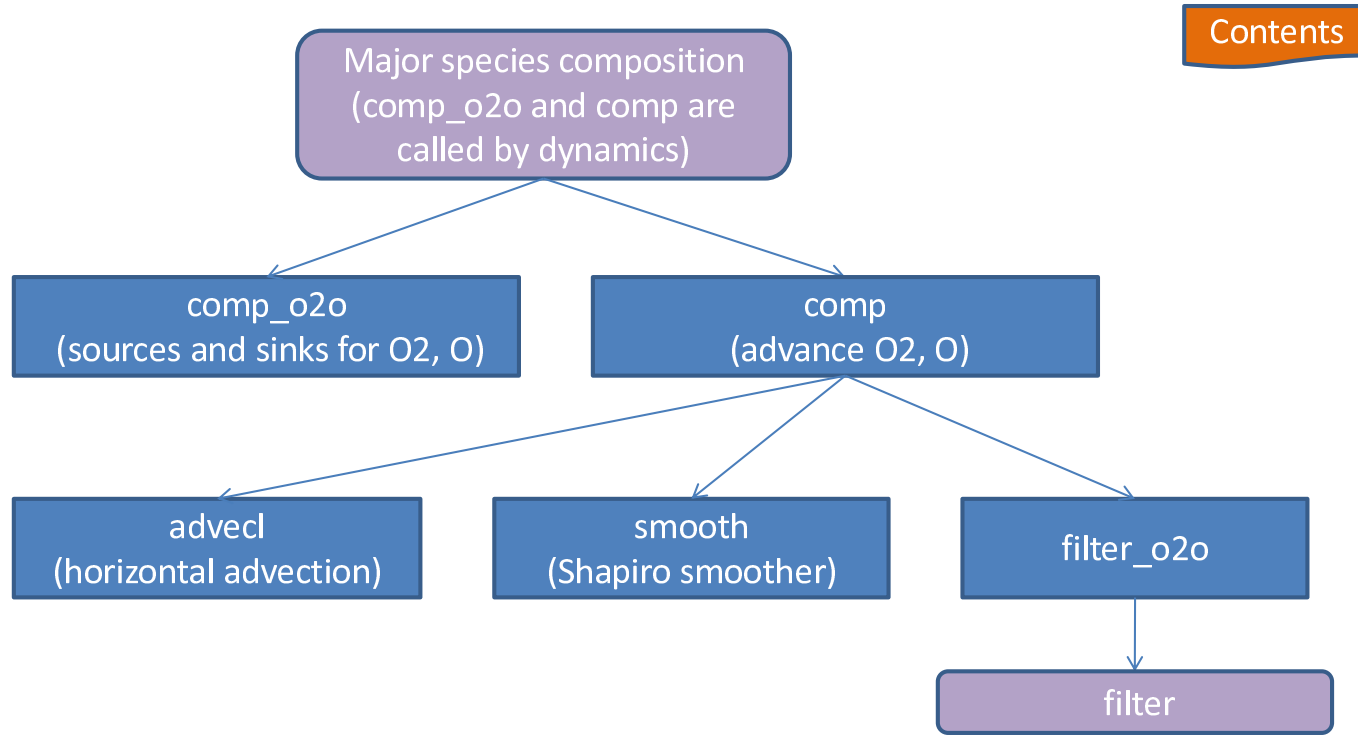


Figure 1.11: major species composition

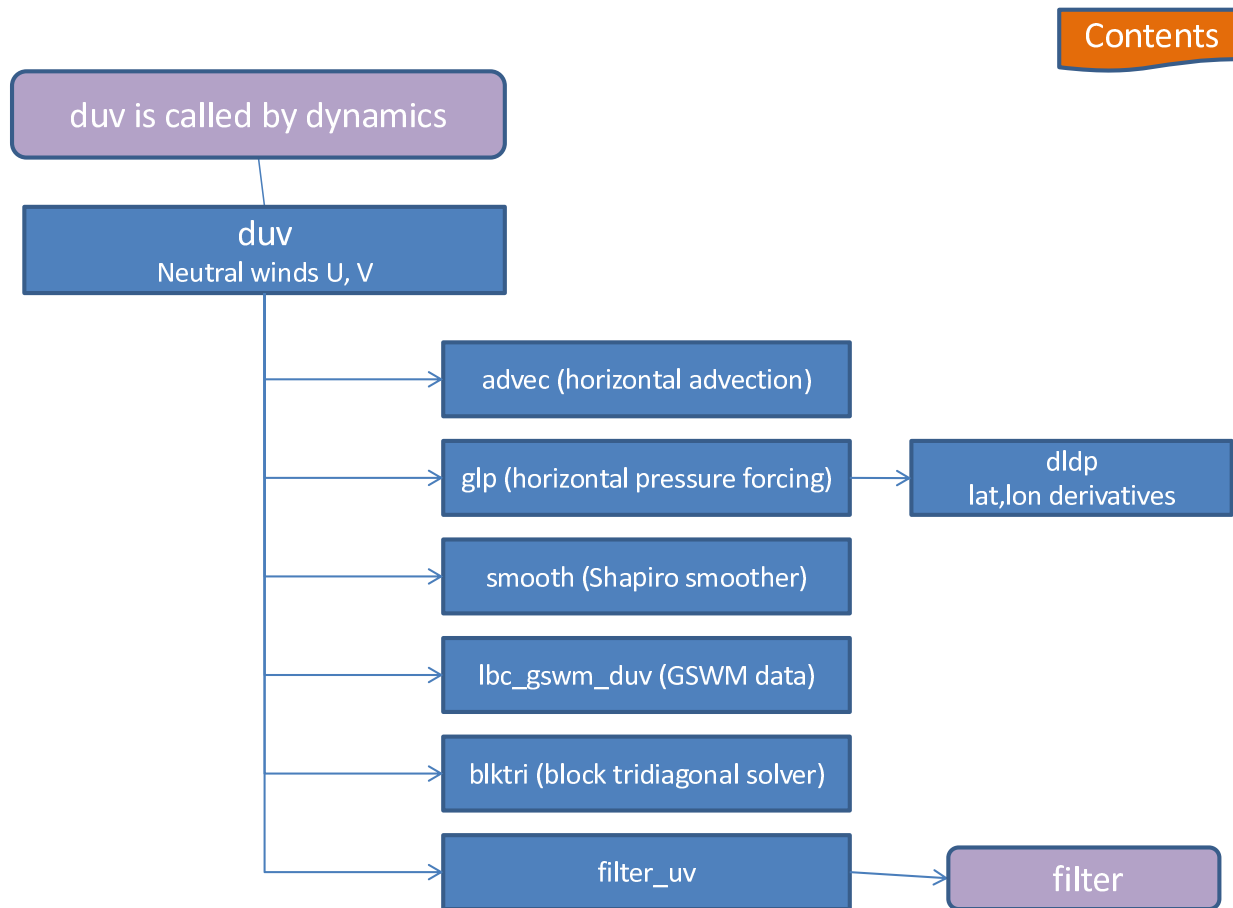


Figure 1.12: duv: calculation of neutral horizontal winds

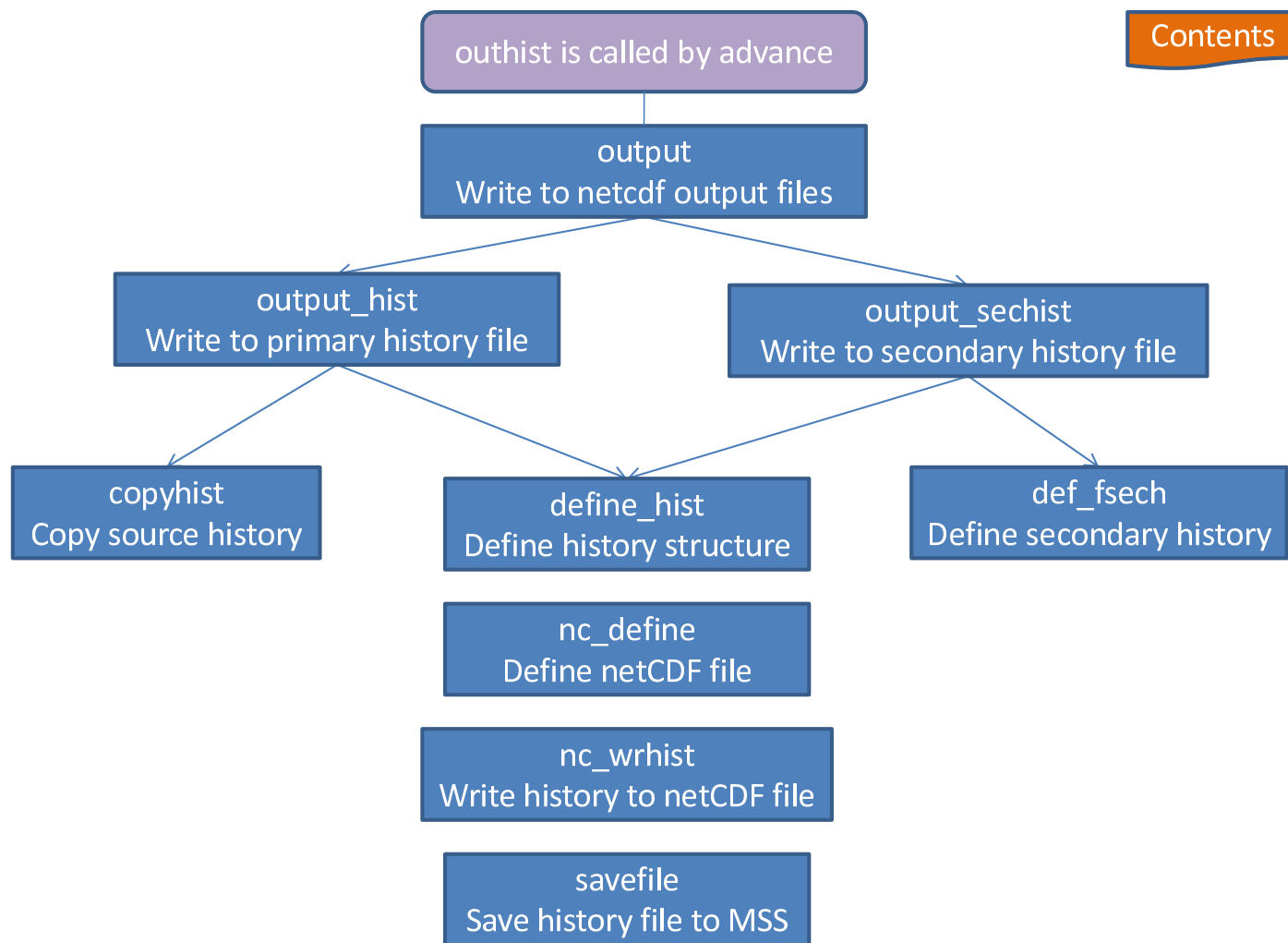


Figure 1.13: output structure

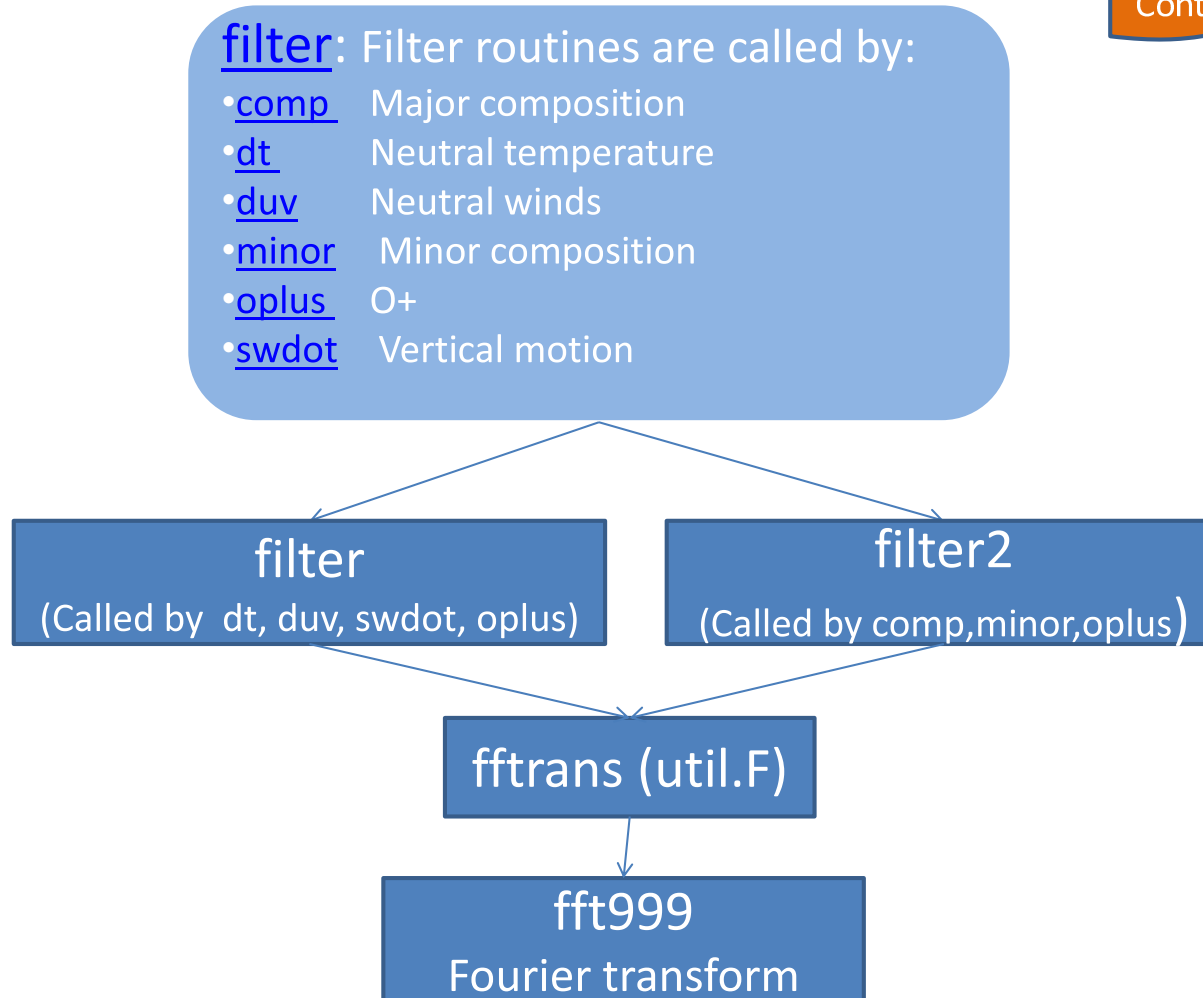
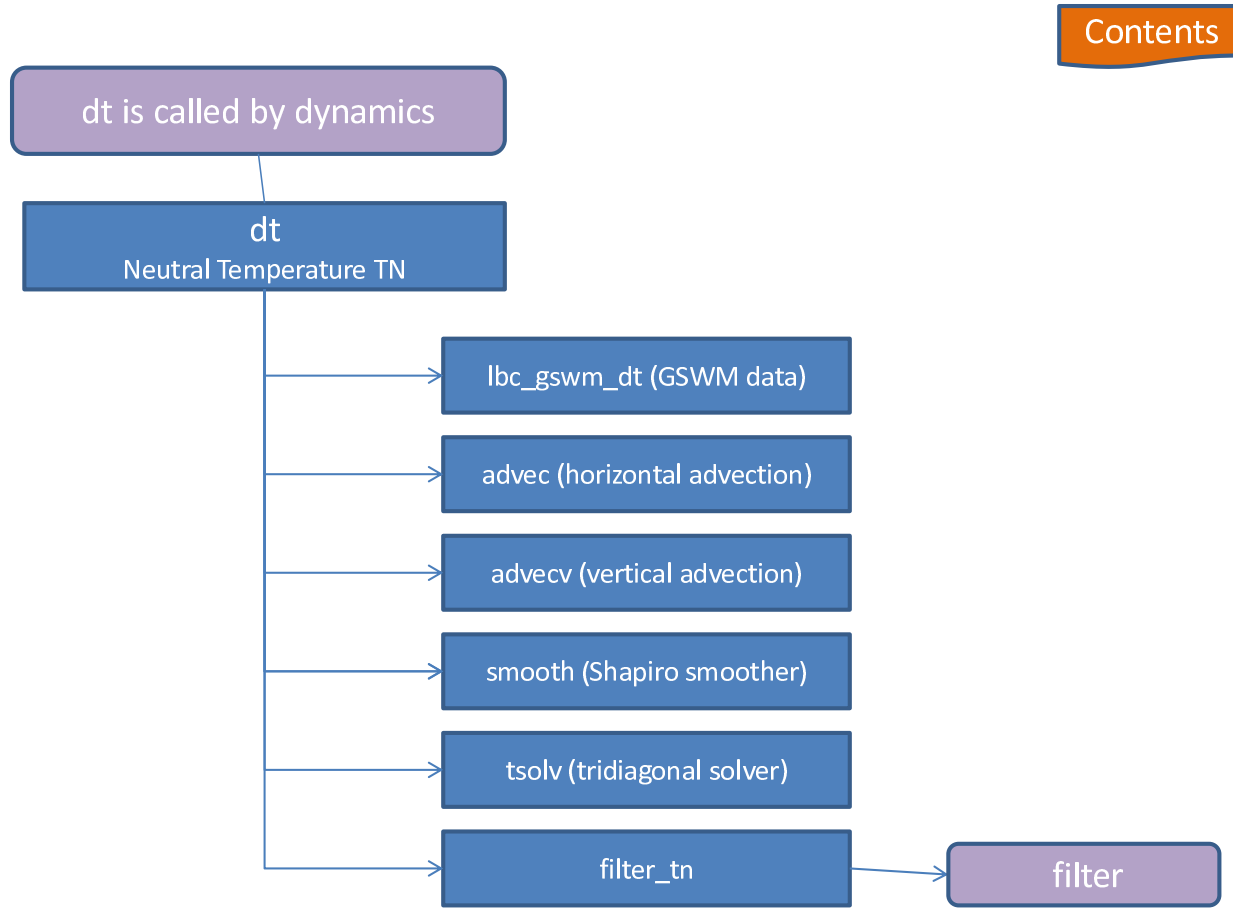


Figure 1.14: filtering in TIEGCM



[Contents](#)Figure 1.15: `dt`: calculation of neutral temperature

# Chapter 2

## Input

### 2.1 Solar Input

## 2.2 Magnetospheric Input

The documentation group for the magnetospheric inputs to the TIEGCM model consists of Barbara Emery, Wenbin Wang and Yue Deng, with help from others as needed.

### 2.2.1 Parameters to define the magnetospheric inputs

Magnetospheric inputs are the high latitude ion convection model (Heelis or Weimer 2005) and the aurora, which are described in the following sections. The aurora depends on the Hemisphere Power (HP), where the auroral radius can depend on the Cross Polar Cap Potential (CPCP) of both hemispheres. The Heelis ion convection [9] depends on the CPCP and the IMF By. The input parameters for the Weimer 2005 model [21] are solar wind density  $N_{sw}$  and speed  $V_{sw}$ , and the IMF By and Bz.

The potential model is specified in the input file as:

1. POTENTIAL\_MODEL = 'NONE'
2. POTENTIAL\_MODEL = 'HEELIS'
3. POTENTIAL\_MODEL = 'WEIMER05'

where 'NONE' means the high-latitude ion drift velocity and electric potential is zero. The aurora is specified in the input file as:

1. AURORA = 0
2. AURORA = 1

where 0 means no aurora and '1' means calculate and use a model aurora ([17]).

The magnetospheric input parameters for the convection and auroral models can be defined in two ways in the namelist input file:

1. Directly specify them in the namelist file as single-valued parameters under the names of: POWER, CTPOTEN, BYIMF, BZIMF, SWVEL, and SWDEN. Multiple-valued parameters can be specified under the

names of: POWER\_TIME, CTPOTEN\_TIME, BYIMF\_TIME, BZ-IMF\_TIME, SWVEL\_TIME, and SWDEN\_TIME, where four values are given for each time as: ut\_daynumber, ut\_hour, ut\_minute, value.

2. Specify and use the "gpi.F" file (GPI\_NCFILE) for the Heelis ion convection model or the "imf.F" (IMF\_NCFILE) for the 2005 Weimer ion convection model in the namelist file, but not both. It is best to comment out the single- or multiple-valued parameters listed above when using this option because the default is to use the listed input namelist values. The code will stop if CTPOTEN is given and 'WEIMER05' is requested.

The GPI\_NCFILE provides 3-h Kp, daily 10.7 cm solar flux data, and 81-day 10.7 cm solar flux data centered on the given day. The "gpi.F" code calculates HP and CPCP from the Kp index. For this case, in the namelist file, comment out the F107, F107A, POWER, and CTPOTEN lines, and select POTENTIAL\_MODEL = 'HEELIS' and the GPI\_NCFILE (a netcdf file). The formulas are [23]

$$\begin{aligned} \text{if } Kp \leq 7 \\ hp &= 16.82 \cdot e^{(0.32kp)} - 4.86 \\ \text{if } Kp > 7 \end{aligned} \tag{2.1}$$

$$hp = 153.13 + \frac{kp - 7}{9 - 7}(300 - 153.13)$$

$$cpcp = 15 + 15kp + 0.8kp^2 \tag{2.2}$$

The IMF\_NCFILE also provides Kp and 10.7 cm solar flux data, but additionally provides hourly interplanetary magnetic field (IMF) data and solar wind speed (Vsw) and density (Dsw). The satellite IMF and plasma data are time-shifted to the bow shock nose of the Earth's magnetosphere as described in the NASA Geophysical Data Center web site for OMNI data at <http://omniweb.gsfc.nasa.gov/ow.html>. All data time-shifted to the bow shock that lie between 0000 and 0100 UT are used in the hourly average centered at 0030 UT. The "imf.F" code interpolates the data to the model time. No lag is done between the bow shock and the polar cap for hourly data, although polar ground magnetometer stations respond between 9 and 25 minutes later (Weimer, 2009 private communication). When we go to higher resolution IMF and plasma data, then we will add a lag time between

the bow shock and the high-latitude ion convection. If the hourly  $B_y$ ,  $B_z$ ,  $V_{sw}$ , or  $N_{sw}$  are missing in the IMF\_NCFILE and also absent (commented out) in the namelist, then the code will stop because there is no provision for filling in IMF or plasma gaps. Since  $N_{sw}$  has little effect on the Weimer 2005 CPCP as described later, it can be set in the namelist ( $SWDEN = 4$ ) to avoid the code stopping during periods when  $N_{sw}$  is missing. If POWER is absent from the namelist, HP is calculated from Emery et al. (2008) [5] from IMF  $B_z$  (in nT) and the solar wind velocity ( $V_{sw}$  in km/s). For this case in the namelist file, comment out the F107, F107A, POWER, CTPOTEN, BXIMF, BYIMF, BZIMF, SWVEL, and SWDEN lines, and select POTENTIAL\_MODEL = 'WEIMER05' and the IMF\_NCFILE (a netcdf file). The formulas are [5]

$$\begin{aligned}
 &\text{if } B_z < 0 \\
 &\quad hp = (6.0 + 3.3 \cdot \text{abs}(B_z) + (0.06 + 0.003 \cdot \text{abs}(B_z)) \\
 &\quad \quad \cdot (\min(V_{sw}, 700) - 300)) \cdot fac \\
 &\text{if } B_z \geq 0 \\
 &\quad hp = 5.0 + 0.05 \cdot (\min(V_{sw}, 700) - 300) \cdot fac
 \end{aligned} \tag{2.3}$$

where  $fac = 2.0$ , so the NOAA/DMSP estimated HP is doubled to be closer to the GUVI estimated HP. Zhang and Paxton (2008) [23] show in their Figure 2. that the GUVI energy flux and the DMSP-F14 energy flux are similar along the cut of the DMSP satellite, but they show in their Figure 11, that the GUVI estimated HP is larger than either the DMSP-F15 estimated HP or the NOAA estimated HP. Their Figure 8a with GUVI HP as a function of  $K_p$  is approximately double the intercalibrated NOAA/DMSP HP versus  $K_p$  in Figure 9 of Emery et al. (2008) [5]. Thus, the factor of 2.0 increase of the NOAA/DMSP HP agrees with the GUVI HP within 10% for  $K_p$  0 to 7 and is approximately 25% lower than GUVI HP for  $K_p$  8 and 9. In addition, TIEGCM modeling studies have shown that the auroral energy flux needs to be increased in order to fit the observed nitric oxide [NO] observations (private communication S. Solomon and L. Qian). Finally, HP is not allowed to be less than 5.0 GW when calculated from IMF  $B_z$  and  $V_{sw}$ . [NOTE: Weimer 2001 model [?] is still in version 1.92. WHY? It relies on calccloc so the calculated convection position is not very good for  $B_z$  positive conditions when  $\text{abs}(B_y)$  is less than  $B_z$ . But it could be improved to use the values in 2005.] The order of calls is:

1. Read namelist and open any netcdf input files in module `init.F`

2. Advance time-step in module `advance.F` and interpolate input parameters with possible calls to `getgpi` in module `gpi.F` or to `getimf` in module `imf.F`. If the potential model is WEIMER (01 or 05), and POWER is not provided by the namelist, then call `hp_from_bz_swvel` in module `util.F`.
3. Call `aurora_cons` in module `aurora.F` from module `advance.F`
4. Call convection model from module `advance.F` (and override auroral constants found in `aurora_cons` if the Weimer 2005 model is used)
5. Call module `dynamics.F` from module `advance.F`, which in turn calls `aurora` in module `aurora.F`.

It is possible to insert different ion convection or auroral patterns into the TIEGCM, such as AMIE derived patterns, but this requires interpolation to the TIEGCM magnetic and auroral circle grids, and is not currently supported in the public version TIEGCM1.92.

### 2.2.2 The Heelis convection pattern

The input to module `heelis` is summarized in table 2.1. The output of module `heelis.F` is summarized in table 2.2.

**\*Note: the following material is from [22], and copyright to the University of Michigan. Some of the material has been modified based on the updated TIEGCM.**

The auroral ion convection pattern in the TIEGCM is parameterized using the Heelis model [9], which is modified to account for IMF  $B_y$  effects on the shape of the convection pattern. In general, only two parameters are needed to define the auroral ion convection pattern: the cross-tail potential  $\Phi$  in kilovolts and the interplanetary magnetic field  $B_y$  component (in nanotesla), where a local variable `byloc` is set to the IMF  $B_y$  in the range  $-11.0 \leq byloc \leq 7.0$  in the northern hemisphere, and in the range  $-7.0 \leq byloc \leq 11.0$  in the southern hemisphere. [NOTE: This  $B_y$  range is only correct for NH in `aurora_cons`, and not for SH!] In versions earlier than version 1.9, the IMF  $B_y$  dependency was removed. Other parameters are set up based on these two parameters that define the convection pattern.

The first parameter defined is the radii  $\theta_0$  of the convection flow reversal

circle where the potential peaks

$$\theta_0 = -3.80^0 + 8.48^0 \Phi^{0.1875} \quad (2.4)$$

Where  $\Phi$  is the cross polar cap potential (CPCP in kV). The center of the circle is located away from the geomagnetic poles by **offc** along the magnetic noon-midnight line and **dskofc** in the dawn-dusk direction

$$\begin{aligned} \text{offc} &= 1.1^0 \\ \text{dskofc} &= -0.08^0 - \pm 0.15^0 \text{byloc} \end{aligned} \quad (2.5)$$

where  $+/-$  applies for southern/northern hemisphere, respectively. The TIEGCM grid is then transformed into grid points in the new ion convection coordinate system defined by **offc** and **dskofc** relative to the geomagnetic poles. In this coordinate the auroral electric potential is generally expressed as

$$\Psi = G(\theta)F(\phi, \theta) \quad (2.6)$$

where  $G$  and  $F$  represent the strongest latitude and local time dependencies, respectively,  $\theta$  and  $\phi$  correspond to the corrected magnetic colatitude and magnetic local time.

Latitude variations of the potential are represented in the TIEGCM by two functions, one describing the variation when colatitude is smaller than  $\theta_0$ , the other one describing the variation when colatitude greater than  $\theta_0$ . The latitude gradient of the potential, and therefore the meridional electric field, is discontinuous at  $\theta_0$  in the TIEGCM implementation of the Heelis model. The TIEGCM neglects a few degrees of turnover region around the ion convection reversal because of the five-by-five degree grid spacing used in the TIEGCM. However, this neglect introduces sharp changes in ion velocity and neutral wind near the convection reversal which are an obvious discrepancy between the calculated and observed convection patterns. In the TIEGCM

$$\begin{aligned} \Psi(\phi, \theta) &= \left( \frac{\sin \theta}{\sin \theta_0} \right)^{r_1} F(\phi, \theta) \quad \text{for } \theta > \theta_0 \\ \Psi(\phi, \theta) &= F_3(\phi, \theta) \left( \frac{\theta}{\theta_0} \right)^3 + F_2(\phi, \theta) \left( \frac{\theta}{\theta_0} \right)^2 + F_1(\phi, \theta) \left( \frac{\theta}{\theta_0} \right) + \text{pcen} \quad \text{for } \theta \leq \theta_0 \end{aligned} \quad (2.7)$$

where  $r_1 = -2.6$ ,  $F(\phi, \theta)$ ,  $F_1(\phi, \theta)$ ,  $F_2(\phi, \theta)$  and  $F_3(\phi, \theta)$  are functions accounting for the local time dependencies of the convection pattern. They are

chosen such that  $\Psi(\phi, \theta)$  is continuous at  $\theta_0$ , **pcen** is the potential at the center of the convection reversal circle due to the  $B_y$  effect

$$\text{pcen} = (-0.168 \pm 0.027 B_y) \Phi \quad (2.8)$$

Positive  $B_y$  increases the evening cell and negative  $B_y$  enlarges the morning cell in the northern hemisphere. The opposite behavior occurs in the southern hemisphere.

The cross tail potential is split between the evening and morning potentials **psie** and **psim**. The evening cell is usually larger than the morning cell based on both satellite and ground measurements, so the normal split used in the TIEGCM is

$$\text{psim} = 0.44\Phi \quad \text{psie} = -0.56\Phi \quad (2.9)$$

The local magnetic time dependencies are described by 6 angles. The longitude  $0^\circ$  (12 MLT) in the TIEGCM ion convection coordinate system is defined at noon. The longitude is positive when rotating clockwise. **phid** and **phin** are local time angles determining the daytime entrance and nighttime exit of the ion convection pattern (zero potential line) across the polar cap. Their position are also affected by the magnitude and orientation of IMF  $B_y$

$$\text{phid} = (9.39 \pm 0.21 \text{byloc} - 12.)15^\circ/\text{hr} \quad \text{phin} = (23.5 \pm 0.15 \text{byloc} - 12.)15^\circ/\text{hr} \quad (2.10)$$

where  $\pm$  applies for the southern/northern hemispheres, respectively. The first expression in each formula is in MLT, where 12 hours is then subtracted because zero is noon MLT. The MLT value is converted first to degrees and then to radians in the code.

The regions over which the flow paths are not parallel to the convection reversal circle are specified by local hour limits on either side of the zero potential line. The dayside convergence region is called the throat region whereas the region on the nightside is the Harang discontinuity. The angular limits of these two convergence zones at  $\theta_0$  are given by positive and negative departures from **phid** and **phin**, respectively, which are denoted by **phidp**, **phidm**, **phinp** and **phinm**. Figure 2.1 is illustration of an example of the Heelis model output marked with various parameters.

It should be noticed that the Heelis model is suitable only for IMF  $B_z$  negative (southward) conditions. As discussed in Chapter 2.2.1, when  $B_z$  is positive (northward), the ion convection patterns can have a configuration



quite different from the two-cell pattern simulated by the Heelis model. Up until now, the latest TIEGCM and TIME-GCM still use this simple model for the parameterization of the convection pattern.

### 2.2.3 The Weimer convection pattern

The input to module `weimer` is summarized in table 2.3. The output of module `weimer.F` is summarized in table 2.4. The input parameters for the 2005 Weimer model [21] are solar wind density ( $N_{sw}$ ) and speed ( $V_{sw}$ ), and the IMF  $B_y$  and  $B_z$ , where the sign of the IMF  $B_y$  is changed for the potential pattern in the southern hemisphere. [ADD A REPRESENTATIVE FIGURE WITH  $B_y$  LARGE,  $B_z$  NEG, NH AND SH?] The ion convection pattern and the `CPCP` are very sensitive to IMF  $B_z$ , IMF  $B_y$ , and  $V_{sw}$ , but `CPCP` is relatively insensitive to  $N_{sw}$ . For example, `CPCP` changes from 158 kV to 155 kV for  $V_{sw}=450$  km/s,  $B_y = 0$  nT, and  $B_z = -15$  nT while  $N_{sw}$  increases from  $1cm^{-3}$  and  $16cm^{-3}$  (Maute, 2008 private communication). Thus, because there are numerous drop-outs of the hourly plasma density  $N_{sw}$ , we recommend setting the namelist `SWDEN = 4` as a constant which is always used. The output parameters are the Weimer convection circle location variables of `theta0` ( $= \text{bndyfitr}$  from the subroutine `setboundary`), `offc` ( $= 4.2^\circ$ ), and `dskofc` ( $= 0.0^\circ$ ), which are set in the Weimer 2005 model, and the convection entrance and exit in MLT-12 hours converted to radians, `phid` and `phin` which were calculated from the Weimer potential patterns. The auroral circle location variables of `rrad`, `offa` ( $= 4.2^\circ$ ), and `dskofa` ( $= \text{diffrac}$  or approximately  $-2.5^\circ$ ) are similar to the parameterizations calculated in `aurora.F`, which are discussed in the next section.

### 2.2.4 High latitude auroral pattern

The input to module `aurora.F` is summarized in table 2.5. The output of module `aurora.F` is summarized in table 2.6. Ion ionization rates and electron heating rate by auroral precipitation are added to the total ionization rates (variables `qo2p`, `qop`, `qn2p` and `qnp`) and electron heating rate (variable `qteaur`) (solar part is calculated in ) within the `auroral.F` module itself (subroutine `xxxx`), so they are not the outputs of the module.

The precipitation in the `auroral.F` module includes electron precipitation, soft electron precipitation, cusp precipitation, polar rain (drizzle), and ion precipitation. The contribution of each precipitation to ion production and

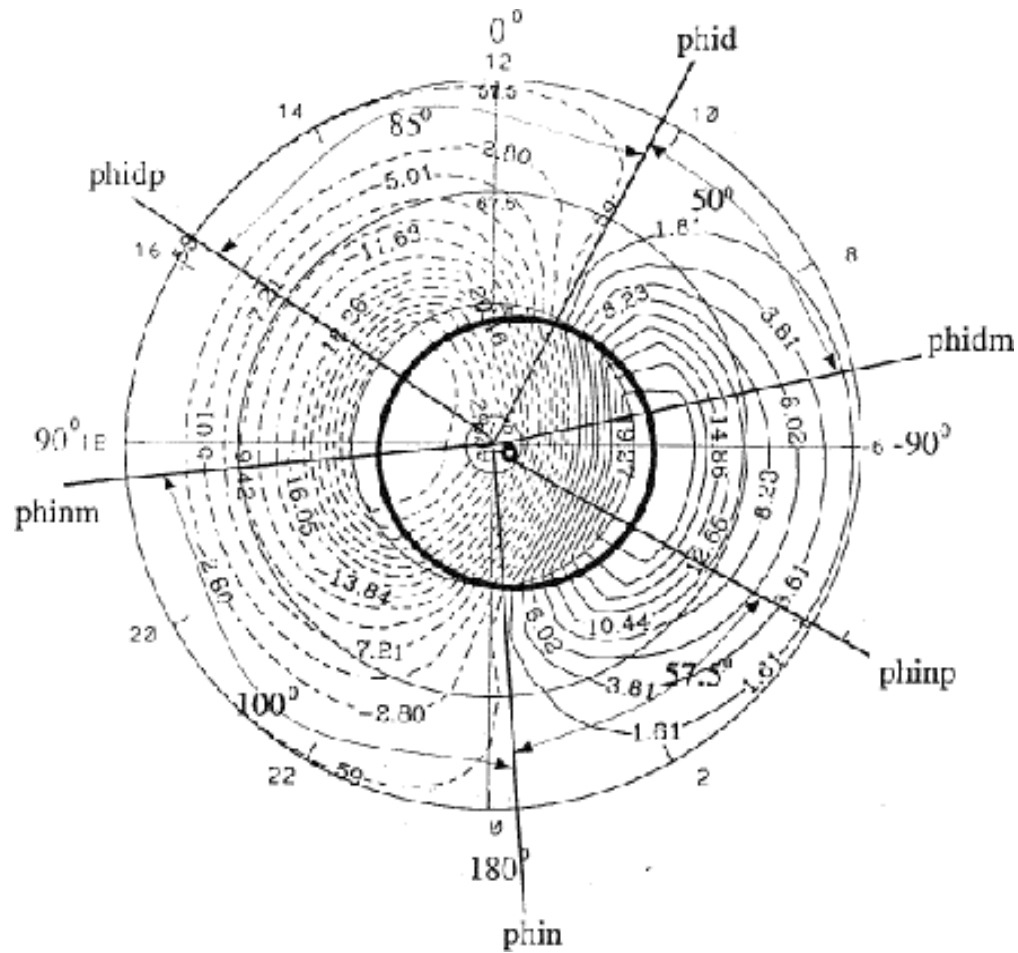


Figure 2.1: The ion convection pattern (northern hemisphere) for cross-tail potential of 60 KV and the IMF  $B_y = 7$  nT. Many of the specification parameters are illustrated.

electron heating is added to the total ionization and heating rates.

The auroral parameterizations described in the following sections are for version 1.9 and later when IMF  $B_y$  effects were restored. **Note: the following material is from [22], and copyright to the University of Michigan. Some of the material has been modified based on the updated TIEGCM.**

### Electron precipitation

The characteristics of the auroral oval used in the TIEGCM are shown in Figure 2.2. The oval is circular and is offset toward the magnetic nighttime by `offa`, which is assumed to be  $1.0^\circ$  with the Heelis convection (`offc` =  $1.1^\circ$ ) and  $4.2^\circ$  with the Weimer 2005 convection (`offc` =  $4.2^\circ$ ). The aurora is shifted towards the dawn with respect to the convection reversal circle, and is larger in radius than the convection circle (e.g. Heelis et al., 1980 [10]). The dawn-dusk offset of the Heelis convection (`dkofc`) is related to the direction and strength of the IMF  $B_y$  component and is given by equation (2.5), and so is  $-0.08$  degrees (negative towards dawn) for  $B_y = 0$ . However, the dawn-dusk offset of the aurora that goes with the Heelis convection is zero (`dkofa` =  $0.0^\circ$ ). There is no IMF  $B_y$  dependance in the Weimer 2005 convection center location, so `dkofc` =  $0.0^\circ$  and similarly `dkofa` =  $0.0^\circ$  also for the location of the aurora. Thus in both convection cases, the ion convection center and the center of the auroral oval is away from the magnetic poles.

The auroral radius ( $R_a$ ) is set by the larger of:

$$Ra(CPCP) = -0.43 + 9.69(CPCP^{0.1875}) \quad (2.11)$$

or

$$Ra(HP) = 14.20 + 0.96P_l \quad (2.12)$$

where  $P_l = 2.09 \ln(HP)$  is the hemisphere power level, and  $HP$  is the hemispheric power in [GW], so

$$Ra = \max(Ra(CPCP), Ra(HP)). \quad (2.13)$$

Recall from Equation (2.4), that the Heelis radius of convection (`theta0`) is similar to  $Ra(CPCP)$  above, where  $CPCP^{0.1875}$  is also used. [CONSIDER adding a plot of  $\theta_0$  and  $Ra(CPCP)$  and  $Ra(HP)$  for Kp formalizations of HP

and CPCP.] For the Weimer 2005 convection model, the Weimer *CPCP* averaged from both hemispheres is used to find the parameterized  $\theta_0(param)$  from Eq.(2.4) , even though the real  $\theta_0 = bndyfitr/2$ .  $Ra(param)$  is the larger of  $Ra(CPCP)$  from Eq. (2.11) or  $Ra(HP)$  from Eq. (2.12). The difference between the larger auroral radius and convection radius, or *difffrac* in *wei05loc*, is approximately 2.5 degrees, but varies. [CONSIDER another plot based on plot above of the difference between  $Ra(param)$  and  $\theta_0(param)$ .] This parameterized difference in the radii is then used to find the auroral radius used with the Weimer 2005 ion convection radius where

$$Ra(with Weimer 2005) = \theta_0(= bndfitr/2.) + difffrac \quad (2.14)$$

The TIEGCM defines the auroral oval in a new auroral coordinate system with poles in the center of the auroral oval. The width of the auroral zone is assumed to be a Gaussian distribution having a half-width of the form

$$h = h_0(1 - r_h \cos \lambda) \quad (2.15)$$

where  $h_0 = 0.5(h_1 + h_2)$ ,  $r_h = \frac{(h_1 - h_2)}{(h_1 + h_2)}$ .  $\lambda$  is the angle clockwise from the entrance of the auroral convection throat, which is away from the magnetic local noon by an angle of  $\chi_h$ .  $h_1$  (daytime) and  $h_2$  (nighttime) are the half-widths of the auroral zone at  $\lambda = 0^\circ$  and  $\lambda = 180^\circ$ , respectively, and given by

$$\begin{aligned} h_1 &= \min(2.35, 0.83 + 0.33P_l) \\ h_2 &= 2.5 + 0.025 \cdot \max(HP, 55) + 0.01 \cdot \min(0, HP - 55) \end{aligned}$$

The angle  $\chi_h$  (variable **rroth** in the code, the clockwise rotation from noon of dayside  $h_1$  Gaussian) is defined as

$$\chi_h = 15^\circ(0.81 - 0.06P_l) \quad (2.16)$$

Thus for  $P_l = 1$ , the thinnest auroral width ( $h_1$ ) is at 12 MLT - 0.75 MLT, or at 1115 MLT, while the maximum auroral width ( $h_2$ ) is 12 hours later at 2315 MLT.

$E_1$  and  $E_2$  are the energy flux of the precipitating particles (ergs cm<sup>-2</sup> s<sup>-1</sup>) in the noon sector and midnight sector, respectively, and given by

$$\begin{aligned} E_1 &= \max(0.5, -2.15 + 0.62P_l) \\ E_2 &= 1. + 0.11HP \end{aligned}$$

Usually  $E_2 > E_1$  so the maximum energy flux is on the nightside and the least is on the dayside.

There is also an angle  $\chi_e$  (variable rrote in the code, the clockwise rotation from noon of peak dayside energy), it is defined as

$$\chi_e = 15^\circ(0.17 - 0.04P_l) \quad (2.17)$$

Thus for  $P_l = 1$ , the minimum (usually) dayside auroral flux ( $E_1$ ) is at 12 MLT - 0.13 MLT, or at 1152 MLT, while the maximum (usually) nightside auroral flux ( $E_2$ ) is 12 hours later at 2352 MLT.

The auroral particle precipitation number flux is then assumed to be a product of functions describing the  $\lambda$  (longitude) variations and a latitudinal Gaussian distribution [17]

$$F = E_0[1 - r_e \cos(\alpha - \chi_e)] \exp[-(\frac{\phi - \phi_0}{h})^2] / (2\alpha_m 1.602 \cdot 10^{-9}) \quad (2.18)$$

where  $\alpha$  is the longitude,  $\phi$  is the colatitude in the newly defined auroral coordinate system,  $\phi_0$  (named `arad` in the code) is the radii of the auroral oval expressed as

$$\phi_0 = \max(-0.43 + 9.69C_p^0.1875, 14.20 + 0.96P_l) \quad (2.19)$$

where  $C_p$  is the cross tail potential in unit of kV and  $\alpha_m$  is the characteristic Maxwellian energy of the precipitating particles in keV and  $2\alpha_m$  is the mean Maxwellian energy. For the Heelis convection,  $C_p$  is the same in both hemispheres, but for the 2005 Weimer convection,  $C_p$  is the average of `CPCP` from both hemispheres. The angle  $\chi_e$  (variable rrote in the code) is defined in 2.17 such that

$$\begin{aligned} E_0[1 - r_e \cos(\alpha - \chi_e)] &= E_1 \quad \text{when } \alpha - \chi_e = 0^\circ \\ E_0[1 - r_e \cos(\alpha - \chi_e)] &= E_2 \quad \text{when } \alpha - \chi_e = 180^\circ \end{aligned} \quad (2.20)$$

where  $E_0 = 0.5(E_1 + E_2)$  and  $r_e = (E_1 - E_2)/(E_1 + E_2)$ .

The characteristic energy  $\alpha_m$  is defined using the statistical patterns measured by satellite (e.g. Hardy et al., 1985). As defined in Roble and Ridley (1987) [17], there is a dayside  $\alpha_1$  and a nightside  $\alpha_2$  that are fixed to the dayside  $E_1$  and nightside  $E_2$  energy fluxes rotated by the angle  $\chi_e$ . Since version 1.8, the characteristic Maxwellian electron energies have been nearly constant at:

$$\begin{aligned} \alpha_1 &= 1.5 \text{ keV} \\ \alpha_2 &= 2.0 \text{ keV} \end{aligned} \quad (2.21)$$

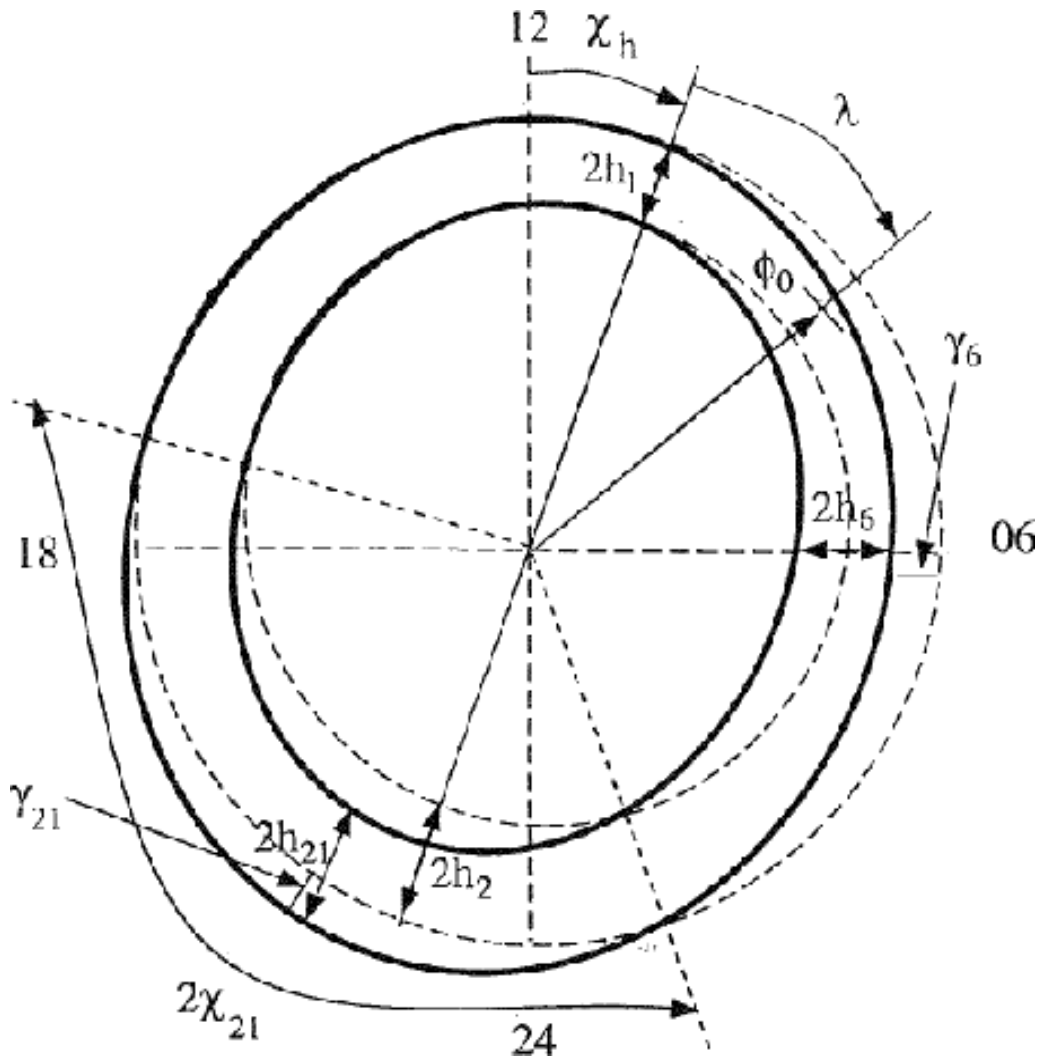


Figure 2.2: Illustration of the parameterization of the auroral oval in the TIGCM - SHOULD REPLACE WITH Roble and Ridley (1987)  $\alpha_{1,2}$  fig.

where

$$\begin{aligned}
 \alpha_0 &= 0.5(\alpha_1 + \alpha_2) \\
 r_a &= (\alpha_1 - \alpha_2)/(\alpha_1 + \alpha_2) \\
 F &= E_0[1 - r_e \cos(\alpha - \chi_e)] \exp[-(\frac{\phi - \phi_0}{h})^2] / \alpha_m = \alpha_0 \cdot [1 - r_a \cos(\alpha - \chi_e)]
 \end{aligned}
 \tag{2.22}$$

Thus the characteristic energy of electron precipitation over the entire auroral oval is not changing with geomagnetic storm intensities (i.e. Kp), although Zhang and Paxton (2008) [23] show in their Figure 8b that  $2\alpha_m$  increases from 1 keV to 3 keV between Kp 0 and 9 from GUVI FUV images.

### Soft electron precipitation

Soft electron precipitation is defined the same as the auroral oval in Section 2.2.4. At present, it is turned off in the TIEGCM by setting the soft electrons to be zero (characteristic energy is set to be 75 eV).

### Cusp Electron precipitation

The polar cusp region is also subject to intense soft particle precipitation with an average energy around 100 eV. (The characteristic energy (not mean energy!) of the cusp precipitation used in TIEGCM is 100 eV.) Most of the energy of the precipitating electrons is deposited in the F-region, causing localized enhanced electron density and temperature, or a so called hot spot (Fontheim et al., 1987; Heikkila and Winningham, 1971). The longitude extent of the polar cusp is about 30 to 40 degrees (2-4 MLT hours) around magnetic local noon. The polar cusp is more constrained in the latitudinal direction with an average width about 2-3 degrees (e.g. Lockwood and Davis, 1995; Newell and Meng, 1992), and is located between  $75^\circ$  and  $80^\circ$  magnetic latitudes. The location and size of the polar cusp may change dramatically under various IMF conditions.

In the TIEGCM cusp precipitation is parameterized by assuming Gaussian distribution in both latitude and longitude. The location of the cusp is assumed to be at the daytime convection reversal throat which is determined by the strength and direction of the IMF  $B_y$  and  $B_z$  components. The Gaussian half width in the longitude direction is  $20^\circ$  and the half width in the latitude direction is  $5^\circ$ . Thus the TIEGCM, because of the limitations of

its grid size, overestimates the latitude extent by about 5 times as compared to the observed average latitude width of  $2^\circ$  to  $3^\circ$  discussed above. One consequence of this parameterization is the overestimation of the sizes of enhanced plasma density and temperature regions produced by the cusp soft precipitation and, in turn, the overestimation of the coupling effect between neutrals and ions, and the amount of plasma transported from the dayside ionosphere into the nighttime polar cap.

The typical energy flux of cusp electron precipitation is about  $0.32 \text{ erg/cm}^2/\text{s}$  varying with geomagnetic and IMF conditions (Hardy et al., 1985; Candidi and Meng, 1984; Heikkila and Winningham, 1971). In the TIEGCM, the energy flux of the cusp precipitation is given by

$$\begin{aligned} E_c &= 3.12 \times 10^8 (2.4 \times 10^{-1} + 6.7 \times 10^{-3} H_p) \text{ eV/cm}^2/\text{s} \\ &= -0.5 (2.4 \times 10^{-1} + 6.7 \times 10^{-3} H_p) \text{ erg/cm}^2/\text{s} \end{aligned} \quad (2.23)$$

(in TIEGCM 1.9  $E_c$  is defined as  $(2.4 \times 10^{-1} + 6.7 \times 10^{-3} H_p)/5$  do not know why) Thus, the energy flux is  $0.14 \text{ erg/cm}^2/\text{s}$  when  $H_p = 5.0 \text{ GW}$  during magnetic quiet times, and  $0.63 \text{ erg/cm}^2/\text{s}$  when is  $150.0 \text{ GW}$  during a storm.

### Polar rain (drizzle)

Spatially homogeneous precipitation of soft particles in the polar cap, the so called polar rain, is also included in the TIEGCM. The polar rain particles come from the solar corona and get into the upper atmosphere through the magnetosheath (Fairfield and Scudder, 1985). The energy fluxes of polar rain commonly vary from  $10^{-3}$  to  $10^{-2} \text{ erg/cm}^2/\text{s}$  (Sotirelis et al., 1997; Hardy et al., 1986; Riehl and Hardy, 1986; Gussenhoven et al., 1984; Winningham and Heikkila, 1974), although sometimes very strong polar rain may occur with energy fluxes up to about  $10 \text{ erg/cm}^2/\text{s}$  (Newell and Meng, 1990, Meng and Kroehl, 1977). The occurrence frequency of polar rain events for the IMF Bz southward is about twice that for IMF Bz northward conditions (Gussenhoven et al., 1984). Polar rain has strong hemispherical asymmetry, with the Earth's north (south) hemisphere favored for away (towards) IMF Bx directions (Hardy et al., 1986; Gussenhoven et al., 1984). The energy flux of polar rain also has a dawn-dusk gradient controlled by IMF  $B_y$  conditions. Polar rain is stronger during magnetic storms than during magnetically quiet times (Winningham and Heikkila, 1974).

The energy spectrum of polar rain can be described by a single or by two Maxwellian distributions. The lower energy component of polar rain has a



very narrow energy distribution centered at 80 eV with a standard deviation of 13 eV. The energy spectrum of the high energy component has a outstanding peak centered at 525 eV but extending over a wide range from 100 eV to several thousand eV. The mean energy of the high energy component of the polar rain is about 1250 eV with a standard deviation of 750 eV (Hardy et al., 1986; Riehl and Hardy, 1986).

In the TIEGCM, polar rain is parameterized by a single Maxwellian distribution with a characteristic (not mean energy) energy of 500 eV. This simple approach may underestimate the contributions of the low energy component of polar rain to the ionization rate of the upper atmosphere, while overestimating the contributions of the high energy component. The peak altitude of the ionization rate is thus moved to lower heights affecting the calculation of the F-region electron density in the winter hemisphere polar cap greatly. The energy flux and its variations with the geomagnetic activity is described in the TIEGCM by

$$\begin{aligned} E_p &= 3.12 \times 10^8 (0.012 + 0.006 H_p) \quad eV/cm^2/s \\ &= 0.5 (0.012 + 0.006 H_p) \quad erg/cm^2/s \end{aligned} \quad (2.24)$$

### Ion precipitation

Solar proton precipitation inside the polar cap is included in TIEGCM. The characteristic energy was assumed to be 10 keV. The energy flux is currently set to be 1.E-20, so practically zero. There is also a logical variable `add_sproton`, which has a default value of `false`. You have to change this to `true` and specify the energy flux `e_sp` if want to include this precipitation in the model calculation.

### Ion ionization and electron heating rates

It is assumed that particle precipitations has a Maxwellian energy distribution. The total energy flux is given by (Roble and Rees, 1977; [17])

$$F_E = 2\alpha F_P \quad (2.25)$$

where  $F_P$  is the total number flux of the precipitating particles,  $\alpha$  is characteristic energy of the energy distribution and  $2\alpha$  is the mean energy. The ionization rate produced by collisions between precipitating particles and neutral particles is then calculated using an analytic relationship derived by

Lazarev (1967). Contributions from both primary and secondary electrons to the production of ionospheric plasma are included. The detailed description of this calculation is given by [17].

The number fluxes of auroral electron precipitation, soft electron precipitation and polar drizzle are calculated in the auroral coordinate system based on 2.25. The coordinate transfer for each geographic grid points, and the final characteristic energies number fluxes (variable `alfa`, `alfa2`, `driz1`, `flux1`, `flux2`) and auroral heating (`qteaur`: used in `subroutine` ) at each grid points are calculated in `subroutine` .

Number flux for the cusp precipitation is obtained in `subroutine` .

The detail of how to obtain ionization rates need to written in detail later. ( `subroutines` `aurora_ions`, `aion` and `bion`). Formulas need to be added here too.

physical field	variable	unit	pressure level	timestep
Radii of convection flow reversal circle	$\theta_0$ <b>theta0</b>	radians		$t_n$
Offset between the center of the convection circle and the geomagnetic pole along the geomagnetic noon and midnight line	<b>offc</b>	radians		$t_n$
Offset between the center of the convection circle and the geomagnetic pole along the geomagnetic dawn-dusk line	<b>dskofc</b>	radians		$t_n$
Potential at the center of the convection circle	<b>pcen</b>			$t_n$
Potential of the evening cell	<b>psie</b>			
Potential of the morning cell	<b>psim</b>			
Daytime entrance of convection in MLT-12 converted to radians	<b>phid</b>	radians		
Daytime exit of convection in MLT-12 converted to radians	<b>phin</b>	radians		
Negative departure from <b>phid</b>	<b>phidm</b>			
Positive departure from <b>phid</b>	<b>phidp</b>			
Positive departure from <b>phin</b>	<b>phinp</b>			
Negative departure from <b>phin</b>	<b>phinm</b>			
Sun's longitude in dipole coordinate ( <b>MAGFIELD.F</b> )	<b>rr1</b> <b>sunlons</b>			
Critical colatitudes ( <b>CONS.F</b> )	<b>crit</b>			

Table 2.1: Input fields to module **heelis**. All these variables but **sunlons** and **crit** are specified in module **AURORA.F**

physical field	variable	unit	pressure level	timestep
Fractional presence of dynamo field	Pfrac (used in )			$t_n$
Heelis potential in geomagnetic coordinates	phihm (used in dynamo.F)			$t_n$

Table 2.2: Output fields of module `heelis.F`

physical field	variable	unit	pressure level	timestep
UT year, daynumber, hour	sunlons			$t_n$
Sun's longitude in dipole coordinate (MAGFIELD.F)				
Solar wind density		$cm^3$		$t_n$
Solar wind speed		$km/s$		$t_n$
IMF $B_y$ , $B_z$		nT		$t_n$

Table 2.3: Input fields to module `weimer`.

physical field	variable	unit	pressure level	timestep
Radii of convection flow reversal circle	$\theta_0$ theta0	radians		$t_n$
Offset between the center of the convection circle and the geomagnetic pole along the geomagnetic noon and midnight line	offc	radians		$t_n$
Offset between the center of the convection circle and the geomagnetic pole along the geomagnetic dawn-dusk line	dskofc	radians		$t_n$
Daytime entrance of convection in MLT-12 converted to radians	phid	radians		
Daytime exit of convection in MLT-12 converted to radians	phin	radians		
Radii of peak energy flux in the auroral circle	rrad	radians		$t_n$
Offset between the center of the auroral circle and the geomagnetic pole along the geomagnetic noon and midnight line	offa	radians		$t_n$
Offset between the center of the auroral circle and the geomagnetic pole along the geomagnetic dawn-dusk line	dskofa	radians		$t_n$
Fractional presence of dynamo field	Pfrac (used in )			$t_n$
Heelis potential in geomagnetic coordinates	phihm (used in dynamo.F)			$t_n$

Table 2.4: Output fields of module `weimer.F`.

physical field	variable	unit	pressure level	timestep
Cross polar cap potential	ctpoten			$t_n$
Hemisphere power	power			$t_n$
IMF By	byimf			
Sun's longitude in dipole coordinate (magfield.F)	sunlons			

Table 2.5: Input fields to module `aurora`.

physical field	variable	unit	pressure level	timestep
Radii of the convection flow reversal circle	$\theta_0$ ( <code>theta0</code> ) (used in <code>heelis.F</code> )	radians		$t_n$
Offset between the center of the convection circle and the geomagnetic pole along the geomagnetic noon and midnight line	<code>offc</code> (used in <code>heelis.F</code> )	radians		$t_n$
Offset between the center of the convection circle and the geomagnetic pole along the geomagnetic dawn-dusk line	<code>dskofc</code> (used in <code>heelis.F</code> )	radians		$t_n$
Potential at the center of the convection circle	<code>pcen</code> (used in <code>heelis.F</code> )			$t_n$
Potential of the evening cell	<code>psie</code> (used in <code>heelis.F</code> )			
Potential of the morning cell	<code>psim</code> (used in <code>heelis.F</code> )			
Daytime entrance of convection in MLT-12 converted to radians	<code>phid</code>	radians		
Daytime exit of convection in MLT-12 converted to radians	<code>phin</code>	radians		
Negative departure from <code>phid</code>	<code>phidm</code> (used in <code>heelis.F</code> )			
Positive departure from <code>phid</code>	<code>phidp</code> (used in <code>heelis.F</code> )			
Positive departure from <code>phin</code>	<code>phinp</code> (used in <code>heelis.F</code> )			
Negative departure from <code>phin</code>	<code>phinm</code> (used in <code>heelis.F</code> )			

Table 2.6: Output fields of module `aurora.F`.

## 2.3 Lower Boundary

At the lower boundary of TI(M)EGCM the background thermosphere has to be specified. In addition tidal perturbations can be optionally added in. Note that not all TIMEGCM option for the lower boundary are describe here since this code is still under development and testing by June 2009.

The lower boundary conditions in TIEGCM are specified at pressure level -7. Note that TIEGCM uses two different height grids. One is called the interface grid, which starts at the pressure level -7, the other one is called the midpoint level grid, which starts at -6.75 (height resolution 2 grid points per scale height), or -6.875 (height resolution 4 grid points per scale height). Except for the geopotential height, the vertical dimensionless velocity and the electron density, all fields are output on the midlevel grid.

In TIEGCM at the lower boundary (pressure level =-7, approximately at 97 km) we specify a constant background field for the geopotential height of 96.37229 *km*, for the neutral temperature of 181.0 *K*, and the neutral zonal and meridional winds are set to zero. The background does not vary with day of the year. These fields are consistent with each other (what does this mean?).

Note that for TIMEGCM the lower boundary is at pressure level -17, approximately at 32 km. However concerning the interface and midpoint pressure levels TIMEGCM and TIEGCM are the same. The background field in TIMEGCM for the geopotential height are from an analytical fit to a model called zatmos (is there any reference or official name?), the neutral temperature is specified by the same model zatmos. Both fields vary with latitude and day of the year. The neutral zonal and meridional winds at the lower boundary are calculated by assuming geostrophic balance. The calculation is done in `subroutine tuvbnd`. At the equator when the Coriolis force is zero, and geostrophic balance is not valid to assume, additional tunable Rayleigh friction is introduced (see `subroutine tuvbnd`).

In TIEGCM as well as TIMEGCM tidal perturbations caused by solar radiation can be added to the background. For classical tidal theory we refer to Chapman and Lindzen [1]. In TIEGCM only migrating tidal components which propagate westward with the apparent motion of the sun should be



specified at either 2.5-degree/4 grid points per scale height or 5-degree/ 2 grid points per scale height resolution until nonmigrating tidal propagation is validated in the high resolution version of the TIEGCM. These components are thermally driven by the periodic absorption of solar radiation throughout the atmosphere, primarily the absorption of UV radiation by stratospheric ozone and of IR by water and water vapor in the troposphere. In TIMEGCM we recommend using migrating and non-migrating tides only with the double resolution version of TIMEGCM (version TIMEGCM1.3 and higher). The single resolution version of TIMEGCM is too coarse to capture the propagation of the tides in the right way. Non-migrating tides which can be include in TIMEGCM are global-scale waves, however they do not follow the apparent motion of the sun. They can either not propagate horizontally, move eastward or westward.

Both models provide two ways of specifying the migrating tidal perturbations:

- Hough Modes
- Global Scale Wave Model (GSWM)

However, we recommend using only the Global Scale Wave Model option to include tidal perturbations, and using Hough Modes only for numerical experiments done by experienced users. Both options will be explained in the following.

### 2.3.1 Migrating tides specified by Hough Modes

Using Hough modes is one way to decompose the tidal perturbations with respect to longitude and latitude for the different wave components. Hough functions are described in e.g. Chapman and Lindzen [1], Flattery [6]. A single tidal mode has a horizontal structure which can be described by a single Hough function. The atmospheric tides which migrate westward with the apparent motion of the Sun are called migrating tides. In TI(M)EGCM only a limited number of upward propagating migrating tidal modes are defined. The modes with a diurnal period have a wavenumber  $s=1$ , and a Hough Mode with  $(s,n)=(1,1)$  can be specified. For the semidiurnal modes with a wavenumber  $s=2$  the following Hough modes can be specified:  $(2,2)$ ,  $(2,3)$ ,  $(2,3)$ ,  $(2,4)$ ,  $(2,5)$ .

To specify the Hough modes the amplitude and phase of the corresponding mode has to be given in the namelist read input for the semidiurnal tides **TIDE**, and the diurnal tides **TIDE2** by setting the amplitude and phase of the component. The order of the semidiurnal Hough mode specification is from  $n=2$  (2,2) to  $n=5$  (2,5). The amplitude has to be in [cm] and the phase of the Hough mode components

$$slt = -bhour + 12 \quad (2.26)$$

with the solar local time  $slt$ , and  $bhour$  the phase of the tidal component in the TI(M)EGCM input. A 24 hrs/12 hrs shift may be applied to the diurnal / semidiurnal components since  $bhour$  should be

$$\begin{aligned} (-12 < bhour < 12) & \text{ for the diurnal} \\ (-6 < bhour < 6) & \text{ for the semidiurnal} \end{aligned} \quad (2.27)$$

### 2.3.2 Migrating and non-migrating tides specified by GSWM

The Global Scale Wave Model (GSWM) [7],[8] is a numerical model of planetary waves and solar tides in the Earth's atmosphere from 0 - 125 km developed at HAO (High Altitude Observatory), NCAR (National Center for Atmospheric Research ) by M. Hagan. GSWM solves for non-migrating or migrating waves with 2-dimensional, linearized, steady-state assumptions and a realistic zonal mean atmosphere. The forcing is due to thermospheric absorption of solar extreme ultraviolet (EUV) radiation, absorption of solar radiation in the Schumann-Runge (S-R) bands and continuum in the mesopause region, strato-mesospheric absorption of solar ultraviolet (UV) radiation, tropospheric absorption of solar infrared (IR) radiation, and tropospheric latent heating associated with deep convective activity (DCA). GSWM also includes dissipation due to ion drag, thermal conductivity, molecular and eddy diffusivity, and gravity wave drag. Both migrating (sun-synchronous) and non-migrating (longitude-dependent) tidal components are included ( $s=-6$  to 6) for both the diurnal and semidiurnal harmonics.

In TI(M)EGCM the use of GSWM at the lower boundary has to be specified by the namelist read parameters

- migrating diurnal tides ( $s=-6$  to 6) **GSWM\_MI\_DI\_NCFILE**

- migrating semidiurnal tides (s=-6 to 6) `GSWM_MI_SDI_NCFILE`
- ONLY TIMEGCM: non-migrating diurnal tides (s=-6 to 6) `GSWM_NM_DI_NCFILE`
- ONLY TIMEGCM: non-migrating semidiurnal tides (s=-6 to 6) `GSWM_NM_SDI_NCFILE`

and the location of the corresponding GSWM file. Note that compared to the Hough mode approach the perturbations at each grid point will be provided, already including the 13 wavenumbers (s=-6 to s=6).

### 2.3.3 Specifics about the Lower Boundary of TIMEGCM

This chapter applies to TIMEGCM version 1.41 and higher. The basic change with respect to the lower boundary compared to older versions is that we separate the background from the perturbations of the geopotential height  $Z$ , the neutral temperature  $T_n$ , and the neutral wind components  $U_n$  and  $V_n$ . The lower boundary in TIME-GCM is at pressure level -17, approximately at 32 km.

#### Background fields

In the model we set the background in `subroutine lbc`. There are three options available, and all have in common that these are daily values, so no tidal perturbations are included.

- ECMWF (only 2.5 deg): sets  $Z$ ,  $T_n$ ,  $U_n$ ,  $V_n$
- NCEP (only 5 deg): sets  $Z$ ,  $T_n$  + calculation of  $U_n$ ,  $V_n$
- model `zatmos` (2.5 and 5 deg): sets  $Z$ ,  $T_n$  + calculation of  $U_n$ ,  $V_n$

`zatmos` is an analytical model which sets the geopotential height and the neutral temperature. For both background cases using NCEP and the model `zatmos` the neutral winds are not specified, and have to be calculated. In TIME-GCM this is done in `subroutine uvbgrd`, and for the first two time steps in `subroutine uvbnd`. The calculation of the neutral winds at the lower boundary is using the background fields of  $Z$ . It's considering horizontal advection, the pressure gradient force, and horizontal diffusion on the left hand side, and the right hand side consists of the Coriolis force, Rayleigh friction and momentum force. It should be added that there is some tuning

friction close to the equator which is set to zero. The time derivative of the neutral winds are discretized and split on the left and right hand side. We are not using the vertical advection term anymore. This term had a neglectable influence on the winds at the lower boundary, and it wouldn't have justified the effort to separate the term into a background and perturbations. The `subroutine uvbnd` calculates the winds fields for the background and the perturbations while `subroutine uvbgrd` calculates it only for the background. Except for the first two time steps, when the splitting into background and perturbations of  $Z$ ,  $U_n$ ,  $V_n$  from the two previous time step is not known, `subroutine uvbgrd` is called to determine the background winds.

### Perturbations fields

The perturbations of tides and waves are set in `subroutine lbc`, after the background is specified. The options are:

- Hough Modes (2.5 and 5 deg): sets  $Z$ ,  $T_n$ ,  $U_n$ ,  $V_n$
- GSWM: sets  $Z$ ,  $T_n$ ,  $U_n$ ,  $V_n$ 
  - migrating (2.5 and 5 deg)
  - nonmigrating (only 5 deg)
- planetary waves etc. (2.5 and 5 deg): sets  $Z$ ,  $T_n$  + calculation of  $U_n$ ,  $V_n$

The planetary wave etc. option is not tested in the model, and the source code is just kept. Also since only the geopotential and neutral temperature from these waves are set the winds have to be calculated like it is done for the background. Therefore only for this perturbation option the perturbations are added to the background field, and then the background + planetary wave neutral winds are determined in `subroutine uvbgrd`. The nonmigrating tides from GSWM should only be used with the 2.5 degree grid resolution since otherwise the tidal propagation is not right.



## Chapter 3

# Neutral Dynamics

The TIE-GCM solves the primitive equations in pressure coordinate, and the detailed information on the equations and the numerics employed can be found in [3]. In this Chapter, we will first give a brief summary of the model dynamics, and then discuss the main components in solving dynamic equations. The solution of the thermodynamics will be discussed in the next Chapter.

The zonal and meridional winds are solved from the momentum equations in the zonal and meridional direction, respectively. The tendencies (acceleration) of the horizontal winds come from horizontal and vertical momentum transport, horizontal gradient of geopotential, eddy and molecular viscosity, Coriolis force, and ion drag (Section 3.3). The vertical wind is determined from the continuity equation by integrating the divergence of the horizontal winds vertically (Section 3.2). The geopotential is calculated from the hydrostatic equation by integrating temperature vertically (Section 3.1).

The equations are solved using 4th order finite difference method. The vertical grid is staggered with horizontal winds, neutral, ion, and electron temperature, and mass mixing ratios defined on the so-called midpoints, and vertical wind and geopotential defined on the interfaces. Leapfrog scheme is used for time integration of momentum transport, geopotential gradient, Coriolis force, and ion drag, and implicit scheme is used for eddy and molecular viscosity in the vertical direction. To achieve better numerical stability, Shapiro filter (reference?) is applied in meridional and zonal directions.

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
mass mixing ration of $O$	$\Psi_O$	—	midpoints	$t_n$
mass mixing ration of $O_2$	$\Psi_{O_2}$	—	midpoints	$t_n$
neutral meridional velocity	$v_n$	$cm/s$	midpoints	$t_n$

Table 3.1: Input fields to subroutine `addiag`

physical field	variable	unit	pressure level	timestep
$\cos \lambda \cdot$ neutral meridional velocity	$\cos \lambda v_n$	$cm/s$	midpoints	$t_n$
mean molecular mass	$\bar{m}$	$g/mole$	interfaces	$t_n + \Delta t$
conversion factor $mmr$ to $\#/cm^3$	$N\bar{m}$ <code>xnmbar</code>	$\#/cm^3 g/mole$	midpoints	$t_n + \Delta t??$
conversion factor $mmr$ to $\#/cm^3$	$N\bar{m}$ <code>xnmbari</code>	$\#/cm^3 g/mole$	interfaces	$t_n + \Delta t??$
conversion factor $mmr$ to $\#/cm^3$	$N\bar{m}$ <code>xnmbarm</code>	$\#/cm^3 g/mole$	midpoints	$t_n + \Delta t??$

Table 3.2: Output fields of subroutine `addiag`

### 3.1 Calculation of geopotential height

The input to subroutine `addiag` is summarized in table 3.1. The output of subroutine `addiag` is summarized in table 3.2. The module data of subroutine `addiag` is summarized in table 3.3. First the term  $\cos \lambda v_n$  is calculated on the midpoint pressure level and stored in the variable `vc`. The mean molecular mass is determined by

$$\bar{m} = \left[ \frac{\Psi_{O_2}}{m_{O_2}} + \frac{\Psi_O}{m_O} + \frac{\Psi_{N_2}}{m_{N_2}} \right]^{-1} \quad (3.1)$$

with the mass mixing ratio of  $N_2$  determined by  $\Psi_{N_2} = 1 - \Psi_O - \Psi_{O_2}$ . Before the mean molecular weight is returned from the subroutine it is transferred



physical field	variable	unit	pressure level	timestep
cosinus	$\cos \lambda$	—	—	—
height step	$\Delta z$	—	—	—
dzgrav	$g/R^*$		interfaces	$t_n$
timestep size	$\Delta t$	$s$	—	—
expz	$e^{-z-\frac{1}{2}\Delta z}$	—	midpoints	—
expzmid	$e^{-\frac{1}{2}\Delta z}$	—	—	—
expzmid_inv	$e^{\frac{1}{2}\Delta z}$	—	—	—
Boltzman constant	$k_B$	$1.38 \cdot 10^{16}$	—	$t_n$
freqsemedi	$\frac{4\Pi}{24 \cdot 60 \cdot 60}$	$rad/s$	—	—
ci		$(0, 1)$	interfaces	$t_n$

Table 3.3: Module data of subroutine `addiag`

to the interface pressure level by averaging.

$$\overline{m}(z) = \frac{1}{2} \left( \overline{m}(z + \frac{1}{2}\Delta z) + \overline{m}(z - \frac{1}{2}\Delta z) \right) \quad (3.2)$$

with the lower boundary value extrapolated

$$\overline{m}(z_{bot}) = 1.5\overline{m}(z_{bot} + \frac{1}{2}\Delta z) - 0.5\overline{m}(z_{bot} + \frac{3}{2}\Delta z) \quad (3.3)$$

The conversion factor from mass mixing ratio to number density is first evaluated at the midpoint level

$$n\overline{m}(z + \frac{1}{2}\Delta z) = p_0 e^{-z-\frac{1}{2}\Delta z} \frac{\overline{m}(z + \frac{1}{2}\Delta z)}{k_B T_n(z + \frac{1}{2}\Delta z)} \quad (3.4)$$

which is stored in the variable `xnmbarm`. I'm not sure why this is done, but again is the conversion factor from mass mixing ratio to number density calculated and stored in `xnmbarm`. The only difference to the above factor is that now the mean molecular mass is already on the interface pressure level and converted back to the midpoint pressure level. Afterward the mean molecular mass on the interface pressure level is determined

$$n\overline{m}(z) = p_0 e^{\frac{1}{2}\Delta z} e^{-z-\frac{1}{2}\Delta z} \frac{\overline{m}(z)}{k_B T_n(z)} \quad (3.5)$$

with  $T_n(z_{top}) = T_n(z_{top} - \frac{1}{2}\Delta z)$ , and the value  $e^{-\frac{1}{2}\Delta z}e^{-z_{top}+\frac{1}{2}\Delta z}$  at the upper boundary.

The geopotential height is calculated by using the hydrostatic equation

$$\frac{\partial Z}{\partial z} = \frac{R^*T_n}{\bar{m}g} = H \quad (3.6)$$

with  $\Delta Z = H\Delta z$ . First the term  $H\Delta z$  is set which is stored in the variable `w1`

$$w1(z + \frac{1}{2}\Delta z) = \frac{\Delta z R^*}{g} \frac{T_n(z + \frac{1}{2}\Delta z)}{\bar{m}(z + \frac{1}{2}\Delta z)} \quad (3.7)$$

The lower boundary values of the geopotential height are set from the Hough modes or GSWM with possible contribution from the semidiurnal migrating tide  $Z_{SD}$ , the migrating diurnal tide  $Z_D$ , the annual tide  $Z_A$ , and the non-migrating semidiurnal and diurnal tides  $Z_{nSD}$  and  $Z_{nD}$ , respectively.

$$Z(z_{bot}) = Z_{SD} + Z_D + Z_A + Z_{nSD} + Z_{nD} \quad (3.8)$$

All the tidal contributions are defined at the lower boundary pressure level  $z = -7$ . The geopotential height is evaluated then by

$$Z(z + \Delta z) = w1(z + \frac{1}{2}\Delta z) + Z(z) \quad (3.9)$$

with  $w1 = \frac{\Delta z R^*}{g} \frac{T_n}{\bar{m}}$  (see eq. (3.7))

physical field	variable	unit	pressure level	timestep
neutral zonal velocity	$u_n$	$cm/s$	midpoints	$t_n$
neutral meridional velocity	$\cos \lambda v_n$	$cm/s$	midpoints	$t_n$

Table 3.4: Input fields to subroutine `swdot`

physical field	variable	unit	pressure level	timestep
'dimensionless' vertical velocity	$W$	$1/s$	interfaces	$t_n + \Delta t$

Table 3.5: Output fields of subroutine `swdot`

## 3.2 Calculation vertical velocity $W$

The input to subroutine `swdot` is summarized in table 3.4. The output of subroutine `swdot` is summarized in table 3.5. The vertical velocity is calculated by solving the continuity equation of the thermospheric neutral gas. The continuity equation takes the following form

$$\frac{1}{R \cos \lambda} \frac{\partial}{\partial \lambda} (v_n \cos \lambda) + \frac{1}{R \cos \lambda} \frac{\partial u_n}{\partial \phi} + e^z \frac{\partial}{\partial Z} (e^{-z} W) = 0 \quad (3.10)$$

with the 'dimensionless' vertical velocity is  $W = \frac{dZ}{dt}$ . The 'real' vertical velocity  $w$  relative to a pressure level (note that for the vertical velocity relative to the ground you have to add the vertical movement of the pressure level) is obtained by integrating the continuity equation over  $Z$  to get  $W$ , and then multiply  $W$  by the scale height  $H$ .

The horizontal divergence  $\nabla_H \cdot \mathbf{v}_n$  is calculated in **subroutine** `divrg`.

$$\begin{aligned} \nabla_H \cdot \mathbf{v}_n = & \frac{1}{R_E \cos \lambda} \left[ \frac{2}{3\Delta\phi} [u_n(\phi + \Delta\phi, \lambda)u_n(\phi - \Delta\phi, \lambda)] - \right. \\ & \frac{1}{12\Delta\phi} [u_n(\phi + 2\Delta\phi, \lambda)u_n(\phi - 2\Delta\phi, \lambda)] \\ & \frac{2}{3\Delta\phi} [\cos(\lambda + \Delta\lambda)v_n(\phi, \lambda + \Delta\lambda)\cos(\lambda - \Delta\lambda)v_n(\phi, \lambda - \Delta\lambda)] - \\ & \left. \frac{1}{12\Delta\lambda} [v_n(\phi, \lambda + 2\Delta\lambda)v_n(\phi, \lambda - 2\Delta\lambda)] \right] \end{aligned} \quad (3.11)$$

The integration is done by an integration from the top to the bottom of the model, with the condition at the upper boundary being

$$\frac{\partial w}{\partial z} = 0 \quad (3.12)$$

and in discretized form

$$W(z_{top}) = \nabla_H \cdot \mathbf{v}_n(z_{top} - \frac{1}{2}\Delta z) \quad (3.13)$$

and then do the integration

$$W(z - \Delta z) = e^{-\frac{1}{2}z} \left[ e^{-\frac{1}{2}z} W(z - 2\Delta z) + \Delta z \nabla_H \cdot \mathbf{v}_n(z + \frac{1}{2}\Delta z) \right] \quad (3.14)$$

The vertical velocity  $W$  is then filtered in longitude to remove the high wave numbers. The filter is in **subroutine** `filter_w` and is part of the file `swdot.F`.

### 3.3 Momentum equation /DUV.F

The input to subroutine `duv` is summarized in table 3.6. The output of subroutine `duv` is summarized in table 3.7. The zonal and meridional momentum equation is solved to get the neutral horizontal velocities  $u_n$  and  $v_n$ . For the vertical velocity the continuity 3.10 equation is solved. In the code the subroutine `addiag` solves for the dimensionless vertical velocity  $w$ .

The momentum equation in the zonal direction can be written as

$$\begin{aligned} \frac{\partial u_n}{\partial t} = & \frac{ge^z}{p_0} \frac{\partial}{\partial Z} \left[ \frac{\mu \partial u_n}{H \partial Z} \right] + f^{cor} v_n + \lambda_{xx}(v_{ExB,x} - u_n) + \lambda_{xy}(v_{ExB,y} - v_n) - \\ & \mathbf{v}_n \cdot \nabla u_n + \frac{u_n v_n}{R_E} \tan \lambda - \frac{1}{R_E \cos \lambda} \frac{\partial \Phi}{\partial \phi} - W \frac{\partial u_n}{\partial Z} - h d_u \end{aligned} \quad (3.15)$$

with  $\lambda_{xx}$  and  $\lambda_{xy}$  the ion drag coefficients. The meridional momentum equation is defined as

$$\begin{aligned} \frac{\partial v_n}{\partial t} = & \frac{ge^z}{p_0} \frac{\partial}{\partial Z} \left[ \frac{\mu \partial v_n}{H \partial Z} \right] - f^{cor} v_n + \lambda_{yy}(v_{ExB,x} - u_n) + \lambda_{yx}(v_{ExB,y} - u_n) - \\ & \mathbf{v}_n \cdot \nabla v_n + \frac{u_n v_n}{R_E} \tan \lambda - \frac{1}{R_E} \frac{\partial \Phi}{\partial \lambda} - W \frac{\partial v_n}{\partial Z} - h d_v \end{aligned} \quad (3.16)$$

Horizontal diffusion  $h d_u$  and  $h d_v$  is also included in the momentum equations (needs documentation look at `hdiff3`; not consistent in equations) The time rate of change in the horizontal velocity on the left hand (1. term) side is equal to the forcing terms on the right hand side. The forcing terms are the following in this order: the vertical viscosity (2. term), the Coriolis force (3. term), the ion-drag force (4.+5. term), the nonlinear horizontal advection (6. term) and momentum force (7. term), the pressure gradient force (8. term), the vertical advection (9. term) and horizontal diffusion (10.term). Using a Leapfrog scheme leads to

$$\begin{aligned} \frac{u_n^{t+\Delta t} - u_n^{t-\Delta t}}{2\Delta t} = & \frac{ge^z}{p_0} \frac{d}{dz} \left[ \frac{\mu \partial u_n^{t+\Delta t}}{H \partial z} \right] + f v_n^{t+\Delta t} + \lambda_{xx}(v_{ExB,x}^t - u_n^{t+\Delta t}) + \\ & \lambda_{xy}(v_{ExB,y}^t - v_n^{t+\Delta t}) - \mathbf{v}_n^t \cdot \nabla u_n^t + \\ & \frac{u_n^{t+\Delta t} v_n^t}{R_E} \tan \lambda - \frac{1}{R_E \cos \lambda} \frac{d\Phi^{t+\Delta t}}{d\phi} - W^{t+\Delta t} \frac{du_n^{t+\Delta t}}{dZ} \end{aligned} \quad (3.17)$$

and

$$\begin{aligned} \frac{v_n^{t+\Delta t} - v_n^{t-\Delta t}}{2\Delta t} = & \frac{ge^z}{p_0} \frac{d}{dZ} \left[ \frac{\mu dv_n^{t+\Delta t}}{HdZ} \right] - fu_n^{t+\Delta t} + \lambda_{yy}(v_{ExB,y}^t - v_n^{t+\Delta t}) + \\ & \lambda_{yx}(v_{ExB,x}^t - u_n^{t+\Delta t}) - \mathbf{v}_n^t \cdot \nabla v_n^t - \\ & \frac{u_n^{t+\Delta t} u_n^t}{R_E} \tan \lambda - \frac{1}{R_E} \frac{d\Phi^{t+\Delta t*}}{d\lambda} - W^{t+\Delta t} \frac{dv_n^{t+\Delta t}}{dZ} \end{aligned} \quad (3.18)$$

The terms of the discretized equation are added to the matrices **Q** at the height level  $k$ , **P** at  $k-1$ , and **R** at  $k+1$ . The first line in the matrices is the zonal equation and the second line the meridional one. In the following text we will describe the contribution to the matrices for each term. The right hand side goes into **rhs**. Note that in the code the two equations are divided by  $e^z$

The time derivatives  $\frac{u_n^{t+\Delta t} - u_n^{t-\Delta t}}{2\Delta t}$  i.e.  $\frac{v_n^{t+\Delta t} - v_n^{t-\Delta t}}{2\Delta t}$  lead to

$$\mathbf{Q}^1 = e^{-z} \begin{pmatrix} \frac{1}{2\Delta t} & 0 \\ 0 & \frac{1}{2\Delta t} \end{pmatrix} \quad (3.19)$$

in units of  $1/s$ , and the right hand side

$$\mathbf{RHS}^1 = e^{-z} \begin{pmatrix} \frac{u_n^{t-\Delta t, smooth}}{2\Delta t} + hd_u \\ \frac{v_n^{t-\Delta t, smooth}}{2\Delta t} + hd_v \end{pmatrix} \quad (3.20)$$

in units of  $cm/s^2$  with  $hd_u$  and  $hd_v$  the horizontal diffusion terms calculated in **subroutine hdiff3**. The velocities  $u_n^{t-\Delta t}$  and  $v_n^{t-\Delta t}$  at the previous timestep  $t - \Delta t$  are smoothed with the Shapiro method. First in meridional direction and then a zonal smoothing is applied.

$$\begin{aligned} f_{merid}^{smooth} = & f(\phi, \lambda) - c_{shapiro} \{ f(\phi, \lambda + 2\Delta\lambda) + f(\phi, \lambda - 2\Delta\lambda) - \\ & 4[f(\phi, \lambda + \Delta\lambda) + f(\phi, \lambda - \Delta\lambda)] + 6f(\phi, \lambda) \} \end{aligned} \quad (3.21)$$

$$\begin{aligned} f_{zonal}^{smooth} = & f_{merid}^{smooth} - c_{shapiro} \{ f_{merid}^{smooth}(\phi + 2\Delta\phi, \lambda) + f_{merid}^{smooth}(\phi - 2\Delta\phi, \lambda) - \\ & 4[f_{merid}^{smooth}(\phi + \Delta\phi, \lambda) + f_{merid}^{smooth}(\phi - \Delta\phi, \lambda)] + 6f_{merid}^{smooth}(\phi, \lambda) \} \end{aligned} \quad (3.22)$$

The Shapiro constant is set to  $c_{shapiro} = 0.03$ . The smoothing is done in the **subroutine smooth**.

The vertical viscosity term includes the eddy  $\mu_{ed}$  and molecular  $\mu_{mol}$  viscosity.

$$\frac{ge^z}{p_0} \frac{d}{dz} \left[ \frac{\mu du_n^{t+\Delta t}}{HdZ} \right] = e^z \frac{g^2(\mu_{ed} + \mu_{mol})\bar{m}}{p_0 k_B T_n^{int} \Delta z^2} \quad (3.23)$$

with  $\frac{1}{H} = \frac{g\bar{m}}{k_B T_n}$ . The term is calculated at the interface level. We substitute in the following in  $[1/s]$

$$\frac{f_{vis}}{\Delta z^2} = \frac{g^2 \mu \bar{m}}{p_0 k_B T_n^{int} \Delta z^2} \quad (3.24)$$

The second derivative is discretized by

$$\begin{aligned} \frac{\partial}{\partial z} \left( f_{vis} \frac{\partial u_n^{t+\Delta t}}{\partial z} \right) (z + \frac{1}{2} \Delta z) &= \frac{\left[ f_{vis}^{int} \frac{\partial u_n^{t+\Delta t}}{\partial z} \right] (z + \Delta z) - \left[ f_{vis}^{int} \frac{\partial u_n^{t+\Delta t}}{\partial z} \right] (z)}{\Delta z} = \\ &= \frac{1}{\Delta z} (f_{vis}(z + \Delta z) \frac{u_n(z + \frac{3}{2} \Delta z) - u_n(z + \frac{1}{2} \Delta z)}{\Delta z} \\ &\quad - f_{vis}(z) \frac{u_n(z + \frac{1}{2} \Delta z) - u_n(z - \frac{1}{2} \Delta z)}{\Delta z}) = \\ &= \frac{1}{\Delta z^2} (f_{vis}(z) u_n(z + \frac{3}{2} \Delta z) \\ &\quad - (f_{vis}(z + \Delta z) + f_{vis}(z)) u_n(z + \frac{1}{2} \Delta z) + f_{vis}(z) u_n(z - \frac{1}{2} \Delta z)) \end{aligned} \quad (3.25)$$

Note that  $f_{vis}$  is at the interface level with  $z$  denoting the index  $k$ , and the neutral velocity on the midpoints with  $z + \frac{1}{2} \Delta z$  being the  $k$  level. The same applies to the derivative of the meridional velocity. The terms from the above equation are added to the matrices  $\mathbf{Q}$  for the height level  $k$ ,  $\mathbf{R}$  for the values at the level  $k + 1$ , and  $\mathbf{P}$  for the  $k - 1$  height level

$$\mathbf{Q}^2 = \mathbf{Q}^1 + \begin{pmatrix} \frac{1}{\Delta z^2} (f_{vis}(z + \Delta z) + f_{vis}(z)) & 0 \\ 0 & \frac{1}{\Delta z^2} (f_{vis}(z + \Delta z) + f_{vis}(z)) \end{pmatrix} \quad (3.26)$$

$$\mathbf{P}^2 = \begin{pmatrix} -\frac{1}{\Delta z^2} f_{vis}(z) & 0 \\ 0 & -\frac{1}{\Delta z^2} f_{vis}(z) \end{pmatrix} \quad (3.27)$$

$$\mathbf{R}^2 = \begin{pmatrix} -\frac{1}{\Delta z^2} f_{vis}(z + \Delta z) & 0 \\ 0 & -\frac{1}{\Delta z^2} f_{vis}(z + \Delta z) \end{pmatrix} \quad (3.28)$$

The third terms in the momentum equations  $f^{cor} v_n^{t+\Delta t}$  and  $-f^{cor} u_n^{t+\Delta t}$  are the Coriolis forcing with the Coriolis parameter  $f^{cor} = 2\Omega \sin \lambda$ . The terms are added to the matrix  $\mathbf{G}$  in units of  $[1/s]$

$$\mathbf{Q}^3 = \mathbf{Q}^2 + e^{-z} \begin{pmatrix} 0 & -f^{cor} \\ f^{cor} & 0 \end{pmatrix} \quad (3.29)$$

The fourth and fifth term in the momentum equation  $\lambda_{xx}(v_{ExB,x} - u_n^{t+\Delta t}) + \lambda_{xy}(v_{ExB,y} - v_n^{t+\Delta t})$  and  $\lambda_{yy}(v_{ExB,x} - u_n^{t+\Delta t}) + \lambda_{yx}(v_{ExB,y} - v_n^{t+\Delta t})$  are the ion drag terms. The terms with the electrodynamic drift velocity are added to the right hand side.

$$\mathbf{RHS}^2 = \mathbf{RHS}^1 + e^{-z} \begin{pmatrix} \lambda_{xx}^{t,mid} v_{ExB,x}^{t,mid} + \lambda_{xy}^{t,mid} v_{ExB,y}^{t,mid} \\ \lambda_{yy}^{t,mid} v_{ExB,x}^{t,mid} - \lambda_{yx}^{t,mid} v_{ExB,y}^{t,mid} \end{pmatrix} \quad (3.30)$$

The values  $\lambda_{**}^{t,mid}$  and  $v_{ExB,*}^{t,mid}$  are the ion drag coefficient and the electrodynamic drift velocity at the time step  $t$  and at the midpoints. Therefore in the code the values from the interface height level  $k$  and  $k+1$  are averaged to get the midpoints values. Both the ion drag coefficients and the electrodynamic drift velocity are on the interface levels.

The terms with the neutral velocity are added to the left hand side in units of  $[1/s]$ .

$$\mathbf{Q}^3 = \mathbf{Q}^2 + e^{-z} \begin{pmatrix} \lambda_{xx}^{t,mid} & \lambda_{xy}^{t,mid} \\ -\lambda_{yx}^{t,mid} & \lambda_{yy}^{t,mid} \end{pmatrix} \quad (3.31)$$

The horizontal advection terms in zonal direction  $-\mathbf{v}_n^t \cdot \nabla u_n^t$  and meridional direction  $-\mathbf{v}_n^t \cdot \nabla v_n^t$  are added to the right hand side in units of  $[cm/s^2]$ .

$$\mathbf{RHS}^3 = \mathbf{RHS}^2 + e^{-z} \begin{pmatrix} -\mathbf{v}_n^t \cdot \nabla u_n^t \\ -\mathbf{v}_n^t \cdot \nabla v_n^t \end{pmatrix} = \mathbf{RHS}^2 + e^{-z} \begin{pmatrix} -u_n^t \frac{\partial u_n^t}{\partial \phi} - v_n^t \frac{\partial u_n^t}{\partial \lambda} \\ -u_n^t \frac{\partial v_n^t}{\partial \phi} - v_n^t \frac{\partial v_n^t}{\partial \lambda} \end{pmatrix} \quad (3.32)$$

The advection term is calculated in the **subroutine** `advect` by taking the fourth order stencil for the derivative. The average velocity is denoted by  $u_n^{avg} = \frac{1}{2}(u_n(\phi + \Delta\phi, \lambda) + u_n(\phi - \Delta\phi, \lambda))$  and  $u_n^{2avg} = \frac{1}{2}(u_n(\phi + 2\Delta\phi, \lambda) +$



$u_n(\phi - 2\Delta\phi, \lambda)$ ). The same is done for the meridional velocity  $v_n$  which leads to  $v_n^{avg} = \frac{1}{2}(v_n(\phi, \lambda + \Delta\lambda) + v_n(\phi, \lambda - \Delta\lambda))$  and  $v_n^{2avg} = \frac{1}{2}(v_n(\phi, \lambda + 2\Delta\lambda) + v_n(\phi, \lambda - 2\Delta\lambda))$ . The discrete advection of the zonal velocity for the point  $(\phi, \lambda)$  is

$$u_n \frac{\partial u_n}{\partial \phi}(\phi, \lambda) = \frac{1}{R_E \cos \lambda} \left( \frac{2}{3\Delta\phi} u_n^{avg}(\phi, \lambda) [u_n(\phi + \Delta\phi, \lambda) - u_n(\phi - \Delta\phi, \lambda)] - \frac{1}{12\Delta\phi} u_n^{2avg}(\phi, \lambda) [u_n(\phi + 2\Delta\phi, \lambda) - u_n(\phi - 2\Delta\phi, \lambda)] \right) \quad (3.33)$$

and

$$v_n \frac{\partial u_n}{\partial \lambda}(\phi, \lambda) = \frac{1}{R_E} \left( \frac{2}{3\Delta\lambda} v_n^{avg}(\phi, \lambda) [u_n(\phi, \lambda + \Delta\lambda) - u_n(\phi, \lambda - \Delta\lambda)] - \frac{1}{12\Delta\lambda} v_n^{2avg}(\phi, \lambda) [u_n(\phi, \lambda + 2\Delta\lambda) - u_n(\phi, \lambda - 2\Delta\lambda)] \right) \quad (3.34)$$

$$u_n \frac{\partial v_n}{\partial \phi}(\phi, \lambda) = \frac{1}{R_E \cos \lambda} \left( \frac{2}{3\Delta\phi} u_n^{avg}(\phi, \lambda) [v_n(\phi + \Delta\phi, \lambda) - v_n(\phi - \Delta\phi, \lambda)] - \frac{1}{12\Delta\phi} u_n^{2avg}(\phi, \lambda) [v_n(\phi + 2\Delta\phi, \lambda) - v_n(\phi - 2\Delta\phi, \lambda)] \right) \quad (3.35)$$

and

$$v_n \frac{\partial v_n}{\partial \lambda}(\phi, \lambda) = \frac{1}{R_E} \left( \frac{2}{3\Delta\lambda} v_n^{avg}(\phi, \lambda) [v_n(\phi, \lambda + \Delta\lambda) - v_n(\phi, \lambda - \Delta\lambda)] - \frac{1}{12\Delta\lambda} v_n^{2avg}(\phi, \lambda) [v_n(\phi, \lambda + 2\Delta\lambda) - v_n(\phi, \lambda - 2\Delta\lambda)] \right) \quad (3.36)$$

The advection term is calculated at midpoints and is in units of  $[cm/s^2]$ .

The 8. term is due to the horizontal momentum in the zonal direction  $\frac{u_n^{t+\Delta t} v_n^t}{R_E} \tan \lambda$  and the meridional one  $\frac{u_n^{t+\Delta t} u_n^t}{R_E} \tan \lambda$ . These terms are added to the left hand side  $\mathbf{G}$  matrix in  $[1/s]$ .

$$\mathbf{Q}^4 = \mathbf{Q}^3 + e^{-z} \begin{pmatrix} 0 & -\frac{v_n^t}{R_E} \tan \lambda \\ \frac{u_n^t}{R_E} \tan \lambda & 0 \end{pmatrix} \quad (3.37)$$

in the code it's  $+\frac{u_n^t}{R_E} \tan \lambda$  due to northward/meridional direction.

The pressure gradient term in the zonal and meridional directions is  $-\frac{1}{R_E \cos \lambda} \frac{d\Phi^{t+\Delta t*}}{d\phi}$

and  $-\frac{1}{R_E} \frac{d\Phi^{t+\Delta t*}}{d\lambda}$  (9. term) which is added to the right hand side matrix **RHS** in units of  $[cm/s^2]$

$$\mathbf{RHS}^3 = \mathbf{RHS}^2 + e^{-z} \left( \begin{array}{c} -\frac{1}{R_E \cos \lambda} \frac{d\Phi^{t+\Delta t*}}{d\phi} \\ -\frac{1}{R_E} \frac{d\Phi^{t+\Delta t}}{d\lambda} \end{array} \right) \quad (3.38)$$

The geopotential is calculated in **subroutine glp**. The input to **subroutine glp** is summarized in table 3.8. The output of **subroutine glp** is summarized in table 3.7. The parameters are summarized in table 3.10. Firstly, an average temperature  $\bar{T}_n$  is calculated by using

$$\bar{T}_n = T_n^t + wgt * [-2T_n^t + T_n^{t-\Delta t} + T_n^{t+\Delta t}] \quad (3.39)$$

The mean molecular weight is determined at the midpoints by

$$\bar{m}(k + \frac{1}{2}) = 0.5 * (\bar{m}(k)\bar{m}(k+1)) = \bar{m}^{mid}(k) \quad (3.40)$$

The geopotential is defined by the hydrostatic equation

$$\frac{\partial \Phi}{\partial z} = \frac{R^* \bar{T}_n}{\bar{m}} \quad (3.41)$$

which is integrated from the bottom of the model to the top.

$$z^*(k) = z^{t+\Delta t*}(k) = \int_{k_{bot}}^{k(z)} \frac{R^* \bar{T}_n}{g \bar{m}^{mid}} \Delta Z \quad (3.42)$$

in units of  $[cm]$  with  $\Phi = Zg$ , the gas constant  $R^*$  in  $[erg/K/mol]$ , and the mean mass  $\bar{m}$  in  $[g/mole]$ . The geopotential height uses already an mix of neutral temperature, which includes  $T_n^{t+\Delta t}$  and there it's neither  $z^t$  not  $z^{t+\Delta t}$ . ??? check units???. Note that  $z^* = z^{t+\Delta t*}$  is at the interfaces, since the value which is integrated is on the midlevels.

The derivatives are determined in **subroutine dldp** by taking the fourth order derivative. In the zonal direction the previous calculated geopotential height  $z^{t+\Delta t*}$  is used while in the latitudinal direction the updated geopoten-

tial height  $z^{t+\Delta t}$  is applied.

$$\begin{aligned} \frac{dz^*}{d\phi}(\phi, \lambda, z) = & \frac{2}{3\Delta\phi} [z^*(\phi + \Delta\phi, \lambda, z) - z^*(\phi - \Delta\phi, \lambda, z)] - \\ & \frac{1}{12\Delta\phi} [z^*(\phi + 2\Delta\phi, \lambda, z) - z^*(\phi - 2\Delta\phi, \lambda, z)] \end{aligned} \quad (3.43)$$

$$\begin{aligned} \frac{dz^*}{d\lambda}(\phi, \lambda, z) = & \frac{2}{3\Delta\lambda} [z^*(\phi, \lambda + \Delta\lambda, z) - z^*(\phi, \lambda - \Delta\lambda, z)] - \\ & \frac{1}{12\Delta\lambda} [z^*(\phi, \lambda + 2\Delta\lambda, z) - z^*(\phi, \lambda - 2\Delta\lambda, z)] \end{aligned} \quad (3.44)$$

in units of  $[cm]$ . The derivatives are transferred from the interface levels to the midpoint level by

$$\frac{1}{R_E \cos \lambda} \frac{d\Phi}{d\phi}(\phi, \lambda, z) = \frac{1}{2} g \frac{1}{R_E \cos \lambda} \left[ \frac{dz^*}{d\phi}(\phi, \lambda, z) + \frac{dz^*}{d\phi}(\phi, \lambda, z + \Delta z) \right] \quad (3.45)$$

$$\frac{1}{R_E} \frac{d\Phi}{d\lambda}(\phi, \lambda, z) = \frac{1}{2} g \frac{1}{R_E} \left[ \frac{dz^*}{d\lambda}(\phi, \lambda, z) + \frac{dz^*}{d\lambda}(\phi, \lambda, z + \Delta z) \right] \quad (3.46)$$

which is in  $[cm/s^2]$ . The periodic points are set to zero.

The final term is the vertical advection term  $-W^{t+\Delta t} \frac{du_n^{t+\Delta t}}{dz}$  and  $-W^{t+\Delta t} \frac{dv_n^{t+\Delta t}}{dz}$ . The terms are added to the left hand side matrix  $\mathbf{P}$  and  $\mathbf{R}$  in  $[1/s]$

$$\mathbf{P}^3 = \mathbf{P}^2 + e^{-z} \begin{pmatrix} -\frac{W^{mid,t+\Delta t}}{2\Delta z} & 0 \\ 0 & -\frac{W^{mid,t+\Delta t}}{2\Delta z} \end{pmatrix} \quad (3.47)$$

$$\mathbf{R}^3 = \mathbf{R}^2 + e^{-z} \begin{pmatrix} \frac{W^{mid,t+\Delta t}}{2\Delta z} & 0 \\ 0 & i \frac{W^{mid,t+\Delta t}}{2\Delta z} \end{pmatrix} \quad (3.48)$$

The lower boundary is taken into account by extrapolating the values of the matrix  $\mathbf{P}$

$$\mathbf{P}(z_{bot} - \frac{1}{2}\Delta z) \mathbf{v}(z_{bot} - \frac{1}{2}\Delta z) = 2\mathbf{P}(z_{bot}) \mathbf{v}_{LB} - \mathbf{P}(z_{bot} + \frac{1}{2}\Delta z) \mathbf{v}(z_{bot} + \frac{1}{2}\Delta z) \quad (3.49)$$

with  $z_{bot} + \frac{1}{2}\Delta z$  on the midpoint level having the height index 1. The value  $\mathbf{P}(z_{bot})$  is set to  $\mathbf{P}(z_{bot} + \frac{1}{2}\Delta z)$ , and the neutral velocity at the lower boundary

is  $\mathbf{v}(z_{bot}) = \mathbf{v}_{LB}$ . Therefore, substituting the lower boundary condition into the equation leads to

$$\mathbf{Q}(z_{bot} + \frac{1}{2}\Delta z)^* = \mathbf{Q}(z_{bot} + \frac{1}{2}\Delta z) - \mathbf{P}(z_{bot} + \frac{1}{2}\Delta z) \quad (3.50)$$

$$\mathbf{RHS}(z_{bot} + \frac{1}{2}\Delta z)^* = \mathbf{RHS}(z_{bot} + \frac{1}{2}\Delta z) - 2\mathbf{P}(z_{bot} + \frac{1}{2}\Delta z)\mathbf{v}_{LB} \quad (3.51)$$

$$\mathbf{P}(z_{bot} + \frac{1}{2}\Delta z) = 0 \quad (3.52)$$

At the upper boundary it's assumed that

$$\mathbf{R}(z_{top} - \frac{1}{2}\Delta z)\mathbf{v}(z_{top} + \frac{1}{2}\Delta z) = \mathbf{R}(z_{top} - \frac{1}{2}\Delta z)\mathbf{v}(z_{top} - \frac{1}{2}\Delta z) \quad (3.53)$$

with  $z_{top} - \frac{1}{2}\Delta z$  on the midpoint level corresponds to the height index  $nlev$ . This which leads to

$$\mathbf{Q}(z_{top} - \frac{1}{2}\Delta z)^* = \mathbf{Q}(z_{top} - \frac{1}{2}\Delta z) - \mathbf{R}(z_{top} - \frac{1}{2}\Delta z) \quad (3.54)$$

$$\mathbf{R}(z_{top} - \frac{1}{2}\Delta z)^* = 0 \quad (3.55)$$

A tridiagonal solver is called in subroutine `trsolv`. It solve the generic equation

$$p(k, i) * v(k - 1, i) + q(k, i) * v(k, i) + r(k, i) * t(k + 1, i) = rhs(k, i) \quad (3.56)$$

with  $p(k, i)$  being the  $(i, j)$  element of the matrix  $\mathbf{P}$ ,  $q(k, i)$  of the matrix  $\mathbf{Q}$ ,  $r(k, i)$  of the matrix  $\mathbf{R}$ ,  $rhs(k, i)$  of the matrix  $\mathbf{RHS}$ , and  $v(k, i)$  of the neutral velocity vector  $\mathbf{v}_n$ . The lower boundary at  $z_{bot} = z_{LB}$  of the neutral velocity is stored at the top level  $nlev + 1$  since this height is above the upper boundary anyway. The upper boundary pressure level is  $-7$  which corresponds to  $z_{top}$ . The neutral velocity is only calculated from  $z_{bot} + \frac{1}{2}\Delta z$  to  $z_{top} - \frac{1}{2}\Delta z$ . Note that the lower boundary is at  $p - lev = -7$ , and all the other values of the neutral velocity are on the midpoints which means at  $p - lev = -6.75, -6.25, -5.75, \dots, 5.75, 6.25, 6.75$ .

The calculated values for the neutral velocity  $\mathbf{u}_n^{upd, t+\Delta t}$  and  $\mathbf{v}_n^{upd, t+\Delta t}$  are smoothed by a Fast Fourier transformation. All the wave numbers larger than a predefined value at each latitude are removed. The wave numbers

are defined in the module `cons.F`. The values of the neutral velocity at the timestep  $t$  are also updated by using

$$u_n^{upd,t} = \frac{1}{2}(1 - c_{smo})(u_n^{t-\Delta t} + u_{n,smo}^{upd,t+\Delta t}) + c_{smo}u_n^t \quad (3.57)$$

$$v_n^{upd,t} = \frac{1}{2}(1 - c_{smo})(v_n^{t-\Delta t} + v_{n,smo}^{upd,t+\Delta t}) + c_{smo}v_n^t \quad (3.58)$$

with  $c_{smo} = 0.95$

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t$
neutral temperature	$T_n^{t-\Delta t}$	$K$	midpoints	$t - \Delta t$
neutral temperature	$T_n^{t+\Delta t}$	$K$	midpoints	$t + \Delta t$
neutral zonal velocity	$u_n$	$cm/s$	midpoints	$t$
neutral meridional velocity	$v_n$	$cm/s$	midpoints	$t$
neutral zonal velocity	$u_n^{t-\Delta t}$	$cm/s$	midpoints	$t - \Delta t$
neutral meridional velocity	$v_n^{t-\Delta t}$	$cm/s$	midpoints	$t - \Delta t$
dimensionless vertical velocity	$W^{t-\Delta t}$	$1/s$	interfaces	$t + \Delta t$
geopotential height	$z$	$cm$	interfaces	$t + \Delta t$
zonal horizontal diffusion	$h_{d,u}$	$cm/s^2$	midpoints	$t - \Delta t$
meridional horizontal diffusion	$h_{d,v}$	$cm/s^2$	midpoints	$t - \Delta t$
zonal electrodynamic drift velocity	$v_{ExB,x}$	$cm/s$	interfaces	$t$
meridional electrodynamic drift velocity	$v_{ExB,y}$	$cm/s$	interfaces	$t$
ion drag coefficients (geographic direction)	$\lambda_{xx}, \lambda_{xy}, \lambda_{yy}, \lambda_{yx}$	$1/s$	interfaces	$t + \Delta t$
molecular viscosity	$k_m$	$\frac{g}{cms}$	interfaces	$t$
mean molecular weight	$\overline{m}$	$g/mol$	interfaces	$t + \Delta t$

Table 3.6: Input fields to subroutine `duv`

physical field	variable	unit	pressure level	timestep
neutral zonal velocity	$u_n^{upd,t+\Delta t}$	$cm/s$	midpoints	$t + \Delta t$
neutral meridional velocity	$v_n^{upd,t+\Delta t}$	$cm/s$	midpoints	$t + \Delta t$
neutral zonal velocity	$u_n^{upd,t}$	$cm/s$	midpoints	$t$
neutral meridional velocity	$v_n^{upd,t}$	$cm/s$	midpoints	$t$

Table 3.7: Output fields of subroutine `duv`

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t$
neutral temperature	$T_n^{t-\Delta t}$	$K$	midpoints	$t - \Delta t$
neutral temperature	$T_n^{t+\Delta t}$	$K$	midpoints	$t + \Delta t$
geopotential height	$z$	$cm$	interfaces	$t + \Delta t$
mean molecular weight	$\overline{m}$	$g/mol$	interfaces	$t + \Delta t$

Table 3.8: Input fields to subroutine `glp`

physical field	variable	unit	pressure level	timestep
zonal derivative of geopotential	$\frac{1}{R_E \cos \lambda} \frac{\partial \Phi^{t+\Delta t*}}{\partial \phi}$	$cm/s^2$	midpoints	$t + \Delta t^*$
meridional derivative of geopotential	$\frac{1}{R_E} \frac{\partial \Phi^{t+\Delta t}}{\partial \lambda}$	$cm/s^2$	midpoints	$t + \Delta t$

Table 3.9: Output fields of subroutine `glp` i.e. subroutine `dldp`

variable	value
$\Delta z$	0.5
$wgt$	0.225
$\frac{g}{R}$	$\frac{870cm/s^2}{8.314e^7 erg/K/mol}$

Table 3.10: Parameters of subroutine `glp` i.e. subroutine `dldp`

## Chapter 4

# Neutral Thermodynamics



physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
mass mixing ratio $O_2$	$\Psi_{O_2}$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi_O$	—	midpoints	$t_n$

Table 4.1: Input fields to subroutine `cpktkm`

physical field	variable	unit	pressure level	timestep
specific heat	$C_p$	$ergs/(Kcm^3)$	interfaces	$t_n +$
molecular viscosity	$\mu$	$gms/(cms)$	interfaces	$t_n +$
thermal conductivity	$K_T$	$ergs/(cmKs)$	interfaces	$t_n$

Table 4.2: Output fields of subroutine `cpktkm`

## 4.1 Calculation of $K_T$ , $\mu$ , $C_p$ /

The input to subroutine `cpktkm` is summarized in table 4.1. The output of subroutine `cpktkm` is summarized in table 4.2. The mean mass at the midpoint level is determined by

$$\bar{m} = \frac{1}{\frac{\Psi_{O_2}}{m_{O_2}} + \frac{\Psi_O}{m_O} + \frac{\Psi_{N_2}}{m_{N_2}}} \quad (4.1)$$

with  $\Psi_{N_2} = 1 - \Psi_O - \Psi_{O_2}$ . The following values are calculated

$$P(O_2) = \bar{m} \frac{\Psi_{O_2}}{m_{O_2}} \quad (4.2)$$

$$P(O) = \bar{m} \frac{\Psi_O}{m_O} \quad (4.3)$$

$$P(N_2) = \bar{m} \frac{\Psi_{N_2}}{m_{N_2}} \quad (4.4)$$

The molecular viscosity is

$$\mu = [4.03 \cdot P(O_2) + 3.42 \cdot P(N_2) + 3.9 \cdot P(O)] T_n^{0.69} \cdot 10^{-6} \quad (4.5)$$

The thermal conductivity is

$$K_T = [56 \cdot (P(O_2) + P(N_2)) + 75.9 \cdot P(O)] T_n^{0.69} \quad (4.6)$$

Note that the value  $T_0$  is set to zero in the code. (This is a holdover from the original TGCM, which only calculated a temperature difference.  $T_0$  was then added to this calculation to get the actual temperature for purposes like this.) The specific heat is

$$C_p = \frac{1}{2} R^* \left[ \frac{7}{32} P(O_2) + \frac{7}{28} P(N_2) + \frac{5}{16} P(O) \right] \quad (4.7)$$

with  $R^*$  the gas constant. At the upper boundary the values are set to

$$\begin{aligned} K_T(z_{top} + \frac{1}{2}\Delta z) &= [56 \cdot (P(O_2) + P(N_2)) + 75.9 \cdot P(O)] \\ &\quad T_n^{0.69}(z_{top} - \frac{1}{2}\Delta z) \end{aligned} \quad (4.8)$$

$$\begin{aligned} \mu(z_{top} + \frac{1}{2}\Delta z) &= [4.03 \cdot P(O_2) + 3.42 \cdot P(N_2) + 3.9 \cdot P(O)] \\ &\quad T_n^{0.69}(z_{top} - \frac{1}{2}\Delta z) \cdot 10^{-6} \end{aligned} \quad (4.9)$$

and all the other values at  $z_{top} + \frac{1}{2}\Delta z$ , and only  $T_n$  at a level below  $z_{top} - \frac{1}{2}\Delta z$ . The values are then transferred to the interface level by averaging

$$K_T(z) = \frac{1}{2} (K_T(z + \frac{1}{2}\Delta z) + K_T(z - \frac{1}{2}\Delta z)) \quad (4.10)$$

$$\mu(z) = \frac{1}{2} (\mu(z + \frac{1}{2}\Delta z) + \mu(z - \frac{1}{2}\Delta z)) \quad (4.11)$$

$$C_p(z) = \frac{1}{2} (C_p(z + \frac{1}{2}\Delta z) + C_p(z - \frac{1}{2}\Delta z)) \quad (4.12)$$

with  $z$  having the height index  $k$  on the interface level,  $z + \frac{1}{2}\Delta z$  has the index  $k$ , and  $z - \frac{1}{2}\Delta z$  has the index  $k - 1$  on the midpoint level. The lower boundary is extrapolated by

$$C_p(z_{bot}) = 2C_p(z_{bot} + \frac{1}{2}\Delta z) - C_p(z_{bot} + \Delta z) \quad (4.13)$$

$$K_T(z_{bot}) = 2K_T(z_{bot} + \frac{1}{2}\Delta z) - K_T(z_{bot} + \Delta z) \quad (4.14)$$

$$\mu(z_{bot}) = 2\mu(z_{bot} + \frac{1}{2}\Delta z) - \mu(z_{bot} + \Delta z) \quad (4.15)$$

$$(4.16)$$

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
neutral temperature	$T_n^{t-\Delta t}$	$K$	midpoints	$t_n - \Delta t$
neutral zonal velocity	$u_n$	$cm/s$	midpoints	$t_n$
neutral meridional velocity	$v_n$	$cm/s$	midpoints	$t_n$
mass mixing ratio $O_2$	$\Psi_{O_2}$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi_O$	—	midpoints	$t_n$
mean molecular mass	$\bar{m}$	$g/mol$	interfaces	$t_n + \Delta t$
specific heat	$C_p$	$\frac{erg}{Kg}$	interfaces	$t_n$
molecular diffusion	$k_t$	$\frac{erg}{cmKs}$	interfaces	$t_n$
molecular viscosity	$k_m$	$\frac{g}{cms}$	interfaces	$t_n$
horizontal diffusion	$h_{d,T}$	$\frac{cm}{s^2}$	midpoints	$t_n - \Delta t$
Joule heating	$Q_{J,T}$	$\frac{erg}{Ks}$	midpoints	$t_n$
implicit cooling	$L_{imp}$	$\frac{1}{s}$	midpoints	$t_n$
explicit cooling	$L_{exp}$	$\frac{erg}{Ks}$	midpoints	$t_n$
dimensionless vertical velocity	$W^{t+\Delta t}$	$1/s$	interfaces	$t + \Delta t$

Table 4.3: Input fields to subroutine `dt`

## 4.2 Thermodynamic equation /

The input to subroutine `dt` is summarized in table 4.3. The output of subroutine `dt` is summarized in table 4.4. The module data of subroutine `dt` is summarized in table 4.5. The thermodynamic equation is solved to get the neutral temperature

$$\begin{aligned}
\frac{\partial T_n}{\partial t} = & \frac{ge^z}{p_0 C_p} \frac{\partial}{\partial Z} \left\{ \frac{K_T}{H} \frac{\partial T_n}{\partial Z} + K_E H^2 C_p \rho \left[ \frac{g}{C_p} + \frac{1}{H} \frac{\partial T}{\partial Z} \right] \right\} - \mathbf{v}_n \cdot \nabla T_n - \\
& W \left( \frac{\partial T_n}{\partial Z} + \frac{R^* T_n}{C_p \bar{m}} \right) + \frac{Q^{exp} - e^z L^{exp}}{C_p} - L^{imp}
\end{aligned} \tag{4.17}$$

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n^{upd,t+\Delta t}$	$K$	midpoints	$t_n + \Delta t$
neutral temperature	$T_n^{upd,t}$	$K$	midpoints	$t_n$

Table 4.4: Output fields of subroutine `dt`

physical field	variable	unit	pressure level	timestep
heating from solar radiation	$Q_{qrj}$	$\frac{erg}{K s}$	interfaces	$t_n$

Table 4.5: Module data of subroutine `dt`

with  $T_n$  the neutral temperature,  $t$  the time,  $g$  the gravitational acceleration,  $C_p$  the specific heat per unit mass,  $p_0$  the reference pressure,  $K_T$  is the molecular thermal conductivity,  $H$  is the pressure scale height,  $K_E$  is the eddy diffusion coefficient,  $\rho$  is the atmospheric mass density,  $\mathbf{v}_n$  is the horizontal neutral velocity with the zonal and meridional components  $u_n$  and  $v_n$ ,  $W$  is the dimensionless vertical velocity given by  $W = \frac{dz}{dt}$ ,  $R^*$  is the universal gas constant,  $\overline{m}$  is the mean atmospheric mass, and  $Q$  and  $L$  are the heating and cooling terms.

The local time variation of the neutral temperature is determined by the heating and cooling terms on the right hand side of the thermodynamic equation. The first term is the heat transfer by vertical molecular heat conduction and adiabatic heating or cooling due to eddy diffusion. The second term is the heat transfer due to horizontal advection, and the third term is the adiabatic heating and cooling caused by the vertical winds. The last terms in equation (4.17) account for all the other heating and cooling terms.

To make it more easy to compare with the code we write the thermody-

namic equation with implicit and explicit terms

$$\begin{aligned} \frac{T_n^{t+\Delta t} - T_n^{t-\Delta t}}{2\Delta t} &= \frac{ge^z}{p_0 C_p} \frac{\partial}{\partial Z} \left\{ \left( \frac{K_T}{H} + \frac{K_E H^2 C_p \rho}{H} \right) \frac{\partial T_n^{t+\Delta t}}{\partial Z} \right\} + \\ &\frac{ge^z}{p_0 C_p} \frac{\partial}{\partial Z} \left\{ K_E H^2 C_p \frac{g}{C_p} \right\} - \mathbf{v}_n^t \cdot \nabla T_n^t - \\ &W^{t+\Delta t} \frac{\partial T_n}{\partial Z} - W^{t+\Delta t} \frac{R^* T_n^{t+\Delta t}}{C_p \bar{m}} + \frac{Q^{exp}}{C_p} - \frac{e^z L^{exp}}{C_p} - L^{imp} T_n^{t+\Delta t} \end{aligned} \quad (4.18)$$

The terms are ordered now by left and right hand side, and the whole equation is multiplied by  $\frac{C_p}{e^z}$ .

$$\begin{aligned} \frac{C_p}{e^z} \left\{ -\frac{T_n^{t-\Delta t, smo}}{2\Delta t} + \mathbf{v}_n^t \cdot \nabla T_n^t + W^{t+\Delta t} \frac{\partial T_n}{\partial Z} - \frac{Q^{exp} - e^z L^{exp}}{C_p} \right\} = \\ \frac{\partial}{\partial Z} \left\{ \frac{g}{H p_0} \left( \frac{K_T}{H} + K_E H^2 C_p \rho \right) \frac{\partial T_n^{t+\Delta t}}{\partial Z} \right\} + \\ \frac{\partial}{\partial Z} \left\{ \frac{g^2 K_E H^2 \rho}{p_0 T_n^t} T_n^{t+\Delta t} \right\} + \frac{C_p}{e^z} \left\{ -\frac{T_n^{t+\Delta t}}{2\Delta t} - w^{t+\Delta t} \frac{R^* T_n^{t+\Delta t}}{C_p \bar{m}} - L^{imp} T_n^{t+\Delta t} \right\} \end{aligned} \quad (4.19)$$

We first describe the known terms on the left hand side. The horizontal advection  $\mathbf{v}_n^t \cdot \nabla T_n^t$  is calculated similar to the horizontal advection in the momentum equation in chapter 3.3 equation (3.3) and following.

The advection term is calculated in the **subroutine** `advec` by taking the fourth order stencil for the derivative. The average velocity is denoted by  $u_n^{avg}(\phi, \lambda) = \frac{1}{2}(u_n(\phi + \Delta\phi, \lambda) + u_n(\phi - \Delta\phi, \lambda))$  and  $u_n^{2avg}(\phi, \lambda) = \frac{1}{2}(u_n(\phi + 2\Delta\phi, \lambda) + u_n(\phi - 2\Delta\phi, \lambda))$ . The same is done for the meridional velocity  $v_n$  which leads to  $v_n^{avg}(\phi, \lambda) = \frac{1}{2}(v_n(\phi, \lambda + \Delta\lambda) + v_n(\phi, \lambda - \Delta\lambda))$  and  $v_n^{2avg}(\phi, \lambda) = \frac{1}{2}(v_n(\phi, \lambda + 2\Delta\lambda) + v_n(\phi, \lambda - 2\Delta\lambda))$ . The horizontal advection of the neutral temperature is

$$\begin{aligned} \mathbf{v}_n^t \cdot \nabla T_n^t &= \frac{1}{R_E \cos \lambda} \left( \frac{2}{3\Delta\phi} u_n^{avg}(\phi, \lambda) [T_n^t(\phi + \Delta\phi, \lambda) - T_n^t(\phi - \Delta\phi, \lambda)] - \right. \\ &\frac{1}{12\Delta\phi} u_n^{2avg}(\phi, \lambda) [T_n^t(\phi + 2\Delta\phi, \lambda) - T_n^t(\phi - 2\Delta\phi, \lambda)] + \\ &\frac{1}{R_E} \left( \frac{2}{3\Delta\lambda} v_n^{avg}(\phi, \lambda) [T_n^t(\phi, \lambda + \Delta\lambda) - T_n^t(\phi, \lambda - \Delta\lambda)] - \right. \\ &\left. \frac{1}{12\Delta\lambda} v_n^{2avg}(\phi, \lambda) [T_n^t(\phi, \lambda + 2\Delta\lambda) - T_n^t(\phi, \lambda - 2\Delta\lambda)] \right) \end{aligned} \quad (4.20)$$

in unit of  $[\frac{K}{s}]$  the values are determined at midpoints.

The vertical advection term  $W^{t+\Delta t} \frac{\partial T_n}{\partial Z}$  is calculated by

$$\begin{aligned} & \frac{1}{2\Delta z} (W^{t+\Delta t}(z) \left[ T_n^t(z + \frac{1}{2}\Delta z) - T_n^t(z - \frac{1}{2}\Delta z) \right] + \\ & W^{t+\Delta t}(z + \Delta z) \left[ T_n^t(z + \frac{3}{2}\Delta z) - T_n^t(z + \frac{1}{2}\Delta z) \right]) = \\ & \frac{1}{2} \left[ W^{t+\Delta t}(z) \frac{\partial T_n^t(z)}{\partial Z} + W^{t+\Delta t}(z + \Delta z) \frac{\partial T_n^t(z + \Delta z)}{\partial Z} \right] = \\ & W^{avg,t+\Delta t}(z + \frac{1}{2}\Delta z) \frac{\partial T_n^{avg,t}(z + \frac{1}{2}\Delta z)}{\partial Z} \end{aligned} \quad (4.21)$$

It takes the average between the values at the level  $z$  and  $z + \Delta z$ . Note that  $T_n$  is on the midpoints levels  $z + \frac{1}{2}\Delta z$  etc. The vertical advection is determined at midpoints and has the units  $[\frac{K}{s}]$ .

The next term is from the time derivative of the neutral temperature  $-\frac{T_n^{t-\Delta t,smo} - T_n^t}{2\Delta t}$ . The smoothed value is calculated similar as in the momentum equation in chapter 3.3 in equation (3.22).

$$\begin{aligned} f_{merid}^{smooth} &= f(\phi, \lambda) - c_{shapiro}(f(\phi, \lambda + 2\Delta\lambda) + f(\phi, \lambda - 2\Delta\lambda) - \\ & 4[f(\phi, \lambda + \Delta\lambda) + f(\phi, \lambda - \Delta\lambda)] + 6f(\phi, \lambda)) \end{aligned} \quad (4.22)$$

$$\begin{aligned} f_{zonal}^{smooth} &= f_{merid}^{smooth} - c_{shapiro}(f_{merid}^{smooth}(\phi + 2\Delta\phi, \lambda) + f_{merid}^{smooth}(\phi - 2\Delta\phi, \lambda) - \\ & 4[f_{merid}^{smooth}(\phi + \Delta\phi, \lambda) + f_{merid}^{smooth}(\phi - \Delta\phi, \lambda)] + 6f_{merid}^{smooth}(\phi, \lambda)) \end{aligned} \quad (4.23)$$

with  $f = T_n^{t-\Delta t}$  which leads to  $T_n^{t-\Delta t,smo}$ .

The heating terms are added together. First the terms from the heating caused by solar radiation, which are calculated in **subroutine qrrj**.

$$Q_{solar} = Q_{EUV} + Q_{SchR} + Q_o \quad (4.24)$$

$$(4.25)$$

with  $Q_{Solar}(z + \frac{1}{2}\Delta z) = \frac{1}{2}[Q_{Solar}(z) + Q_{Solar}(z + \Delta z)]$  to calculate the value on the midpoint level  $z + \frac{1}{2}\Delta z$ . The solar radiation has contributions from the EUV and from the Schuman Runge bands and continuum, and the O????.

$$Q = Q_{Solar} + 1.5Q_{JH} + h_{d,T} + Q_{OR} + Q_{md} \quad (4.26)$$

$$(4.27)$$

with the Joule heating term denoted by  $Q_{JH}$  which is multiplied by 1.5 to take the heating due to the small scale electric field into account. The horizontal diffusion term is denoted by  $h_{dT}$ .

The heating due to atomic oxygen recombination is determined by

$$Q_{OR} = f_T r_{km} \frac{N_A}{\bar{m}} \left[ \frac{p_0 e^{-z\bar{m}} \Psi_o}{k_B T_n m_o} \right]^2 \quad (4.28)$$

with the Boltzman constant  $k_B = 1.38 \cdot 10^{-16} \frac{cm^2 g}{s^2 K}$ , and  $f_T = 5.11 eV = 5.11 \cdot 1.602 \cdot 10^{-12} ergs$ , which is the surplus heating and set in **subroutine cons**. The loss of O to  $O_2$  is captured by  $r_{km}$  and set in the source code file **chemrates.F** according to Dickinson et al. 1984.

The photoelectron heating is determined by

$$Q_{photo} = q_{ionize} 0.05 \times 35 N_A \frac{1.602 \cdot 10^{-12}}{\bar{m}} \quad (4.29)$$

where  $q_{ionize}$  is the ionization rate.

The heating resulting from ion chemistry is of the type

$$Q_i^{chem} = N_A 1.602 \cdot 10^{-12} n_{neutral} r_k n_i q_{heat} \quad (4.30)$$

where  $n_{neutral}$  is the number density of the neutral species,  $n_i$  is the number density of the ion species,  $r_k$  is the reaction rate, and  $q_{heat}$  is the heat emitted by the reaction.

The heating resulting from neutral chemistry of the minor species is

$$Q_i^{chem} = N_A 1.602 \cdot 10^{-12} n_{neutral} \beta n_{neutral} q_{heat} \quad (4.31)$$

where  $\beta$  is the reaction rate.

The heating from electron-neutral and electron-ion collisions are

$$Q_{en}^{chem} = L_{en} (T_e - T_n) \frac{N_A}{\bar{m}} \quad (4.32)$$

$$Q_{ei}^{chem} = L_{ei} (T_e - T_i) \frac{N_A}{\bar{m}} \quad (4.33)$$

The loss term due to NO cooling is

$$L_{NO} = 4.956 \cdot 10^{-12} N_A n_{NO} \frac{ANO}{ANO + 13.3} e^{\frac{-2700}{T_n}} \quad (4.34)$$

where  $ANO = \bar{m}N_A 5 \cdot 10^{-4} e^{-z} (6.5 \cdot 10^{-11} \frac{n_o}{m_o} + 2.4 \cdot 10^{-14} \frac{n_{o2}}{m_{o2}}) / (RT_n)$   
The loss due to  $CO_2$  cooling is

$$L_{CO2_{cool}} = 2.65 \cdot 10^{-13} n_{CO2} e^{\frac{-960}{T_n}} N_A \left( \left( \frac{n_{O2}}{m_{O2}} + \frac{n_{N2}}{m_{N2}} \right) ACO2 + \frac{n_O}{m_O} BCO2 \right) \quad (4.35)$$

where

$$\begin{aligned} ACO2 &= 2.5 \cdot 10^{-15} & T_n < 200K \\ &2.5 \cdot 10^{-15} (1 + 0.03(T_n - 200)) & T_n > 200K \\ BCO2 &= 1. \cdot 10^{-12} & T_n < 300K \\ &1. \cdot 10^{-12} \frac{T_n}{300} & T_n > 300K \end{aligned}$$

The loss due to  $O(^3P)$  cooling is

$$L_{O(^3P)_{cool}} = \frac{ANO3P(1) \times XO(k) \frac{N_A}{m_o} n_o e^{\frac{-BNO3P(1)}{T_n}}}{1 + ANO3P(2) e^{\frac{-BNO3P(2)}{T_n}} + ANO3P(3) e^{\frac{-BNO3P(3)}{T_n}}} \quad (4.36)$$

with  $XO$  is a pressure level dependent set of coefficients.  $XO = (3 \times 0.01, 0.05, 0.1, 0.2, 0.4, 0.55, 0.7, 0.75, 15 \times 0.0)$ .  $ANO3P$  is a 3 element array of constants  $ANO3P = (1.67 \cdot 10^{-18}, 0.6, 0.2)$ .  $BNO3P$  is a three element array of constants  $BNO3P = (228, 228, 325)$ .

The heating due to molecular diffusion is determined by

$$Q_{md} = \frac{g^2 \bar{m} K_m^{mid}}{p_0 R^* e^{-z} T_n^t} \left\{ \left( \frac{\partial u_n}{\partial Z} \right)^2 + \left( \frac{\partial v_n}{\partial Z} \right)^2 \right\} = \quad (4.37)$$

$$\frac{e^z g \bar{m} K_m^{mid}}{p_0 H} \left\{ \left( \frac{\partial u_n}{\partial Z} \right)^2 + \left( \frac{\partial v_n}{\partial Z} \right)^2 \right\} \quad (4.38)$$

with the gas constant  $R^* = 8.31410^7 \frac{ergs}{Kmol}$  and  $\frac{1}{H} = \frac{g \bar{m}}{R^* T_n}$ . The vertical change in the neutral velocity is calculated by

$$\frac{du_n}{dZ} \left( z + \frac{1}{2} \Delta z \right) = \frac{u_n \left( z + \frac{3}{2} \Delta z \right) - u_n \left( z - \frac{1}{2} \Delta z \right)}{2 \Delta z} \quad (4.39)$$

$$\frac{dv_n}{dZ} \left( z + \frac{1}{2} \Delta z \right) = \frac{v_n \left( z + \frac{3}{2} \Delta z \right) - v_n \left( z - \frac{1}{2} \Delta z \right)}{2 \Delta z} \quad (4.40)$$



At the lower boundary the derivative is determined by

$$\frac{du_n}{dZ}(z_{LB}) = \frac{1}{\Delta z} \left( u_n(z_{LB} + \frac{1}{2}\Delta z) + \frac{1}{3}u_n(z_{LB} + \frac{3}{2}\Delta z) - \frac{4}{3}u_n(z_{LB}) \right) \quad (4.41)$$

$$\frac{dv_n}{dZ}(z_{LB}) = \frac{1}{\Delta z} \left( v_n(z_{LB} + \frac{1}{2}\Delta z) + \frac{1}{3}v_n(z_{LB} + \frac{3}{2}\Delta z) - \frac{4}{3}v_n(z_{LB}) \right) \quad (4.42)$$

At the top the derivatives are set to

$$\frac{du_n}{dZ}(z_{top} - \Delta z) = \frac{1}{3} \frac{du_n}{dZ}(z_{top} - 2\Delta z) \quad (4.43)$$

$$\frac{dv_n}{dZ}(z_{top} - \Delta z) = \frac{1}{3} \frac{dv_n}{dZ}(z_{top} - 2\Delta z) \quad (4.44)$$

All the terms of the right hand side are added together which leads to

$$RHS = \frac{C_p}{e^z} \left[ \mathbf{v}_n^t \cdot \nabla T_n^t + W^{t+\Delta t} \frac{\partial T}{\partial Z} - \frac{1}{2\Delta t} T_n^{t-\Delta t, smo} \right] - e^{-z} Q^{exp} + L^{exp} \quad (4.45)$$

Next we discuss the terms on the left hand side starting with the second derivative terms  $\frac{\partial}{\partial Z} \left\{ \frac{g}{H p_0} \left( \frac{K_T}{H} + K_E H^2 C_p \rho \right) \frac{\partial T_n^{t+\Delta t}}{\partial Z} \right\}$ . In the source code and in this description we substitute for simplicity  $g_c = \frac{g}{H p_0} \left( \frac{K_T}{H} + K_E H^2 C_p \rho \right)$ . First the mass density  $\rho$  and the scale height  $H$  are calculated. The neutral temperature at the interface level is

$$T_n^t(z) = \frac{1}{2} \left[ T_n^t(z - \frac{1}{2}\Delta z) + T_n^t(z + \frac{1}{2}\Delta z) \right] \quad (4.46)$$

and the scale height  $H$  is

$$H(z) = \frac{R^* T_n^t(z)}{\overline{m}(z)g} \quad (4.47)$$

and the mass density  $\rho$

$$\rho(z) = \frac{p_0 e^{-z} \overline{m}(z)}{e^{-0.5\Delta z} R^* T_n^t(z)} = \frac{p}{H(z)g} \quad (4.48)$$

with the pressure  $p = p_0 e^{-\int_o^z dz'/H}$ . At the boundaries the values are set to

$$T_n^t(z_{LB}) = T_{n,LB}^t \quad (4.49)$$

$$T_n^t(z_{top}) = T_n^t(z_{top} - \frac{1}{2}\Delta z) \quad (4.50)$$

$$gH(z_{LB}) = \frac{RT_n^t(z_{LB})}{\bar{m}(z_{LB})} \quad (4.51)$$

$$gH(z_{top}) = \frac{R^*T_n^t(z_{top})}{\bar{m}(z_{top})} \quad (4.52)$$

$$\rho_{LB} = \frac{p_0 e^{-z_{LB}}}{e^{-0.5\Delta z}} \frac{1}{H(z_{LB})g} \quad (4.53)$$

$$\rho_{top} = \frac{p_0 e^{-z_{top}}}{e^{-0.5\Delta z}} \frac{1}{H(z_{top})g} \quad (4.54)$$

The second derivative  $\frac{\partial}{\partial Z} \left\{ g_c \frac{\partial T_n^{t+\Delta t}}{\partial Z} \right\}$  is approximated at midpoint level by

$$\begin{aligned} \frac{\partial}{\partial Z} \left\{ g_c \frac{\partial T_n^{t+\Delta t}}{\partial Z} \left( z + \frac{1}{2}\Delta z \right) \right\} &\approx \frac{1}{\Delta z^2} [T_n^{t+\Delta t} \left( z - \frac{1}{2}\Delta z \right) g_c(z) + \\ &\quad T_n^{t+\Delta t} \left( z + \frac{1}{2}\Delta z \right) \{ -g_c(z + \Delta z) - g_c(z) \} + \\ &\quad T_n^{t+\Delta t} \left( z + \frac{3}{2}\Delta z \right) g_c(z + \Delta z)] \end{aligned} \quad (4.55)$$

Note that  $g_c$  are calculated at the interface levels  $z, z + \Delta z \dots$  and the neutral temperature is on the midpoint level. For a derivation of the discrete second order derivative we refer to chapter 3.3 equation (3.26).

The first order derivative  $\frac{\partial}{\partial Z} \left\{ \frac{g^2}{p_0} \frac{K_E H^2 \rho}{T_n^t} T_n^{t+\Delta t} \right\}$  is expanded by  $\frac{T_n^{t+\Delta t}}{T_n^t}$ . The term  $\frac{g^2}{p_0} \frac{K_E H^2 \rho}{T_n^t}$  is substituted by  $f_c$  with  $f$  in the source code denotes  $f = \frac{f_c}{2\Delta z}$ . The first order derivative is determined by

$$\begin{aligned} \frac{\partial}{\partial Z} \{ f_c T_n^{t+\Delta t} \} \left( z + \frac{1}{2}\Delta z \right) &\approx \frac{1}{2\Delta z} [ -T_n^{t+\Delta t} \left( z - \frac{1}{2}\Delta z \right) f_c(z) + \\ &\quad T_n^{t+\Delta t} \left( z + \frac{1}{2}\Delta z \right) \{ f_c(z + \Delta z) - f_c(z) \} + \\ &\quad T_n^{t+\Delta t} \left( z + \frac{3}{2}\Delta z \right) f_c(z + \Delta z) ] \end{aligned} \quad (4.56)$$

Note that  $f_c$  is on the interface level, and the neutral temperature on the midpoint level. The first order derivative derived from

$$\frac{\partial f T_n^{t+\Delta t}}{\partial Z}(z + \frac{1}{2}\Delta z) = \frac{f(z + \Delta z)T_n^{t+\Delta t}(z + \Delta z) - f(z)T_n^{t+\Delta t}(z)}{\Delta z} \quad (4.57)$$

with the values at the interface level  $T_n^{t+\Delta t}(z) = \frac{1}{2}(T_n^{t+\Delta t}(z - \frac{1}{2}\Delta z) + T_n^{t+\Delta t}(z + \frac{1}{2}\Delta z))$  and  $T_n^{t+\Delta t}(z + \Delta z) = \frac{1}{2}(T_n^{t+\Delta t}(z + \frac{3}{2}\Delta z) + T_n^{t+\Delta t}(z + \frac{1}{2}\Delta z))$ . The tridiagonal solver need the equation in the following form:

$$P(k, i)T_n^{t+\Delta t}(k - 1, i) + Q(k, i)T_n^{t+\Delta t}(k, i) + R(k, i)T_n^{t+\Delta t}(k + 1, i) = RHS(k, i) \quad (4.58)$$

with the height index  $k$  for  $z + \frac{1}{2}\Delta z$ ,  $k + 1$  for  $z + \frac{3}{2}\Delta z$ , and  $k - 1$  for  $z - \frac{1}{2}\Delta z$ . The longitude index is denoted by  $i$ . Note that the equation is solved at each latitude  $\lambda$  with the index  $j$ .

The left hand side terms discussed above are sorted according to the height index which leads to

$$P(k, i) = g_c(k, i) - f_c(k, i) \quad (4.59)$$

$$Q^*(k, i) = -g_c(k + 1, i) - g_c(k, i) - f_c(k, i) + f(k + 1, i) \quad (4.60)$$

$$R = g_c(k + 1, i) + f(k + 1, i) \quad (4.61)$$

At the upper boundary the values are set to

$$R(z_{top} - \frac{1}{2}\Delta z) = 0 \quad (4.62)$$

$$P(z_{top} - \frac{1}{2}\Delta z) = g_c(z_{top} - \frac{1}{2}\Delta z) - f(z_{top} - \frac{1}{2}\Delta z) \quad (4.63)$$

$$Q(z_{top} - \frac{1}{2}\Delta z) = -g_c(z_{top} - \frac{1}{2}\Delta z) - f(z_{top} - \frac{1}{2}\Delta z) \quad (4.64)$$

The right hand side is

$$RHS = C_p^{mid} e^{-z} \left[ \mathbf{v}_n^t \nabla T_n^t + w^{t+\Delta t} \frac{\partial T_n^t}{\partial Z} - \frac{1}{2\Delta t} T_n^{t-\Delta t, smo} \right] - e^{-z} Q^{exp} + L^{exp} \quad (4.65)$$

At the height level  $k$  the following terms are added to  $Q$

$$Q(k, i) = Q^*(k, i) + C_p^{mid} \left\{ \frac{1}{2\Delta t} + L^{imp} \right\} + w^{mid} \frac{R}{\overline{m}} \quad (4.66)$$

with the values at the midpoint level  $C_p^{mid}(z + \frac{1}{2} + \Delta z) = C_p(z) + C_p(z + \Delta z)$  and  $w^{mid}(z + \frac{1}{2} + \Delta z) = w(z) + w(z + \Delta z)$ . At the lower boundary the following condition is used

$$P(z_{bot} - \frac{1}{2}\Delta z)T_n(z_{bot} - \frac{1}{2}\Delta z) = 2P(z_{bot})T_n(z_{LB}) - P(z_{bot} + \frac{1}{2}\Delta z)T_n(z_{bot} + \frac{1}{2}\Delta z) \quad (4.67)$$

$$P(z_{bot} + \frac{1}{2}\Delta z) = 0 \quad (4.68)$$

with  $z_{bot} + \frac{1}{2}\Delta z$  corresponding to the midpoint level and the height index  $k = 1$ .  $P(z_{bot})$  is set to  $P(z_{bot} + \frac{1}{2}\Delta z)$ , and  $T_n(z_{bot})$  is equal to the lower boundary with the value  $T_n(z_{LB})$ . This which leads to

$$Q^*(z_{bot} + \frac{1}{2}\Delta z) = Q(z_{bot} + \frac{1}{2}\Delta z) - P(z_{bot} + \frac{1}{2}\Delta z) \quad (4.69)$$

$$RHS^*(z_{bot} + \frac{1}{2}\Delta z) = RHS(z_{bot} + \frac{1}{2}\Delta z) - 2P(z_{bot} + \frac{1}{2}\Delta z)T_n^t(z_{LB}) \quad (4.70)$$

$$P^*(z_{bot} + \frac{1}{2}\Delta z) = 0 \quad (4.71)$$

Solving for the neutral temperature at each latitude leads to the updated neutral temperature  $T_n^{upd,t_n+\Delta t}$  at the midpoints. The lower boundary of the neutral temperature is stored at the top level with the height index  $nlev + 1$  which is above the upper boundary of the model with pressure level  $-7$ . Note that the lower boundary is at pressure level  $-7$  which is  $z_{bot}$  or  $z_{LB}$ , however all the other values of the neutral temperature are on the midpoints which means at the pressure levels  $-6.75, -6.25, -5.75, \dots, 5.75, 6.25, 6.75$ . The calculated values for the neutral temperature  $T_n^{upd,t+\Delta t}$  are smoothed by a Fast Fourier transformation. All the wave numbers larger than a predefined value at each latitude are removed. The wave numbers are defined in the module `cons.F`. The values of the neutral temperature at the timestep  $t_n$  are also updated by using

$$T_n^{upd,t} = \frac{1}{2}(1 - c_{smo})(T_n^{t-\Delta t} + T_{n,smo}^{upd,t+\Delta t}) + c_{smo}T_n^t \quad (4.72)$$

with  $c_{smo} = 0.95$



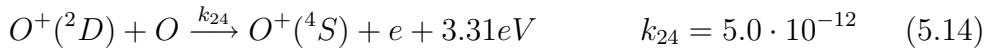
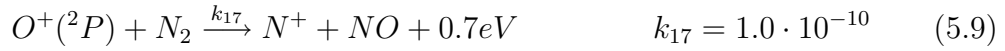
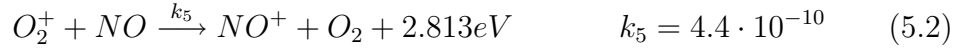
# Chapter 5

## Chemistry

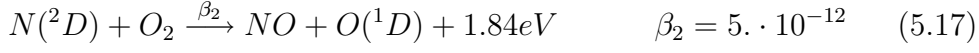
## 5.1 Calculation of chemical reaction rates /

The chemical reaction rates can be found in [16], and [17] In this module the time independent reaction rates are set as module data. The time dependent rates are calculated in the subroutine `chemrates_tdep`. First we describe the time independent rates for the ion chemistry:

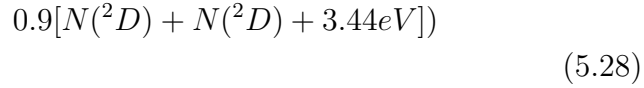
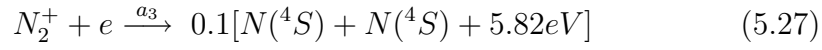
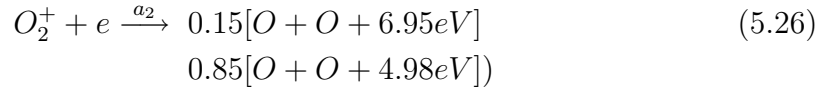
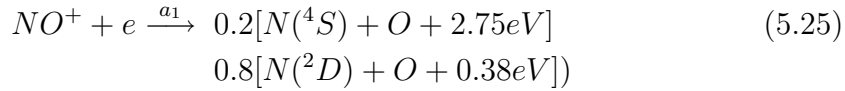
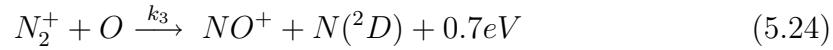
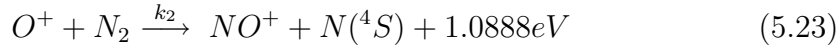
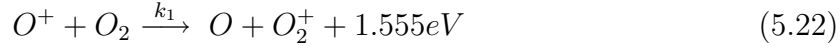
### 5.1.1 Module data



The time independent rates for the neutral chemistry are

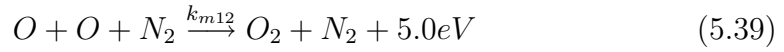
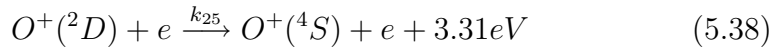
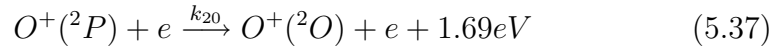
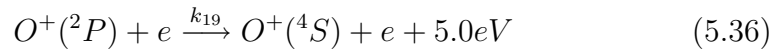
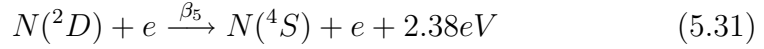
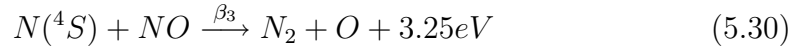
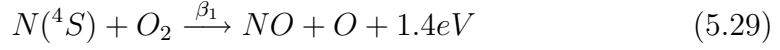


The temperature dependent rates are calculated at every timestep and every latitude. For the ion chemistry these reaction rates are:





The time dependent reactions for the neutral chemistry are



### 5.1.2 Calculation of time dependent reaction rates

The time dependent rates, mentioned in the previous section 5.1.1 are calculated in the subroutine `chemrates_tdep`. The temperatures are set by

$$\begin{aligned} T_1 &= \frac{1}{300} \left( \frac{2}{3} T_i + \frac{1}{3} T_n \right) \\ T_2 &= \frac{1}{300} (0.6363 T_i + 0.3637 T_n) \\ T_3 &= \frac{1}{2} \frac{1}{300} (T_i + T_n) \end{aligned} \quad (5.40)$$

with  $T_i$ ,  $T_e$  and  $T_n$  denoting the ion, electron and neutral temperature, respectively.

$$k_1 = 1.6 \cdot 10^{-11} T_1^{-0.52} + 5.5 \cdot 10^{-11} e^{-22.85/T_1} \quad (5.41)$$

$$k_2^* = (8.6 \cdot 10^{-11} T - 2 - 5.92 \cdot 10^{-13}) T_2 + 1.533 \cdot 10^{-12} \quad (5.42)$$

$$e^t = e^{-3353/t_n}$$

$$k_2 = [(\{[(270 \cdot e^t + 220) e^t + 85] e^t + 38\} e^t + 1) k_2^* e^t + k_2^*] (1 - e^t) \quad (5.43)$$

$$k_3 = 5.2 \cdot 10^{-11} T_3^{0.2} \text{for } \frac{1}{2}(T_i + T_n) > 1500K$$

$$k_3 = 1.4 \cdot 10^{-10} T_3^{-0.44} \text{for } \frac{1}{2}(T_i + T_n) \leq 1500K \quad (5.44)$$

$$k_{19} = 4.10^{-8} \sqrt{300/T_e} \quad (5.45)$$

$$k_{20} = 1.510^{-7} \sqrt{300/T_e} \quad (5.46)$$

$$k_{25} = 6.610^{-8} \sqrt{300/T_e} \quad (5.47)$$

$$k_{m,12} = 9.5910^{-34} e^{480/T_n} \quad (5.48)$$

$$a_1 = 4.210^{-7} (300/T_e)^{0.85} \quad (5.49)$$

$$a_2 = 1.610^{-7} (300/T_e)^{0.55} \quad T_e \geq 1200K$$

$$a_2 = 2.710^{-7} (300/T_e)^{0.7} \quad T_e < 1200K \quad (5.50)$$

$$a_3 = 1.810^{-7} (300/T_e)^{0.39} \quad (5.51)$$

$$\beta_1 = 1.510^{-11} e^{-3600/T_n} \quad (5.52)$$

$$\beta_3 = 3.410^{-11} \sqrt{T_n/300} \quad (5.53)$$

$$\beta_5 = 3.610^{-10} \sqrt{T_e/300} \quad (5.54)$$

$$\beta_8 = 4.5^{-6} (1 + 0.11 \frac{F_{10.7} - 65}{165}) e^{-110^{-8} f n O_2^{0.38}} f l s \quad (5.55)$$

with  $F n O_2$  the  $O_2$  line integral from `chapman.F`,  $F N v O_2$  the column number density of  $O_2$  from `chapman.F`, and  $f l s$  denotes the flux variation due to orbital excentricity (from `init_module`). The 10.7 cm flux is denoted by

$F_{10.7}$ .

$$\beta_9 = 2.9110^{11} \left(1 + 0.2 \frac{F_{10.7} - 65}{100}\right) 210^{-18} e^{1-8.10^{-21} F_{nO_2}} fls \quad (5.56)$$

$$\beta_{9n} = 510^9 \left(1 + 0.2 \frac{F_{10.7} - 65}{100}\right) 210^{-18} e^{1-8.10^{-21} F_{nvO_2}} fls \quad (5.57)$$

$$(5.58)$$

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
mass mixing ratio $O_2$	$\Psi_{O_2}$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi_O$	—	midpoints	$t_n$
mean molecular mass	$\overline{m}$	$g/mol$	interfaces	$t_n + \Delta t$
number density of $O^+$	$n(O^+)$	$\#/cm^3$	midpoints	$t_n$
number density of $O^{+,t_n+\Delta t}$	$n(O^+)$	$\#/cm^3$	midpoints	$t_n$
number density of $N(^2D)$	$n(N(^2D))$	$\#/cm^3$	midpoints	$t_n$
number density of $NO$	$n(NO)$	$\#/cm^3$	midpoints	$t_n$
number density of $N(^4S)$	$n(N(^4S))$	$\#/cm^3$	midpoints	$t_n$
number density of $XIO^+(^2P)$	$n(XIO^+(^2P))$	$\#/cm^3$	midpoints	$t_n + \Delta t$
number density of $XIO^+(^2D)$	$n(XIO^+(^2D))$	$\#/cm^3$	midpoints	$t_n + \Delta t$

Table 5.1: Input fields to subroutine `elden`

## 5.2 Calculation of electron density $N_e$ , $N^+$ , $N_2^+$ , $NO^+$ /

The input to subroutine `elden` is summarized in table 5.1. The output of subroutine `settei` is summarized in table 5.2. The module data of subroutine `elden` is summarized in table 5.3.

The electron density is calculated by

$$N_e = n(O^+) + n(N_2^+) + n(N^+) + n(O_2^+) + n(NO^+) \quad (5.59)$$

physical field	variable	unit	pressure level	timestep
number density of $N^+$	$n(N^+)$	$\#/cm^3$	midpoints	$t_n + \Delta t$
number density of $N_2^+$	$n(N_2^+)$	$\#/cm^3$	midpoints	$t_n + \Delta t$
number density of $NO^+$	$n(NO^+)$	$\#/cm^3$	midpoints	$t_n + \Delta t$
number density of $O_2^+$	$n(O_2^+)$	$\#/cm^3$	midpoints	$t_n + \Delta t$
electron density	$N_e$	$\#/cm^3$	midpoints	$t_n + \Delta t$

Table 5.2: Output fields of **subroutine elden**

physical field	variable	unit	pressure level	timestep
QRJ: production due to $N^+$	$Q(N^+)$	$cm^{-3}s^{-1}$	interfaces	$t_n$
QRJ: production due to $NO^+$	$Q(NO^+)$	$cm^{-3}s^{-1}$	interfaces	$t_n$
CHEMRATES: reaction rates	$k_i$	$cm^3s^{-1}$	midpoints	—
CHEMRATES: N) production coefficient	$\beta_9$	$s^{-1}$	interface	—

Table 5.3: Module data of **subroutine elden**

with

$$n(O^+) = F \quad (5.60)$$

$$n(N_2^+) = \frac{D}{E' + \alpha_3 N_e} \quad (5.61)$$

$$n(N^+) = G \quad (5.62)$$

$$n(O_2^+) = \frac{B + \frac{HD}{E' + \alpha_3 N_e}}{C + \alpha_2 N_e} \quad (5.63)$$

$$n(NO^+) = \left[ A + \frac{E'D - HD}{E' + \alpha_3 N - e} + \frac{C}{C + \alpha_2 N - e} \frac{B + HD}{E' + \alpha_3 N_e} \right] \frac{1}{\alpha_1 N_e} \quad (5.64)$$

This leads to an fourth order equation

$$a_4 N_e^4 + a_3 N_e^3 + a_2 N_e + a_1 N_e + a_0 = 0 \quad (5.65)$$

with

$$a_4 = \alpha_1 \alpha_2 \alpha_3 \quad (5.66)$$

$$a_3 = \alpha_1 (\alpha_2 E' + \alpha_3 C) - \alpha_1 \alpha_2 \alpha_3 (F + G) \quad (5.67)$$

$$a_2 = \alpha_1 E' C - \alpha_1 (\alpha_2 E' + \alpha_3 C) (F + G) - \alpha_1 \alpha_2 D - \alpha_2 \alpha_3 A - \alpha_1 \alpha_3 B \quad (5.68)$$

$$a_1 = -\alpha_1 [E' C (F + G) + DC + BE' + HD] - \alpha_2 [E' (A + D) - HD] - \alpha_3 C (A + B) \quad (5.69)$$

$$a_0 = -E' C (A + B + D) \quad (5.70)$$

and

$$A = Q(NO^+) + k_2 n(O^+) n(N_2) + k_7 n(N^+) n(O_2) + \beta_9 n(NO) \quad (5.71)$$

$$B = Q(O_2^+) + k_1 n(O^+) + n(O_2) + k_6 n(N^+) n(O_2) + k_{26} n(O_2) n(xiO^+(^2D)) \quad (5.72)$$

$$C = k_4 n(N(^4S)) + k_5 n(NO) \quad (5.73)$$

$$D = Q(N_2^+) + n(N_2) [k_{16} n(xiO^+(^2P)) + k_{23} n(xiO^+(^2D))] \quad (5.74)$$

$$E = k_3 n(O) \quad (5.75)$$

$$F = n(O^+) \quad (5.76)$$

$$G = n(N^+) \quad (5.77)$$

$$H = k_9 n(O_2) \quad (5.78)$$

$$E' = E + H \quad (5.79)$$

Then the electron density is

$$N_e = F + \frac{D}{E' + \alpha_3 N_e} + G + \frac{B}{C + \alpha_2 N_e} + \frac{HD}{(E' + \alpha_3 N_e)(C + \alpha_2 N_e)} + \frac{1}{\alpha_1 N_e} \left[ A + \frac{E'D - HD}{E' + \alpha_3 N_e} + \frac{CB}{C + \alpha_2 N_e} + \frac{CHD}{(E' + \alpha_3 N_e)(C + \alpha_2 N_e)} \right] \quad (5.80)$$

The values  $A, B, C, D, E, F, G$  and  $H$  are evaluated at midpoint level

$$A(z + \frac{1}{2}\Delta z) = \frac{1}{2}(Q(NO^+)(z) + Q(NO^+)(z + \Delta z)) + \\ N\bar{m} \left[ k_2 n(O^+)^{t+\Delta t} \frac{\Psi_{N_2}}{m_{N_2}} + k_7 n(N^+) \frac{\Psi_{O_2}}{m_{O_2}} \right] + \\ \frac{1}{2} [\beta_9(z) + \beta_9(z + \Delta z)] \frac{\Psi_{NO}}{m_{NO}} \quad (5.81)$$

$$B(z + \frac{1}{2}\Delta z) = \frac{1}{2}(Q(O_2^+)(z) + Q(O_2^+)(z + \Delta z)) + \\ N\bar{m} [k_1 n(O^+)^{T+\Delta t} + k_6 n(N^+) + \\ k_{26} n(xiO^+(^2D))] \frac{\Psi_{O_2}}{m_{O_2}} \quad (5.82)$$

$$C(z + \frac{1}{2}\Delta z) = N\bar{m} \left[ k_4 \frac{\Psi_{N(^4S)}}{m_{N(^4S)}} + k_5 \frac{\Psi_{NO}}{m_{NO}} \right] \quad (5.83)$$

$$D(z + \frac{1}{2}\Delta z) = \frac{1}{2} [Q(N_2^+)(z) + Q(N_2^+)(z + \Delta z)] + \\ N\bar{m} \frac{\Psi_{N_2}}{m_{N_2}} [k_{16} n(xiO^+(^2P) + k_{23} n(xiO^+(^2D)))] \quad (5.84)$$

$$E'(z + \frac{1}{2}\Delta z) = N\bar{m} \left[ k_3 \frac{\Psi_O}{m_O} + k_9 \frac{\Psi_{O_2}}{m_{O_2}} \right] \quad (5.85)$$

$$(F + G)(z + \frac{1}{2}\Delta z) = n(O^+) + n(N^+) \quad (5.86)$$

$$H(z + \frac{1}{2}\Delta z) = N\bar{m} k_9 \frac{\Psi_{O_2}}{m_{O_2}} \quad (5.87)$$

First the conversion factor from mass mixing ratio to number density is calculated at the midpoint level

$$N\bar{m}(z + \frac{1}{2}\Delta z) = \frac{p_o e^{-z - \frac{1}{2}\Delta z} \bar{m}(z + \Delta z)}{k_B T_n(z + \Delta z)} \quad (5.88)$$

The mass mixing ratio of  $N_2$  at the midpoint level is determined by

$$\Psi(N_2)(z + \frac{1}{2}\Delta z) = 1 - \Psi(O_2)(z + \frac{1}{2}\Delta z) - \Psi(O)(z + \frac{1}{2}\Delta z) \quad (5.89)$$

The number density of  $N^+$  is

$$n(N^+) = \frac{Q(N^+) + k_{10} n(O^+) n(N(^2D))}{(k_6 + k_7) n(O_2) + k_8 n(O)} \quad (5.90)$$

## 5.2. CALCULATION OF ELECTRON DENSITY $N_E$ , $N^+$ , $N_2^+$ , $NO^+$ / 87

which is calculated at the midpoint level in the code by

$$n(N^+)(z + \frac{1}{2}\Delta z) = \frac{\frac{1}{2}[Q(N^+)(z) + Q(N^+)(z + \Delta z)] + k_{10}n(O^+)N\overline{m}\frac{\Psi(N(^2D))}{m_{N(^2D)}}}{N\overline{m}(k_6 + k_7)\frac{\Psi(O_2)}{m_{O_2}} + k_8\frac{\Psi(O)}{m_O}} \quad (5.91)$$

The quadric solver solves for the electron density  $N_e$ , with  $N_e \geq 3 \cdot 10^3$ . Then, the number densities of  $N_2^+$ ,  $O_2^+$  and  $NO^+$  can be determined on the midpoint level

$$n(N_2^+) = \frac{D}{E' + \alpha_3 N_e} \quad (5.92)$$

$$n(O_2^+) = \left[ B + \frac{HD}{E' + \alpha_3 N_e} \right] \frac{1}{C + \alpha_2 N_e} \quad (5.93)$$

$$n(NO^+) = \frac{A + \frac{D(E'-H)}{E' + \alpha_3 N_e} + C \left( B + \frac{HD}{E' + \alpha_3 N_e} \right)}{C + \alpha_2 N_e} \frac{1}{\alpha_1 N_e} \quad (5.94)$$

with  $N_e$  still on the midpoint level. The electron density at the interface level is determined by

$$N_e(z) = \sqrt{N_e(z - \frac{1}{2}\Delta z)N_e(z + \frac{1}{2}\Delta z)} \quad (5.95)$$

with the midpoint level  $z - \frac{1}{2}\Delta z$  denoted by index  $k$ ,  $z + \frac{1}{2}\Delta z$  then by the height index  $k + 1$ , and on the interface level  $z$  has the index  $k + 1$ . The upper and lower boundary are set by

$$N_e(z_{bot}) = \sqrt{\frac{N_e^3(z_{bot} + \frac{1}{2}\Delta z)}{N_e(z_{bot} + \frac{3}{2}\Delta z)}} \quad (5.96)$$

$$N_e(z_{top}) = \sqrt{\frac{N_e^3(z_{top} - \frac{1}{2}\Delta z)}{N_e(z_{top} - \frac{3}{2}\Delta z)}} \quad (5.97)$$



physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n$
mass mixing ratio $X$	$\Psi(X)^{t_n}$	—	midpoints	$t_n$
mass mixing ratio $X$	$\Psi(X)^{t_n+\Delta t}$	—	midpoints	$t_n + \Delta t$
upward number flux at upper boundary	$F_x^{upw,top}$	$\#/cm^3$	$z_{top}$	$t_n + \Delta t$
diffusive vector	$D_v$	???	midpoints??	$t_n??$
molecular weight of species $X$	$m_X$	$g/mole$	—	—
thermal diffusion coefficient	$D_T$	???	midpoints???	$t_n???$
loss of $X$	$L_X$	???	midpoints???	$t_n????$
production of $X$	$P_X$	???	midpoints???	$t_n???$
???coefficient of upward flux $A, B, C$	$A \frac{\partial \Psi_X}{\partial Z} + B \Psi_X + C = 0$	???	$z_{bot}$	$t_n + \Delta t$

Table 5.4: Input fields to subroutine `minor`

### 5.3 Calculation minor species $N(^4S)$ and $NO$ , (and $HOx$ in TIMEGCM)

The input to subroutine `minor` is summarized in table 5.4. The output of subroutine `minor` is summarized in table 5.5. The module data of subroutine `minor` is summarized in table 5.6. Since the minor species  $N(^4S)$  and  $NO$  (and  $HOx$  in TIMEGCM) have longer life times, the neutral wind transport effects have to taken into account. The governing equation

physical field	variable	unit	pressure level	timestep
mass mixing ratio of species $X$	$\Psi(X)^{t_n, upd}$	—	interfaces???	$t_n$
mass mixing ratio of species $X$	$\Psi(X)^{t_n + \Delta t, upd}$	—	interfaces???	$t_n + \Delta t$

Table 5.5: Output fields of **subroutine minor**

physical field	variable	unit	pressure level	timestep
background eddy diffusion	$K_E$	???	interfaces	—

Table 5.6: Module data of **subroutine minor**

is (see [?]) Roble et al. 1988

$$\begin{aligned}
\frac{\partial \Psi}{\partial t} = & -e^z \frac{\partial}{\partial Z} \left[ A \left( \frac{\partial}{\partial Z} - E \right) \Psi \right] \\
& + S\Psi - R - \left[ \mathbf{v}_n \cdot \nabla \Psi + W_n \frac{\partial \Psi}{\partial Z} \right] \\
& + e^z \left[ e^{-z} K_E \left( \frac{\partial}{\partial Z} + \frac{1}{\bar{m}} \frac{\partial \bar{m}}{\partial Z} \right) \Psi \right] + H_{sub}
\end{aligned} \tag{5.98}$$

with

$$\tilde{E} = \left( 1 - \frac{m}{\bar{m}} - \frac{1}{\bar{m}} \frac{\partial \bar{m}}{\partial Z} \right) - \tilde{\alpha} \frac{1}{T_n} \frac{\partial T_n}{\partial Z} + \tilde{F} \tilde{\Psi} \tag{5.99}$$

The vertical molecular diffusion coefficient is  $A$ , the production term is  $S$ , the loss term is  $R$ , the term  $E$  includes the effects of gravity, thermal diffusion and friction with the major species on the vertical profile of the two species ( $O_x, O_2$ ). The matrix operator for frictional interaction is  $\tilde{F}$ , the thermal diffusion coefficient is  $\alpha$ , and the mean molecular mass is  $\bar{m}$ , and  $\Psi$  stands for the mass mixing ratio of either  $NO$ ,  $N(^4S)$  or  $HOx$ . In TIEGCM  $O_x$  is simply  $O$ , whereas in TIMEGCM, it is  $O_3 + O$ . The horizontal diffusion caused by sub-grid processes which cannot be resolved by the model is added in by  $H_{sub}$ , and calculated in **subroutine hdif**

The temporal change in the mass mixing ratio on the left hand side of eq.(5.98) is equal to the vertical molecular diffusion which is denoted by

the first term on the right hand side, the production and loss of the minor species (term two and three in eq.(5.98)), the horizontal and vertical nonlinear advection term (fourth term), and the vertical eddy diffusion (fifth term). The temporal term and all terms dependent with  $Z$  derivatives are treated implicit. The solver needs the equation in the following form

$$P_k \Psi_{k-1}^{t+\Delta t} + Q_k \Psi_k^{t+\Delta t} + R_k \Psi_{k+1}^{t+\Delta t} = f_k \quad (5.100)$$

where  $P_k$ ,  $Q_k$ ,  $R_k$ , and  $f_k$  are determined at timestep  $t$  at midpoints.  $\Psi_{k-1,k+1}^{t+\Delta t}$  are also at midpoints but at the next timestep  $t + \Delta t$ ,  $k$  stands for the index of the vertical grid. The equation 5.98) can be rearranged and multiplied by  $e^{-z}$  which will lead to

$$\begin{aligned} e^{-z} \frac{\Psi_n^{t+\Delta t}}{2\Delta t} + \frac{\partial}{\partial Z} \left[ A_n \frac{\partial}{\partial Z} \Psi_n^{t+\Delta t} - E_n \Psi_n^{t+\Delta t} \right] \\ - e^{-z} S \Psi_n^{t+\Delta t} + e^{-z} W_n \frac{\partial \Psi_n^{t+\Delta t}}{\partial Z} - \frac{\partial}{\partial Z} \left\{ e^{-z} K_E \frac{\partial}{\partial Z} + \frac{1}{\bar{m}} \frac{\partial \bar{m}}{\partial Z} \Psi_n^{t+\Delta t} \right\} = \\ - e^{-z} R - e^{-z} \{ \mathbf{v}_n \cdot \nabla \Psi^t \} + e^{-z} \frac{\Psi_n^{t-\Delta t}}{2\Delta t} + e^{-z} H_{sub} \end{aligned} \quad (5.101)$$

The second term is discretized by

$$\begin{aligned} \frac{\partial}{\partial Z} \left[ A_n \frac{\partial}{\partial Z} \Psi_n^{t+\Delta t} \right] = \frac{1}{\Delta z^2} \{ A_n(z - \frac{1}{2}\Delta z) \Psi^{t+\Delta t}(z - \Delta z) - \\ \left[ A_n(z + \frac{1}{2}\Delta z) + A_n(z - \frac{1}{2}\Delta z) \right] \Psi^{t+\Delta t}(z) + \\ A_n(z + \frac{1}{2}\Delta z) \Psi^{t+\Delta t}(z + \Delta z) \} \end{aligned} \quad (5.102)$$

The third term by

$$\begin{aligned} - \frac{\partial}{\partial Z} [A_n E_n \Psi_n^{t+\Delta t}] = \frac{1}{\Delta z} \{ -A_n(z - \frac{1}{2}\Delta z) E_n(z - \frac{1}{2}\Delta z) \Psi^{t+\Delta t}(z - \Delta z) - \\ \left[ -A_n(z + \frac{1}{2}\Delta z) E_n(z + \frac{1}{2}\Delta z) + A_n(z - \frac{1}{2}\Delta z) E_n(z - \frac{1}{2}\Delta z) \right] \Psi^{t+\Delta t}(z) + \\ A_n(z + \frac{1}{2}\Delta z) E_n(z + \frac{1}{2}\Delta z) \Psi^{t+\Delta t}(z + \Delta z) \} \end{aligned} \quad (5.103)$$

The fifth term is discretized by

$$e^{-z}W_n\frac{\partial\Psi^{t+\Delta t}}{\partial Z}=\frac{1}{2\Delta z}e^{-z}W_n(z)\Psi^{t+\Delta t}(z+\Delta z)-\frac{1}{2\Delta z}e^{-z}W_n(z)\Psi^{t+\Delta t}(z-\Delta z) \quad (5.104)$$

the sixth term by

$$-\frac{\partial}{\partial Z}\left[e^{-z}K_E\frac{\partial}{\partial Z}\Psi^{t+\Delta t}\right]=-\frac{1}{\Delta z^2}[e^{-z+\frac{1}{2}\Delta z}K_E(z-\frac{1}{2}\Delta z)\Psi^{t+\Delta t}(z-\Delta z)-\left\{e^{-z-\frac{1}{2}\Delta z}K_E(z+\frac{1}{2}\Delta z)+e^{-z+\frac{1}{2}\Delta z}K_E(z-\frac{1}{2}\Delta z)\right\}\Psi^{t+\Delta t}(z)+e^{-z-\frac{1}{2}\Delta z}K_E(z+\frac{1}{2}\Delta z)\Psi^{t+\Delta t}(z+\Delta z)] \quad (5.105)$$

and the seventh term is

$$-\frac{\partial}{\partial Z}e^{-z}K_E\frac{1}{\bar{m}}\frac{\partial\bar{m}}{\partial Z}\Psi^{t+\Delta t}=-\frac{1}{\Delta z^2}[e^{-z+\frac{1}{2}\Delta z}K_E(z-\frac{1}{2}\Delta z)\frac{m(z-\Delta z)}{\bar{m}(z-\frac{1}{2}\Delta z)}\Psi^{t+\Delta t}(z-\Delta z)-\left\{e^{-z-\frac{1}{2}\Delta z}K_E(z+\frac{1}{2}\Delta z)\frac{m(z)}{\bar{m}(z+\frac{1}{2}\Delta z)}+e^{-z+\frac{1}{2}\Delta z}K_E(z-\frac{1}{2}\Delta z)\frac{m(z)}{\bar{m}(z-\frac{1}{2}\Delta z)}\right\}\Psi^{t+\Delta t}(z)+e^{-z-\frac{1}{2}\Delta z}K_E(z+\frac{1}{2}\Delta z)\frac{m(z+\Delta z)}{\bar{m}(z+\frac{1}{2}\Delta z)}\Psi^{t+\Delta t}(z+\Delta z)] \quad (5.106)$$

and

$$-e^{-z}S\Psi^{t+\Delta t}(z) \quad (5.107)$$

Rearranging according to eq. (5.100) leads to the coefficients

$$P = \frac{1}{\Delta^2 z} \tilde{A}(z) + \frac{1}{\Delta z} \tilde{A}(z) \tilde{E}(z) - \frac{1}{2\Delta z} e^{-z} W(z + \frac{1}{2}\Delta z) - \frac{1}{\Delta^2 z} e^{-z+\Delta z} K_E(z) - \frac{1}{\Delta^2 z} e^{-z+\Delta z} K_E(z) \frac{m(z - \frac{1}{2}\Delta z)}{\bar{m}(z)} \quad (5.108)$$

$$R = \frac{1}{\Delta^2 z} \tilde{A}(z + \Delta z) - \frac{1}{\Delta z} \tilde{A}(z + \Delta z) \tilde{E}(z + \Delta z) + \frac{1}{2\Delta z} e^{-z} W(z + \frac{1}{2}\Delta z) - \frac{1}{\Delta^2 z} e^{-z} K_E(z + \Delta z) - \frac{1}{\Delta^2 z} e^{-z} K_E(z + \Delta z) \frac{m(z - \frac{3}{2}\Delta z)}{\bar{m}(z + \Delta z)} \quad (5.109)$$

$$Q = \frac{e^{-z}}{2\Delta t} - \frac{1}{\Delta^2 z} [\tilde{A}(z + \Delta z) + \tilde{A}(z)] + \frac{1}{\Delta z} [\tilde{A}(z + \Delta z) \tilde{E}(z + \Delta z) + \tilde{A}(z) \tilde{E}(z)] - e^{-z} S + \frac{1}{\Delta^2 z} [e^{-z} K_E(z + \Delta z) + e^{-z+\Delta z} K_E(z)] - \frac{1}{\Delta^2 z} [e^{-z} K_E(z + \Delta z) \frac{m(z + \frac{1}{2}\Delta z)}{\bar{m}(z + \Delta z)} + e^{-z+\frac{1}{2}\Delta z} K_E(z) \frac{m(z + \frac{1}{2}\Delta z)}{\bar{m}(z)}] \quad (5.110)$$

$$f = -e^{-z} R - e^{-z} \mathbf{v}_n \cdot \Psi^{t_n} + e^{-z} \frac{\Psi^{t_n - \Delta t}}{2\Delta t} \quad (5.111)$$

The lower boundary condition is ??? not used in the code????

$$\frac{1}{2}(\Psi(z_{bot} - \Delta z) + \Psi(z_{bot} + \Delta z)) = \Psi(z_{bot}) \quad (5.112)$$

which leads to

$$\Psi(z_{bot} - \Delta z) = 2\Psi(z_{bot}) - \Psi(z_{bot} + \Delta z) \quad (5.113)$$

Inserting into the equation (5.100)

$$\{-P(z_{bot}) + Q(z_{bot})\} \Psi(z_{bot}) + R(z_{bot}) \Psi(z_{bot} + \Delta z) = f(z_{bot}) - 2\Psi(z_{bot}) P(z_{bot}) \quad (5.114)$$

The upper boundary is ??? not used in the code ????

$$\frac{\partial}{\partial Z}\Psi = \epsilon\Psi \quad (5.115)$$

which leads to

$$\frac{\Psi(z_{top}) - \Psi(z_{top} - \Delta z)}{\Delta z} = \frac{\epsilon(z_{top} - \frac{1}{2}\Delta z)}{2} (\Psi(z_{top}) + \Psi(z_{top} - \Delta z)) \quad (5.116)$$

and the value for  $\Psi(z_{top})$

$$\Psi(z_{top}) = \frac{1 + \Delta z \frac{\epsilon(z_{top} - \frac{1}{2}\Delta z)}{2}}{1 - \Delta z \frac{\epsilon(z_{top} - \frac{1}{2}\Delta z)}{2}} \Psi(z_{top} - \Delta z) \quad (5.117)$$

Inserting into the equation (5.100)

$$\begin{aligned} & P(z_{top} - \Delta z)\Psi(z_{top} - 2\Delta z) + \{Q(z_{top} - \Delta z) + \\ & R(z_{top} - \Delta z)\} \frac{1 + \Delta z \frac{\epsilon(z_{top} - \frac{1}{2}\Delta z)}{2}}{1 - \Delta z \frac{\epsilon(z_{top} - \frac{1}{2}\Delta z)}{2}} \Psi(z_{top} - \Delta z) = f(z_{top} - \Delta z) \end{aligned} \quad (5.118)$$

In the code first the thermal diffusion coefficient  $\tilde{\alpha}$  is set with the diffusion vector  $\Phi_1 = (0, 1.35, 1.11)$  and  $\Phi_2 = (0.673, 0, 0.769)$  independent of the species, and the vector  $\Phi_x$  depending on the species.

$$\begin{aligned} \alpha_{12} &= \Phi_{12} - \Phi_{13} \\ \alpha_{21} &= \Phi_{21} - \Phi_{23} \\ \alpha_{x1} &= \Phi_{x1} - \Phi_{x3} \\ \alpha_{x2} &= \Phi_{x2} - \Phi_{x13} \end{aligned} \quad (5.119)$$

The values  $\Psi_x^{t_n - \Delta t}$  are smoothed with the Shapiro smoother, first in latitude,

$$\begin{aligned} \Psi_x^{t_n - \Delta t, lat} &= \Psi_x^{t_n - \Delta t} - 0.003[\Psi_x^{t_n - \Delta t}(\phi, \lambda - 2\Delta\lambda) + \Psi_x^{t_n - \Delta t}(\phi, \lambda + 2\Delta\lambda) - \\ & 4(\Psi_x^{t_n - \Delta t}(\phi, \lambda + \Delta\lambda) + \Psi_x^{t_n - \Delta t}(\phi, \lambda - \Delta\lambda)) + 6\Psi_x^{t_n - \Delta t}(\phi, \lambda)] \end{aligned} \quad (5.120)$$

and then in longitude

$$\begin{aligned} \Psi_x^{t_n - \Delta t, smo} &= \Psi_x^{t_n - \Delta t, lat} - 0.003[\Psi_x^{t_n - \Delta t, lat}(\phi - 2\Delta\phi, \lambda) + \\ & \Psi_x^{t_n - \Delta t, lat}(\phi + 2\Delta\phi, \lambda) - 4(\Psi_x^{t_n - \Delta t, lat}(\phi - \Delta\phi, \lambda) + \\ & \Psi_x^{t_n - \Delta t, lat}(\phi + \Delta\phi, \lambda)) + 6\Psi_x^{t_n - \Delta t, lat}(\phi, \lambda)] \end{aligned} \quad (5.121)$$

The horizontal advection  $\mathbf{v}_n \cdot \nabla \Psi_x$  is calculated in subroutine `advec`, with

$$\begin{aligned} u_n^\phi(\phi, \lambda) &= \frac{1}{2}[u_n(\phi + \Delta\phi, \lambda) + u_n(\phi - \Delta\phi, \lambda)] \\ u_n^{2\phi}(\phi, \lambda) &= \frac{1}{2}[u_n(\phi + 2\Delta\phi, \lambda) + u_n(\phi - 2\Delta\phi, \lambda)] \\ v_n^\lambda(\phi, \lambda) &= \frac{1}{2}[v_n(\phi, \lambda + \Delta\lambda) + v_n(\phi, \lambda - \Delta\lambda)] \\ v_n^{2\lambda}(\phi, \lambda)e &= \frac{1}{2}[v_n(\phi, \lambda + 2\Delta\lambda) + v_n(\phi, \lambda - 2\Delta\lambda)] \end{aligned} \quad (5.122)$$

and the terms

$$\begin{aligned} T_1(\phi, \lambda) &= \frac{1}{R_E \cos \lambda} \left\{ \frac{2}{3\Delta\phi} u_n^\phi(\phi, \lambda) [\Psi_x(\phi + \Delta\phi, \lambda) - \Psi_x(\phi - \Delta\phi, \lambda)] - \right. \\ &\quad \left. \frac{1}{12\Delta\phi} u_n^{2\phi}(\phi, \lambda) [\Psi_x(\phi + 2\Delta\phi, \lambda) - \Psi_x(\phi - 2\Delta\phi, \lambda)] \right\} \end{aligned} \quad (5.123)$$

$$\begin{aligned} T_2(\phi, \lambda) &= \frac{1}{R_E} \left\{ \frac{2}{3\Delta\lambda} v_n^\lambda(\phi, \lambda) [\Psi_x(\phi, \lambda + \Delta\lambda) - \Psi_x(\phi, \lambda - \Delta\lambda)] - \right. \\ &\quad \left. \frac{1}{12\Delta\lambda} v_n^{2\lambda}(\phi, \lambda) [\Psi_x(\phi, \lambda + 2\Delta\lambda) - \Psi_x(\phi, \lambda - 2\Delta\lambda)] \right\} \end{aligned} \quad (5.124)$$

The advection  $\mathbf{v}_n \cdot \nabla \Psi_x$  is then

$$\mathbf{v}_n \cdot \nabla \Psi_x = T_1 + T_2 \quad (5.125)$$

At the lower boundary the following values are set ??? which level  $z_{bot} - \frac{1}{2}\Delta z$  such that it fits afterward????

$$\begin{aligned} \Psi(O_2)(z_{bot} - \frac{1}{2}\Delta z) &= b_{11}\Psi(O_2)(z_{bot} + \frac{1}{2}\Delta z) + \\ &\quad b_{12}\Psi(O)(z_{bot} - \frac{1}{2}\Delta z) + F_b(1) \end{aligned} \quad (5.126)$$

$$\begin{aligned} \Psi(O)(z_{bot} - \frac{1}{2}\Delta z) &= b_{21}\Psi(O_2)(z_{bot} + \frac{1}{2}\Delta z) + \\ &\quad b_{22}\Psi(O)(z_{bot} - \frac{1}{2}\Delta z) + F_b(2) \end{aligned} \quad (5.127)$$

with  $b_{11}, b_{12}, b_{22}, b_{21}$  and  $\mathbf{F}_b$  from the file `bndry.F` and subroutine `bndcmp`. The mean molecular mass is

$$\begin{aligned} \overline{m}(z_{bot} - \frac{1}{2}\Delta z) &= \left[ \frac{\Psi(O_2)}{m_{O_2}}(z_{bot} - \frac{1}{2}\Delta z) + \frac{\Psi(O)}{m_O}(z_{bot} - \frac{1}{2}\Delta z) + \right. \\ &\quad \left. \frac{1 - \Psi(O_2) - \Psi(O)}{m_{N_2}}(z_{bot} - \frac{1}{2}\Delta z) \right]^{-1} \end{aligned} \quad (5.128)$$

The  $N_2$  number density is

$$\Psi(N_2)(z + \frac{1}{2}\Delta z) = 1 - \Psi(O_2)(z + \frac{1}{2}\Delta z) - \Psi(O)(z + \frac{1}{2}\Delta z) \quad (5.129)$$

and the mean molecular mass is

$$\begin{aligned} \bar{m}(z + \frac{1}{2}\Delta z) = & [\frac{\Psi(O_2)}{m_{O_2}}(z + \frac{1}{2}\Delta z) + \frac{\Psi(O)}{m_O}(z + \frac{1}{2}\Delta z) + \\ & \frac{\Psi(N_2)}{m_{N_2}}(z + \frac{1}{2}\Delta z)]^{-1} \end{aligned} \quad (5.130)$$

At the lower boundary the following quantities are calculated

$$\bar{m}(z_{bot}) = \frac{1}{2}[\bar{m}(z_{bot} - \frac{1}{2}\Delta z) + \bar{m}(z_{bot} + \frac{1}{2}\Delta z)] \quad (5.131)$$

$$\frac{d\bar{m}}{dz}(z_{bot}) = \frac{\bar{m}(z_{bot} + \frac{1}{2}\Delta z) - \bar{m}(z_{bot} - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.132)$$

$$\Psi(O)(z_{bot}) = \frac{1}{2}[\Psi(O)(z_{bot} - \frac{1}{2}\Delta z) + \Psi(O)(z_{bot} + \frac{1}{2}\Delta z)] \quad (5.133)$$

$$\Psi(O_2)(z_{bot}) = \frac{1}{2}[\Psi(O_2)(z_{bot} - \frac{1}{2}\Delta z) + \Psi(O_2)(z_{bot} + \frac{1}{2}\Delta z)] \quad (5.134)$$

$$\frac{d\Psi(O)}{dz}(z_{bot}) = \frac{\Psi(O)(z_{bot} + \frac{1}{2}\Delta z) - \Psi(O)(z_{bot} - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.135)$$

$$\frac{d\Psi(O_2)}{dz}(z_{bot}) = \frac{\Psi(O_2)(z_{bot} + \frac{1}{2}\Delta z) - \Psi(O_2)(z_{bot} - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.136)$$

At all other levels these quantities are

$$\bar{m}(z) = \frac{1}{2}[\bar{m}(z + \frac{1}{2}\Delta z) + \bar{m}(z - \frac{1}{2}\Delta z)] \quad (5.137)$$

$$\frac{d\bar{m}}{dz}(z) = \frac{\bar{m}(z + \frac{1}{2}\Delta z) - \bar{m}(z - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.138)$$

$$\Psi(O)(z) = \frac{1}{2}[\Psi(O)(z + \frac{1}{2}\Delta z) + \Psi(O)(z - \frac{1}{2}\Delta z)] \quad (5.139)$$

$$\Psi(O_2)(z) = \frac{1}{2}[\Psi(O_2)(z + \frac{1}{2}\Delta z) + \Psi(O_2)(z - \frac{1}{2}\Delta z)] \quad (5.140)$$

$$\frac{d\Psi(O)}{dz}(z) = \frac{\Psi(O)(z + \frac{1}{2}\Delta z) - \Psi(O)(z - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.141)$$

$$\frac{d\Psi(O_2)}{dz}(z) = \frac{\Psi(O_2)(z + \frac{1}{2}\Delta z) - \Psi(O_2)(z - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.142)$$



The neutral temperature at the interfaces is set by

$$\begin{aligned} T_n(z_{bot}) &= T_n(z_{LB}) \\ T_n(z_{top}) &= T_n(z_{top} - \frac{1}{2}\Delta z) \\ T_n(z) &= \frac{1}{2}[T_n(z + \frac{1}{2}\Delta z) + T_n(z - \frac{1}{2}\Delta z)] \end{aligned} \quad (5.143)$$

The production is calculated by

$$P_0 = P_x \frac{m_x k_B T_n(z + \frac{1}{2}\Delta z)}{p_0 e^{-z - \frac{1}{2}\Delta z} \bar{m}(z + \frac{1}{2}\Delta z)} \quad (5.144)$$

and stored in `s0prod`. The production  $P_x$  for the specie  $x$  is input to the subroutine, and is multiplied by  $\frac{m_x}{N\bar{m}}$ . does this make sense? The final thermal diffusion coefficients are determined

$$\begin{aligned} \alpha_{11,f} &= -[\phi_{13} + \alpha_{12}\Psi(O)(z)] \\ \alpha_{12,f} &= -\alpha_{12}\Psi(O_2)(z) \\ \alpha_{21,f} &= -[\alpha_{21}\Psi(O)(z) \\ \alpha_{22,f} &= -[\phi_{23} + \alpha_{21}\Psi(O_2)(z)] \end{aligned} \quad (5.145)$$

The quantity  $1 - \frac{\tilde{m}}{\bar{m}} - \frac{1}{\bar{m}} \frac{\bar{m}}{\partial Z} + \tilde{F}\tilde{\Psi}$  is calculated and stored in the variable `ex`

$$\begin{aligned} T_{ex} = & \{(\alpha_{x1}\alpha_{22,f} - \alpha_{x2}\alpha_{21,f}) \left[ \frac{d\Psi(O_2)}{dZ} - \left(1 - \frac{m_{O_2} + \frac{d\bar{m}}{dZ}}{\bar{m}}\right) \Psi(O_2) \right] + \\ & (\alpha_{x2}\alpha_{11,f} - \alpha_{x1}\alpha_{12,f}) \left[ \frac{d\Psi(O)}{dZ} - \left(1 - \frac{m_O + \frac{d\bar{m}}{dZ}}{\bar{m}}\right) \Psi(O) \right] \} \\ & \frac{1}{\alpha_{11,f}\alpha_{22,f} - \alpha_{12,f}\alpha_{21,f}} + 1 - \frac{m_X + \frac{d\bar{m}}{dZ}}{\bar{m}} \end{aligned} \quad (5.146)$$

The vertical molecular diffusion coefficient  $\tilde{A}$  is determined by

$$\tilde{A} = -\frac{\bar{m}(z)}{\tau m_{N_2}} \left( \frac{T_0}{T_n(z)} \right)^{0.25} \{\phi_{x3} + \alpha_{x1}\Psi(O_2)(z) + \alpha_{x2}\Psi(O)\}^{-1} \quad (5.147)$$

with  $\tau = 1.86 \cdot 10^3$ , and  $T_0 = 273K$ . The value is stored in the variable `ax` in the source code. The effects of gravity, thermal diffusion and the frictional interaction with the major species is expressed by the variable  $\tilde{E}$  given by eq. (5.99)

$$T_{thdiff}(z) = T_{ex} - \alpha_X \frac{T_n(z + \Delta z) - T_n(z - \Delta z)}{2\delta z T_n(z)} \quad (5.148)$$

and  $T_{ex}$  given by the expression in eq. (5.146). The quantity  $T_{thdiff}$  is stored in the variable `thdiff` in the source code. At the lower boundary the value is

$$\begin{aligned} T_{thdiff}(z_{bot}) &= T_{ex}(z_{bot}) - \alpha_X \frac{T_n(z_{bot} + \Delta z) - T_n(z_{bot})}{\Delta z T_n(z_{bot})} \\ T_{thdiff}(z_{top}) &= T_{ex}(z_{top}) - \alpha_X \frac{T_n(z_{top}) - T_n(z_{top} - \Delta z)}{\Delta z T_n(z_{top})} \end{aligned} \quad (5.149)$$

If the INPUT flag `difhor` is set (i0) then the horizontal variation of the eddy diffusion and thermal conductivity is set by

$$\begin{aligned} |\lambda_r| \geq 40^\circ \quad d_{fac} &= hor(\lambda) + 1.0 \\ |\lambda_r| < 40^\circ \quad d_{fac} &= hor(\lambda) + \frac{1}{2} \left( 1 + \sin \Pi \frac{|\lambda_r| - \frac{\Pi}{9}}{\Pi/4.5} \right) \end{aligned} \quad (5.150)$$

with  $\lambda_r$  going from the south pole to the north pole check  $|\lambda_r|$

The coefficients for the equation (5.100) which is solved for the mass mixing ratio are check the pressure levels and with the equation at the beginning

$$\begin{aligned} P &= \frac{\tilde{A}(k)}{\Delta z} \left( \frac{1}{\Delta z} + \frac{1}{2} T_{thdiff}(k) \right) - \\ &e^{-z - \frac{1}{2} \Delta z} [e^{\frac{1}{2} \Delta z} K_E(k) d_{fac} \left\{ \frac{1}{\Delta z} - \frac{1}{2} \frac{d\bar{m}}{dz}(k) \right\} + \\ &\frac{1}{4} \{W(z) + W(z + \Delta z)\}] \frac{1}{\Delta z} \end{aligned} \quad (5.151)$$

$$\begin{aligned}
R = & \frac{\tilde{A}(k+1)}{\Delta z} \left( \frac{1}{\Delta z} - \frac{1}{2} T_{thdiff(k+1)} \right) - \\
& e^{-z-\frac{1}{2}\Delta z} [e^{-\frac{1}{2}\Delta z} K_E(k+1) d_{fac} \left\{ \frac{1}{\Delta z} + \frac{1}{2} \frac{d\bar{m}}{dz}(k+1) \right\} - \\
& \frac{1}{4} \{W(z) + W(z + \Delta z)\}] \frac{1}{\Delta z}
\end{aligned} \tag{5.152}$$

$$\begin{aligned}
Q = & - \left\{ \frac{\tilde{A}(k)}{\Delta z} \left( \frac{1}{\Delta z} - \frac{1}{2} T_{thdiff(k)} + \frac{\tilde{A}(k+1)}{\Delta z} \left( \frac{1}{\Delta z} + \frac{1}{2} T_{thdiff(k+1)} \right) \right) \right\} + \\
& e^{-z-\frac{1}{2}\Delta z} (e^{\frac{1}{2}\Delta z} K_E(k) d_{fac} \left\{ \frac{1}{\Delta z} + \frac{1}{2} \frac{d\bar{m}}{dz}(k) \right\} + \\
& e^{-\frac{1}{2}\Delta z} K_E(k+1) d_{fac} \left\{ \frac{1}{\Delta z} - \frac{1}{2} \frac{d\bar{m}}{dz}(k) \right\}) \frac{1}{\Delta z} - L(l) + \frac{1}{2\Delta t}
\end{aligned} \tag{5.153}$$

$$f = e^{-z-\frac{1}{2}\Delta z} \left\{ \frac{\Psi_X^{t-\Delta t, smo}}{2\Delta t} - \mathbf{v}_n \cdot \nabla \Psi(k) + R(k) \right\} \tag{5.154}$$

At the lower boundary

$$\begin{aligned}
Q^*(k_{bot}) &= Q(k_{bot}) + P(k_{bot}) \frac{F(1) + 0.5F(2)\Delta z}{F(1) - 0.5F(2)\Delta z} \\
f^*(k_{bot}) &= f(k_{bot}) - P(k_{bot}) \frac{F(3)\Delta z}{F(1) - 0.5F(2)\Delta z} \\
P^*(k_{bot}) &= 0
\end{aligned} \tag{5.155}$$

with  $F$  the coefficient  $A, B, C$  of the upward flux which are input to the subroutine `minor`. The upper boundary is set by

$$\begin{aligned}
P^*(k_{top}) &= 1 + \frac{1}{2} \Delta z T_{thdiff}(k_{top}) \\
Q^*(k_{top}) &= P^*(k_{bot}) - 2. \\
R^*(k_{top}) &= 0. \\
f^*(k_{top}) &= - \frac{gm_x F_x^{upw, top} \Delta z}{p_0 \tilde{A} N_A}
\end{aligned} \tag{5.156}$$

with  $F_x^{upw,top}$  the upward number flux at the upper boundary which is input to **subroutine minor**.

Solving for the mass mixing ratio  $\Psi$  at each latitude leads to the updated mass mixing ratio  $\Psi^{upd,t_n+\Delta t}$  at the midpoints. The calculated values for the mass mixing ratio  $\Psi^{upd,t+\Delta t}$  are smoothed by a Fast Fourier transformation, which is part of the **minor module**. All the wave numbers larger than a predefined value at each latitude are removed. The wave numbers are defined in the **subroutine minor**. The values of the mass mixing ratio at the time step  $t_n$  are also updated by using

$$\Psi^{upd,t_n} = \frac{1}{2}(1 - c_{smo})(\Psi^{t_n-\Delta t} + \Psi_{smo}^{upd,t_n+\Delta t}) + c_{smo}\Psi^{t_n} \quad (5.157)$$

with  $c_{smo} = 0.95$ . All the values of  $\Psi^{upd,t_n}$  and  $\Psi^{upd,t_n+\Delta t}$  have to be at least as larger as  $10^{-12}$

physical field	variable	unit	pressure level	timestep
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n$
mass mixing ratio $NO$	$\Psi(NO)$	—	midpoints	$t_n$
electron density	$Ne$	$1/cm^3$	interfaces	$t_n$
number density $O^+$	$n(O^+)$	$1/cm^3$	midpoints	$t_n$
number density $N(^2P)$	$n(N(^2P))$	$1/cm^3$	midpoints	$t_n$
number density $NO^+$	$n(NO^+)$	$1/cm^3$	midpoints	$t_n$
conversion factor	$N\overline{m}$	$\#/cm^3 g/mole$	midpoints	$t_n$

Table 5.7: Input fields to subroutine `comp_n2d`

physical field	variable	unit	pressure level	timestep
mass mixing ratio $N(^2D)$	$\Psi(N(^2D))$	—	midpoints	$t_n + \Delta t$

Table 5.8: Output fields of subroutine `comp_n2d`

## 5.4 Calculation of Minor species $N(^2D)$ , $N(^4S)$ , and $NO$

### 5.4.1 calculation of $N(^2D)$

The input to subroutine `comp_n2d` is summarized in table 5.7. The output of subroutine `comp_n2d` is summarized in table 5.8.  $N(^2D)$  is assumed to be in photochemical equilibrium, such that the production  $P(N(^2D))$  and loss rate  $L(N(^2D))$  of  $N(^2D)$  is balanced.

$$n(N(^2D)) = \frac{P(N(^2D))}{L(N(^2D))} \quad (5.158)$$

The production is due to solar EUV photodissociation of  $N_2$ , and ion and neutral chemistry

$$\begin{aligned}
 P(N(^2D))(z + \frac{1}{2}\Delta z) = & \frac{1}{2} [Q_{tef}(z) + Q_{tef}(z + \Delta z)] br_{N^2D} + \\
 & k_3 n(N_2^+) N \bar{m} \frac{\Psi(O)}{m_o} + (\alpha_1 n(NO^+) 0.85 + \\
 & \alpha_3 n(N_2^+) 0.9) \sqrt{Ne(z) Ne(z + \Delta z)} \quad (5.159)
 \end{aligned}$$

with the branching ratio of producing  $N(^2D)$  which is set to 0.6. The chemical reaction rates are  $\alpha$  and  $k$  defined in the `chemrates_module`. The total production rate due to solar radiation and auroral particle precipitation is denoted by  $Q_{tef}$  which is calculated in subroutine `qrj`.

The loss term  $L(N(^2D))$  is determined by

$$\begin{aligned}
 L(N(^2D))(z + \frac{1}{2}\Delta z) = & N \bar{m} \left[ \beta_2 \frac{\Psi(O_2)}{m_{O_2}} + \beta_4 \frac{\Psi(O)}{m_O} + \beta_6 \frac{\Psi(NO)}{m_{NO}} \right] + \\
 & \beta_7 + \beta_5 \sqrt{Ne(z) Ne(z + \Delta z)} + k_{10} n(O^+) \quad (5.160)
 \end{aligned}$$

The chemical rates  $\beta$  are defined in the module `chemrates_module`.

The number density  $n(N(^2D))$  is converted to the mass mixing ratio by

$$\Psi(N(^2D)) = \frac{m_{N^2D}}{N \bar{m}} \frac{P(N(^2D))}{L(N(^2D))} \quad (5.161)$$

### 5.4.2 calculation of $N(^4S)$

The input to subroutine `comp_n4s` is summarized in table 5.9. The output of subroutine `comp_n4s` are the factor which define the lower boundary calculated in subroutine `minor` by solving  $A \frac{dX}{dz} + BX + C = 0$ . Also the upward flux at the upper boundary is defined, and the production  $P$  and loss rate  $L$  of  $N(^4S)$ . These values are stored in module data of the module `comp_n4s`. After subroutine `comp_n4s` the subroutine `minor_n4s` is called to calculate the mass mixing ratio of  $N(^4S)$ . Subroutine `minor_n4s` is not described here since it just calls subroutine `minor`. For information about subroutine `minor` please see chapter 5.3. The input to subroutine `minor` is described in table 5.4 and the output in table 5.5, substituting the species  $X$  by  $N(^4S)$ .

physical field	variable	unit	pressure level	timestep
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n$
mass mixing ratio $NO$	$\Psi(NO)$	—	midpoints	$t_n$
mass mixing ratio $N(^2D)$	$\Psi(N(^2D))$	—	midpoints	$t_n$
electron density	$Ne$	$1/cm^3$	interfaces	$t_n$
number density $O_2^+$	$n(O_2^+)$	$1/cm^3$	midpoints	$t_n$
number density $O^+$	$n(O^+)$	$1/cm^3$	midpoints	$t_n$
number density $N_2^+$	$n(N_2^+)$	$1/cm^3$	midpoints	$t_n$
number density $N^4$	$n(N^4)$	$1/cm^3$	midpoints	$t_n$
number density $NO^+$	$n(NO^+)$	$1/cm^3$	midpoints	$t_n$
neutral temperature	$Tn$	$K$	midpoints	$t_n$
mean molecular mass	$\overline{m}$	$g/mole????$	midpoints	$t_n$
conversion factor	$N\overline{m}$	$\#/cm^3 g/mole$	midpoints	$t_n$

Table 5.9: Input fields to subroutine `comp_n4s`

$N(^4S)$  has longer life time and is therefore influenced by the neutral winds.

The lower boundary is given by photochemical equilibrium. The factors  $A$ ,  $B$ , and  $C$  for the equation solved in subroutine `minor`  $A \frac{d\Psi(N(^4S))}{dz} + B\Psi(N(^4S)) + C = 0$  are

$$A = 0$$

$$B = 1.$$

$$C = (N(^4S)) = \frac{P(N(^4S))}{L(N(^4S))} \quad (5.162)$$

The conversion factor from number density to mass mixing ratio  $N\overline{m}(z_{LB})$

at the lower boundary is

$$N\overline{m}(z_{LB}) = p_0 e^{-z_{bot}-1/2\Delta z} e^{1/2\Delta z} \frac{\overline{m}(z_{bot})}{k_B T_n(z_{bot})} \quad (5.163)$$

The mass mixing ratio ????? or number density at the lower boundary is then

$$\begin{aligned} C = n(N(^4S))(z_{lbc}) &= \frac{m_{n(^4S)}}{N\overline{m}} [Q_{tef}(1 - br_{N^2D}) \frac{1}{N\overline{m}(z_{bot})} + \\ &\frac{\Psi(N(^2D))}{m_{N^2D}} (\beta_4 N\overline{m}(z_{bot}) \frac{\Psi(NO)}{m_o} + \beta_5 Ne + \beta_7) + \beta_8 \frac{\Psi(NO)}{m_{NO}}] \\ &\frac{1}{\beta_1 \frac{\Psi(O_2)}{m_{O_2}} + \beta_3 \frac{\Psi(NO)}{m_{NO}} + N\overline{m} \beta_{17} \frac{\Psi(O)}{m(O)} \frac{\Psi(N_2)}{m_{N_2}}} \end{aligned} \quad (5.164)$$

At the upper boundary the upward diffusive flux is set

$$n(N(^4S))(z_{ubc}) = 0. \quad (5.165)$$

The production rate  $P$  of  $N(^4S)$  is

$$\begin{aligned} P(N(^4S)) &= \frac{1}{2} (Q_{tef}(z) + Q_{tef}(z + \Delta z)) (1 - br_{N^2D}) + \\ &N\overline{m} \left[ \frac{\Psi(N^2D)}{m_{N^2D}} \left\{ \beta_5 \frac{1}{2} (Ne(z) + Ne(z + \Delta z) + \beta_7) \right\} + \right. \\ &\frac{1}{2} (\beta_8(z) + \beta_8(z + \Delta z)) \frac{\Psi(NO)}{m_{NO}} \left. \right] + \\ &N\overline{m} \left[ k_2 n(O^+) \frac{\Psi(xN_2)}{m_{N_2}} + k_6 n(N^+) \frac{\Psi(O_2)}{m_{O_2}} k_8 n(N^+) \frac{\Psi(O)}{m_O} + \right. \\ &\left. \sqrt{Ne(z) \cdot Ne(z + \Delta z)} (\alpha_1 n(NO^+) 0.15 + \alpha_3 n(N_2^+) 1.1) \right] \end{aligned} \quad (5.166)$$

and the loss rate  $L$  of  $N(^4S)$  is

$$\begin{aligned} L(N(^4S)) &= - N\overline{m} \left[ \beta_1 \frac{\Psi(O_2)}{m_{O_2}} + \beta_3 \frac{\Psi(NO)}{m_{NO}} + N\overline{m} \beta_{17} \frac{\Psi(O)}{m_O} \frac{\Psi(xN_2)}{m_{N_2}} \right] - \\ &k_4 n(O_2^+) \end{aligned} \quad (5.167)$$



physical field	variable	unit	pressure level	timestep
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n$
mass mixing ratio $N(^4S)$	$\Psi(N(^4S))$	—	midpoints	$t_n$
mass mixing ratio $N(^2D)$	$\Psi(N(^2D))$	—	midpoints	$t_n$
electron density	$Ne$	$1/cm^3$	interfaces	$t_n$
number density $O_2^+$	$n(O_2^+)$	$1/cm^3$	midpoints	$t_n$
neutral temperature	$Tn$	$K$	midpoints	$t_n$
mean molecular mass	$\overline{m}$	$g/mole????$	midpoints	$t_n$
conversion factor	$N\overline{m}$	$\#/cm^3 g/mole$	midpoints	$t_n$

Table 5.10: Input fields to subroutine `comp_no`

### 5.4.3 calculation of $NO$

The input to subroutine `comp_no` is summarized in table 5.10. The output of subroutine `comp_no` are the factors  $A$ ,  $B$ , and  $C$  which define the lower boundary condition of  $NO$ , the upper boundary upward diffusive flux, and the production  $P$  and loss rate  $L$  of  $NO$ . These values are stored in module data of the module `comp_no`. After subroutine `comp_no` the subroutine `minor_no` is called to calculate the mass mixing ratio of  $NO$ . Subroutine `minor_no` is not described here since it just calls subroutine `minor`. For information about subroutine `minor` please see chapter 5.3. The input to subroutine `minor` is described in table 5.4 and the output in table 5.5, substituting the species  $X$  by  $NO$ .

$NO$  has longer life time and is therefore influenced by the neutral winds. The lower boundary is given by photochemical equilibrium. The factors  $A$ ,  $B$ , and  $C$  for the equation solved in subroutine `minor`  $A \frac{d\Psi(N(^4S))}{dz} +$

$B\Psi(N(^4S)) + C = 0$  are

$$A = 0$$

$$B = 1.$$

$$C = \Psi(NO) = -\frac{n(NO)(z_{LB})m_{NO}k_B T_n(z_{LBC})}{p_0 e^{1/2\Delta z} e^{-z-1/2\Delta z} \bar{m}(z_{LBC})} \quad (5.168)$$

with  $n(NO)(z_{LB}) = 4 \cdot 10^6$ . At the upward diffusive flux at the upper boundary is set to zero

$$n(N(^4S))(z_{ubc}) = 0. \quad (5.169)$$

The production rate  $P$  of  $NO$  is

$$\begin{aligned} P(NO) = & (N\bar{m})^2 \frac{\Psi(O_2)}{m_{O_2}} \left( +\beta_2 \frac{\Psi(N(^2D))}{m_{N^2D}} \right) + \\ & (N\bar{m})^3 \beta_{17} \frac{\Psi(N_2)}{m_{N_2}} \frac{\Psi(N(^4S))}{m_{N^4S}} \end{aligned} \quad (5.170)$$

and the loss rate  $L$  of  $NO$  is

$$\begin{aligned} L(NO) = & -N\bar{m} \left[ \beta_3 \frac{\Psi(N(^4S))}{m_{N(^4S)}} + \beta_6 \frac{\Psi(N(^2D))}{m_{N(^2D)}} \right] - \frac{1}{2} (\beta_8(z) + \beta_8(z + \Delta z)) + \\ & \frac{1}{2} (\beta_9(z) + \beta_9(z + \Delta z)) - k_9 n(O_2^+) \frac{1}{2} (\beta_{9n}(z) + \beta_{9n}(z + \Delta z)) \end{aligned} \quad (5.171)$$

physical field	variable	unit	pressure level	timestep
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n$
electron density	$Ne$	$1/cm^3$	interfaces	$t_n$
number density $O^+$	$n(O^+)$	$1/cm^3$	midpoints	$t_n$
number density $N_2^+$	$n(N_2^+)$	$1/cm^3$	midpoints	$t_n$
number density $NO^+$	$n(NO^+)$	$1/cm^3$	midpoints	$t_n$
number density $NO$	$n(NO)$	$1/cm^3$	midpoints	$t_n$
number density $N(^4S)$	$n(N(^4S))$	$1/cm^3$	midpoints	$t_n$
number density $N^+$	$n(N^+)$	$1/cm^3$	midpoints	$t_n$

Table 5.11: Input fields to subroutine `comp_o2o`

physical field	variable	unit	pressure level	timestep
matrix coefficients for rhs?	$fs$	—	midpoints?	$t_n + \Delta t$

Table 5.12: Output fields of subroutine `comp_o2o`

## 5.5 Calculation of Major species $O_2$ , and $O$ /

,

### 5.5.1 Calculation of source and sinks for $O_2$ and $O$

The input to subroutine `comp_O2O` is summarized in table 5.11. The output of subroutine `comp_o2o` is summarized in table 5.12. The module data of subroutine `comp_o2o` is summarized in table 5.13. The source and sink terms for the neutral composition are calculated in this subroutine, and stored in the coefficient matrix  $fs$ , which is module data of `chemrates_module`.

Firstly, the total dissociation frequency and the production rates are

transferred from the interface level to the midpoint level.

$$\begin{aligned} rj(z + \frac{1}{2}\Delta z) &= \frac{1}{2}[rj(z) + rj(z + \Delta z)] \\ Q(O_2^+)(z + \frac{1}{2}\Delta z) &= \frac{1}{2}[Q(O_2^+)(z) + Q(O_2^+)(z + \Delta z)] \\ Q(O^+)(z + \frac{1}{2}\Delta z) &= \frac{1}{2}[Q(O^+)(z) + Q(O^+)(z + \Delta z)] \end{aligned} \quad (5.172)$$

The conversion factor  $N\overline{m}$  from number density to mass mixing ratio is evaluated at the midpoint level

$$N\overline{m}(z + \frac{1}{2}\Delta z) = \frac{p_0 e^{-z-1/2\Delta z}}{k_B T_n(z + 1/2\Delta z)} \left( \frac{\Psi(O_2)}{m_{O_2}} + \frac{\Psi(O)}{m_O} + \frac{\Psi(N_2)}{m_{N_2}} \right) \quad (5.173)$$

with  $\Psi(N_2) = 1 - \Psi(O_2) - \Psi(O)$ , and  $1/\overline{m}(z + \frac{1}{2}\Delta z) = \frac{\Psi(O_2)}{m_{O_2}} + \frac{\Psi(O)}{m_O} + \frac{\Psi(N_2)}{m_{N_2}}$ . The  $O_x$  production is

$$\begin{aligned} P(O_x) &= (N\overline{m})^2 \left[ \beta_3 \frac{n(N^4S)}{m_{N^4S}} \frac{n(NO)}{m_{NO}} + \beta_6 \frac{n(N^2D)}{m_{N^2D}} \frac{n(NO)}{m_{NO}} \right] + \\ &\quad \frac{1}{2}(\beta_8(z) + \beta_8(z + \Delta z)) \frac{n(NO)}{m_{NO}} N\overline{m}(z + \frac{1}{2}\Delta z) + \\ &\quad N\overline{m}(z + \frac{1}{2}\Delta z) \left[ k_4 n(O_2^+) \frac{n(N^4S)}{m_{N^4S}} + k_4 n(O^+) \frac{n(N^2D)}{m_{N^2D}} \right] + \\ &\quad \sqrt{Ne(z)Ne(z + \Delta z)} (a_1 n(NO^+) = 2a_2 n(O_2^+)) \end{aligned} \quad (5.174)$$

???? what is mass mixing ratio and what number density ??? and

$$\begin{aligned} P(O_{x2}) &= (N\overline{m})(z + \frac{1}{2}\Delta z) \left[ \beta_1 \frac{n(N^4S)}{m_{N^4S}} + \beta_2 \frac{n(N^2D)}{m_{N^2D}} \right] + \\ &\quad k_1 n(O^+) + k_7 n(N^+) + 2rj(z + \frac{1}{2}\Delta z) \end{aligned} \quad (5.175)$$

The  $O_x$  loss rates are

$$L(O_{x1}) = 2k_{m12} N\overline{m} \frac{1}{\frac{1}{2}(\overline{m}(z) + \overline{m}(z + \Delta z))} \quad (5.176)$$

$$L(O_{x2}) = k_3 n(N_2^+) + k_8 n(N^+) \quad (5.177)$$

$$L(O_{x3}) = Q(O^+)(z + \frac{1}{2}\Delta z) \quad (5.178)$$

The  $O_2$  production rates are

$$P(O_2)_1 = k_{m12} \frac{N\overline{m}(z + \frac{1}{2}\Delta z)}{\frac{1}{2}(\overline{m}(z) + \overline{m}(z + \Delta z))} \quad (5.179)$$

$$P(O_2)_2 = 0 \quad (5.180)$$

$$P(O_2)_3 = k_5 \frac{n(NO)}{m_{NO}} n(O_2^+) N\overline{m}(z + \frac{1}{2}\Delta z) \quad (5.181)$$

The  $O_2$  loss rates are

$$L(O_2)_1 = N\overline{m}(z + \frac{1}{2}\Delta z) \left[ \beta_1 \frac{n(N^4S)}{m_{N^4S}} + \beta_2 \frac{n(N^2D)}{m_{N^2D}} \right] + k_1 n(O^+) + (k_6 + k_7) n(N^+) + k_9 n(N_2^+) + rj \quad (5.182)$$

$$l(O_2)_2 = Q(O_2^+)(z + \frac{1}{2}\Delta z) \quad (5.183)$$

The coefficients of the matrix ( $fs$ ) are then

$$fs_{11} = -L(O_2) \quad (5.184)$$

$$fs_{12} = N\overline{m}(z + \frac{1}{2}\Delta z) P(O_2)_1 \frac{\Psi(O)}{m_O} \frac{m_{O_2}}{m_O} \quad (5.185)$$

$$fs_{21} = P(O_x)_2 \frac{m_O}{m_{O_2}} \quad (5.186)$$

$$fs_{22} = -L(O_x)_2 - L(O_x)_1 \frac{\Psi(O)}{m_O} N\overline{m}(z + \frac{1}{2}\Delta z) \quad (5.187)$$

$$fs_{10} = (P(O_2)_3 - L(O_2)_2) \frac{m_{O_2}}{N\overline{m}} \quad (5.188)$$

$$fs_{20} = (P(O_x)_1 - L(O_x)_3) \frac{m_O}{N\overline{m}} \quad (5.189)$$

$$(5.190)$$

### 5.5.2 Calculation of major species $O_2$ and $O$ / COMP.F

The input to subroutine `comp` is summarized in table 5.14. The output of subroutine `comp` is summarized in table 5.15. The module data of subroutine `comp` is summarized in table 5.16. The calculation of the composition is explained in [4] The major neutral constituents of the thermosphere

are  $O_2$ ,  $O$ , and  $N_2$ . The mass mixing ratio of these are

$$\Psi_i = n_i m_i \left( \sum_{j=1}^3 n_j m_j \right)^{-1} \quad (5.191)$$

with  $n_i$  the number density of the  $i$ th species, with  $i = 1, 2$ , and  $3$  corresponding to  $O_2$ ,  $O$ , and  $N_2$ . The molecular mass of the  $i$ th species is  $m_i$ . The vector of mass mixing ratios is defined by

$$\mathbf{\Psi} = \begin{pmatrix} \Psi_{O_2} \\ \Psi_O \end{pmatrix} \quad (5.192)$$

The  $N_2$  mass mixing ratio is determined by

$$\Psi_{N_2} = 1 - \Psi_{O_2} - \Psi_O \quad (5.193)$$

The coupled vector equation for the mass mixing ratio vector [4]

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{\Psi} = & -e^z \tau^{-1} \frac{\partial}{\partial z} \left[ \frac{\bar{m}}{m_{N_2} \left( \frac{T_{00}}{T_n} \right)^{0.25}} \alpha^{-1} \mathbf{L} \mathbf{\Psi} \right] + \\ & e^z \frac{\partial}{\partial z} \left( K(z) e^{-z} \frac{\partial}{\partial z} \mathbf{\Psi} \right) - \\ & \left( \mathbf{v}_n \cdot \nabla \mathbf{\Psi} + W \frac{\partial}{\partial z} \mathbf{\Psi} \right) + \mathbf{S} - \mathbf{R} \end{aligned} \quad (5.194)$$

with time  $t$ , the vertical coordinate  $z = \ln(p_0/p)$ , the pressure  $p$  and  $p_0$  the reference pressure. The diffusion time scale is  $\tau = (p_0 H_0 / p_{00} D_0) = 1.8610^3 s$ , with  $H_0$  the characteristic molecular nitrogen scale height at  $T_{00} = 273K$ ,  $p_{00} = 10^5 Pa$ , the characteristic diffusion coefficient at  $p_{00}$  and temperature  $T_{00}$  is  $D_0 = 210^{-5} m^2/s$ . The mean molecular mass is  $\bar{m}$ , the molecular mass of each species is  $m_i$ . The horizontal neutral velocity is  $\mathbf{v}_n$ , and the "vertical" velocity is  $W = \frac{dz}{dt}$ .  $K(z)$  is the eddy diffusion coefficient, the effective mass source is  $\mathbf{S}$ , and the removal rate is  $\mathbf{R}$ .

The matrix  $\alpha$  varies as the inverse of the diffusion coefficients according to

$$\begin{aligned} \alpha_{11} &= -[\phi_{13} + (\phi_{12} - \phi_{13})\Phi_2] \\ \alpha_{22} &= -[\phi_{23} + (\phi_{21} - \phi_{23})\Phi_1] \\ \alpha_{12} &= (\phi_{12} - \phi_{13})\Phi_1 \\ \alpha_{21} &= (\phi_{12} - \phi_{13})\Phi_2 \end{aligned} \quad (5.195)$$

where  $i = 1, 2$ , and  $3$  denotes  $O_2$ ,  $O$ , and  $N_2$  respectively. The value  $\phi_{ij}$  is determined by

$$\phi_{ij} = \frac{D}{D_{ij}} \frac{m_3}{m_j} \quad (5.196)$$

with  $D_{ij}$  is the mutual diffusion coefficient for gases  $i$  and  $j$  with  $D_{12}$ ,  $D_{13}$ ,  $D_{23}$ , and  $D_0$  being 0.26, 0.18, 0.26 [2], and  $0.2 \times 10^{-4} m^2/s$ , respectively.  $D$  is the characteristic diffusion coefficient, which has the same temperature and pressure dependence as  $D_{ij}$

$$D = D_0 \frac{P_{00}}{P} \left( \frac{P}{T_{00}} \right)^{1.75} \quad (5.197)$$

The matrix operator  $\mathbf{L}$  is diagonal with elements

$$\mathbf{L} = \delta_{ij} \left( \frac{\delta}{\delta z} - \epsilon_{ii} \right) \quad (5.198)$$

and

$$\epsilon_{ii} = 1 - \frac{m_i}{m} - \frac{1}{m} \frac{\partial}{\partial z} \quad (5.199)$$

The matrix  $\mathbf{L}$  defines diffusive equilibrium through  $\mathbf{L}\Phi = 0$ . at the upper boundary diffusive equilibrium is assumed, so that  $\mathbf{L}\Phi = 0$ . At the lower boundary the atomic oxygen concentration  $n(O)$  peaks, which was observed, and therefore it is assumed  $\partial n(O)/\partial z = 0$ . Together with the the conservation of total oxygen atoms, this assumption leads to the following condition at the lower boundary

$$\begin{aligned} \frac{\partial}{\partial z} \Psi_2 &= \Psi_2 \\ \Psi_1 + \Psi_2 &= constant \end{aligned} \quad (5.200)$$

In the source code in `comp.F` first the values  $\phi_{ij}$  from equation (5.195) are set

$$\begin{aligned} \phi_{21} &= \frac{0.2}{0.26} \frac{28}{32} = & 0.673 \\ \phi_{12} &= \frac{0.2}{0.26} \frac{28}{10} = & 1.35 \\ \phi_{13} &= \frac{0.2}{0.18} \frac{28}{28} = & 1.11 \\ \phi_{23} &= \frac{0.2}{0.26} \frac{28}{28} = & 0.769 \end{aligned} \quad (5.201)$$

The diffusive time scale  $\tau$  is set to  $1.86 \times 10^3 s$ , and the standard temperature  $T_{00} = 273K$ . A  $\delta$  matrix is set up as the identity matrix

$$\delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.202)$$

The horizontal advection term  $\mathbf{v}_n \cdot \nabla \Psi$  is determined in the **subroutine** **advec1** which is part of the file **comp.F**. The input to the **subroutine** **advec1** is the mass mixing ratios  $\Psi(O_2)^{t_n}$  and  $\Psi(O)^{t_n}$ , as well as the horizontal neutral velocities  $u_n$  and  $v_n$ .

$$\begin{aligned} \mathbf{v}_n \cdot \Psi_i = & \frac{1}{2} \frac{1}{R_e \cos \lambda} \left[ \frac{2}{3\Delta\phi} (\Psi_i(\phi + \Delta\phi, \lambda) - \Psi_i(\phi - \Delta\phi, \lambda)) \right. \\ & (u_n(\phi + \Delta\phi, \lambda) + u_n(\phi - \Delta\phi, \lambda)) - \\ & \frac{1}{12\Delta\phi} (\Psi_i(\phi + 2\Delta\phi, \lambda) - \Psi_i(\phi - 2\Delta\phi, \lambda)) (u_n(\phi + 2\Delta\phi, \lambda) + u_n(\phi - 2\Delta\phi, \lambda))] + \\ & \frac{1}{2} \frac{1}{R_e} \left[ \frac{2}{3\Delta\lambda} (\Psi_i(\phi, \lambda + \Delta\lambda) - \Psi_i(\phi, \lambda - \Delta\lambda)) (v_n(\phi, \lambda + \Delta\lambda) + v_n(\phi, \lambda - \Delta\lambda)) - \right. \\ & \left. \frac{1}{12\Delta\lambda} (\Psi_i(\phi, \lambda + 2\Delta\lambda) - \Psi_i(\phi, \lambda - 2\Delta\lambda)) (v_n(\phi, \lambda + \Delta\lambda) + v_n(\phi, \lambda - \Delta\lambda)) \right] \end{aligned} \quad (5.203)$$

for  $i = 1, 2$  which corresponds to  $O_2$  and  $O$ , respectively. The mass mixing ratios at timestep  $t_n - \Delta t$  are smoothed with a two part Shapiro smoother. The smoothing in latitude is

$$\begin{aligned} \Psi_i^{t-\Delta t, \lambda_s} = & \Psi_i^{t-\Delta t} - 0.03 \{ \Psi_i^{t-\Delta t}(\phi, \lambda + 2\Delta\lambda) + \Psi_i^{t-\Delta t}(\phi, \lambda - 2\Delta\lambda) - \\ & 4[\Psi_i^{t-\Delta t}(\phi, \lambda + \Delta\lambda) + \Psi_i^{t-\Delta t}(\phi, \lambda - \Delta\lambda) + 6\Psi_i^{t-\Delta t}(\phi, \lambda)] \} \end{aligned} \quad (5.204)$$

and afterwards a zonal smoothing is applied

$$\begin{aligned} \Psi_i^{t-\Delta t, smo} = & \Psi_i^{t-\Delta t, \lambda_s} - 0.03 \{ \Psi_i^{t-\Delta t, \lambda_s}(\phi + 2\Delta\phi, \lambda) + \Psi_i^{t-\Delta t, \lambda_s}(\phi - 2\Delta\phi, \lambda) - \\ & 4[\Psi_i^{t-\Delta t, \lambda_s}(\phi + \Delta\phi, \lambda) + \Psi_i^{t-\Delta t, \lambda_s}(\phi - \Delta\phi, \lambda) + 6\Psi_i^{t-\Delta t, \lambda_s}(\phi, \lambda)] \} \end{aligned} \quad (5.205)$$

for  $i = 1, 2$  which corresponds to  $O_2$  and  $O$ , respectively. The horizontal diffusion factor is set by

$$\begin{aligned} |\lambda| > 40^\circ & \quad d_{fac} = 0.25 + 1.0 \\ |\lambda| \leq 40^\circ & \quad d_{fac} = 0.25 + \frac{1}{2} \left( 1 + \sin\left(\frac{\Pi(|\lambda| - 20^\circ)}{40^\circ}\right) \right) \end{aligned} \quad (5.206)$$



If the input flag *DIFHOR* is set to zero, in the input file then  $d_{fac} = 0$ . The mean molecular mass  $\overline{m}$  is calculated at the midpoint level

$$\overline{m}(z + \frac{1}{2}\Delta z) = \left( \frac{\Psi(O_2)}{m_{O_2}} + \frac{\Psi(O)}{m_O} + \frac{\Psi(N_2)}{m_{N_2}} \right)^{-1} \quad (5.207)$$

with  $\Psi(N_2) = 1 - \Psi(O_2) - \Psi(O)$ . Note that the mass mixing ratios are also on the midpoint levels.

The lower boundary values for the mass mixing ratios are set by

$$\Psi_i(z_{LB}) = b(i, 1)\Psi(O_2)(z_{LB} + \frac{1}{2}\Delta z) + b(i, 2)\Psi(O)(z_{LB} + \frac{1}{2}\Delta z) + f_b(i) \quad (5.208)$$

for  $i = 1, 2$  which corresponds to  $O_2$  and  $O$ , respectively. The values  $b(i, 1)$ ,  $b(i, 2)$  and  $f_b(i)$  are set in the `boundary_module`. With the mass mixing ratios at the lower boundary the mean molecular mass can be determined at the lower boundary

$$\overline{m}(z_{LB}) = \left( \sum_{i=1}^3 \frac{\Psi_i(z_{LB})}{m_i} \right)^{-1} \quad (5.209)$$

for  $i = 1, 2$  and  $3$  which corresponds to  $O_2$ ,  $O$  and  $N_2$ , respectively. The term  $\frac{1}{\overline{m}} \frac{\partial \overline{m}}{\partial z}$  at the bottom is determined

$$wk_4 = \frac{1}{\overline{m}(z_{LB}) + \overline{m}(z_{LB} + \frac{1}{2}\Delta z)} \frac{\overline{m}(z_{LB} + \frac{1}{2}\Delta z) + \overline{m}(z_{LB})}{\Delta z} \quad (5.210)$$

???? where is the factor of  $1/2$  and  $1/2$  in  $wk_4$  which level. Is the LB below the LB level??????. The *epsilon* terms  $1 - \frac{1}{\overline{m}}[m_i + \frac{\partial \overline{m}}{\partial z}]$  are

$$\epsilon_i(k_m) = 1 - \frac{2}{\overline{m}(z_{LB}) + \overline{m}(z_{LB} + \frac{1}{2}\Delta z)} \left[ m_i + \frac{\overline{m}(z_{LB} + \frac{1}{2}\Delta z) - \overline{m}(z_{LB})}{\Delta z} \right] \quad (5.211)$$

for  $i = 1, 2$  which corresponds to  $O_2$  and  $O$ , respectively, and  $k_m = 2$ . The value

$$zz_1(k_m) = zz_1(k_m) = 0 \quad (5.212)$$

??? how does the algorithm goes?????. Next the matrix  $\alpha$  at the height level  $z + 0.25\Delta z$  is determined

$$\alpha_{1,1}^*(k_m) = \alpha_{22} = -\Delta_{11}[\phi_{2,3} + \{\phi_{2,1} - \phi_{2,3}\}] \frac{1}{2} \{ \Psi_1(z_{LB}) + \Psi_1(z_{LB} + \frac{1}{2}\Delta z) \} \quad (5.213)$$

$$\alpha_{1,2}^*(k_m) = -\alpha_{12} = [1 - \Delta_{12}][\phi_{1,2} - \phi_{1,3}] \frac{1}{2} \{ \Psi_1(z_{LB}) + \Psi_1(z_{LB} + \frac{1}{2}\Delta z) \} \quad (5.214)$$

$$\alpha_{2,2}^*(k_m) = \alpha_{11} = -\Delta_{22}[\phi_{1,3} + \{\phi_{1,2} - \phi_{1,3}\}] \frac{1}{2} \{ \Psi_2(z_{LB}) + \Psi_2(z_{LB} + \frac{1}{2}\Delta z) \} \quad (5.215)$$

$$\alpha_{2,1}^*(k_m) = -\alpha_{21} = [1 - \Delta_{22}][\phi_{2,2} - \phi_{2,3}] \frac{1}{2} \{ \Psi_2(z_{LB}) + \Psi_2(z_{LB} + \frac{1}{2}\Delta z) \} \quad (5.216)$$

Note, that the indices in the source code already take into account the inverse of the matrix with  $\alpha^{-1} = \alpha^*/\det|\alpha|$ , and therefore the diagonal values are switches and the off-diagonal terms have an minus sign. The determinant  $\det|\alpha|$  is the same as  $\det|\alpha^*(k_m)| = \alpha_{1,1}^*(k_m)\alpha_{2,2}^*(k_m) - \alpha_{1,2}^*(k_m)\alpha_{2,1}^*(k_m)$ . The matrix  $\alpha^*$  is multiplied by the factor  $\frac{1}{\tau} \frac{\overline{m}}{m_{N_2}} \left( \frac{T_{00}}{T_n} \right)^{0.25} \frac{1}{\det|\alpha^*|}$

$$wk_1 = \frac{1}{\tau} \frac{1}{2} [\overline{m}(z_{LB}) + \overline{m}(z_{LB} + \frac{1}{2}\Delta z)] \frac{1}{m_{N_2}} \left( \frac{T_{00}}{T_n(z_{LB})} \right)^{0.25} \frac{1}{\det|\alpha^*(k_m)|} \quad (5.217)$$

which lead to the quantity defined as  $A = \frac{1}{\tau} \frac{\overline{m}}{m_{N_2}} \left( \frac{T_{00}}{T_n} \right)^{0.25} \alpha^{-1}$ . The value  $\gamma$  at the bottom are set to

$$\gamma_{ij}(k=1) = 0. \quad (5.218)$$

for  $i = 1, 2$  and  $j = 1, 2$ , which corresponds to  $O_2$  and  $O$ , respectively.

After setting all the values at the bottom of the model, the height loops starts from the bottom to the top of the model ( $k = 1/z = -6.75$  to  $k =$

$nlev - 1/z = 6.75$ ). The *epsilon* terms  $1 - \frac{1}{\bar{m}}[m_i + \frac{\partial \bar{m}}{\partial z}]$  are set at  $z$  by

$$\epsilon_i(k_p) = 1 - \frac{2}{\bar{m}(z - \frac{1}{2}\Delta z) + \bar{m}(z + \frac{1}{2}\Delta z)} [m_i + \frac{\bar{m}(z + \frac{1}{2}\Delta z) - \bar{m}(z - \frac{1}{2}\Delta z)}{\Delta z}] \quad (5.219)$$

for  $i = 1, 2$  which corresponds to  $O_2$  and  $O$ , respectively, and  $k_p = 1$ . Note that before the value  $\epsilon_i(k_m)$  was determined, with  $k_m = 2$ . The values of  $k_m$  and  $k_p$  are alternating between 1 and 2 to get the values at the previous height level  $k_m = k - 1$ , and the height level  $k_p = k + 1$ . The  $\alpha$  is determined at  $k_p/z$  by

$$\alpha_{1,1}^*(k_p) = \alpha_{22} = -\Delta_{11}[\phi_{2,3} + \{\phi_{2,1} - \phi_{2,3}\}] \quad (5.220)$$

$$\frac{1}{2}\{\Psi_1(z - \frac{1}{2}\Delta z) + \Psi_1(z + \frac{1}{2}\Delta z)\}$$

$$\alpha_{1,2}^*(k_p) = -\alpha_{12} = [1 - \Delta_{12}][\phi_{1,2} - \phi_{1,3}] \quad (5.221)$$

$$\frac{1}{2}\{\Psi_1(z - \frac{1}{2}\Delta z) + \Psi_1(z + \frac{1}{2}\Delta z)\}$$

$$\alpha_{2,2}^*(k_p) = \alpha_{11} = -\Delta_{22}[\phi_{1,3} + \{\phi_{1,2} - \phi_{1,3}\}] \quad (5.222)$$

$$\frac{1}{2}\{\Psi_2(z - \frac{1}{2}\Delta z) + \Psi_2(z + \frac{1}{2}\Delta z)\}$$

$$\alpha_{2,1}^*(k_p) = -\alpha_{21} = [1 - \Delta_{22}][\phi_{2,2} - \phi_{2,3}] \quad (5.223)$$

$$\frac{1}{2}\{\Psi_2(z - \frac{1}{2}\Delta z) + \Psi_2(z + \frac{1}{2}\Delta z)\}$$

The matrix  $\alpha^*$  is multiplied by the factor  $\frac{1}{\tau} \frac{\bar{m}}{m_{N_2}} \left( \frac{T_{00}}{T_n} \right)^{0.25} \frac{1}{\det|\alpha^*|}$

$$wk_1 = \frac{1}{\tau} \frac{1}{2} [\bar{m}(z - \frac{1}{2}\Delta z) \bar{m}(z + \frac{1}{2}\Delta z)] \frac{1}{m_{N_2}} \left( \frac{T_{00}}{T_n(z)} \right)^{0.25} \frac{1}{\det|\alpha^*(k_p)|} \quad (5.224)$$

which lead to the quantity defined as  $A = \frac{1}{\tau} \frac{\bar{m}}{m_{N_2}} \left( \frac{T_{00}}{T_n} \right)^{0.25} \alpha^{-1}$ . The term  $\frac{1}{\bar{m}} \frac{\partial \bar{m}}{\partial z}$  at is determined, but first the value  $wk_4$  which holds the value for  $k_p/z$  is copied into  $wk_3$  which holds the value for  $k_m/z - \Delta z$ .

$$wk_4 = \frac{1}{\bar{m}(z - \frac{1}{2}\Delta z) + \bar{m}(z + \frac{1}{2}\Delta z)} \frac{\bar{m}(z + \frac{1}{2}\Delta z) + \bar{m}(z - \frac{1}{2}\Delta z)}{\Delta z} \quad (5.225)$$

???? where is the factor of 1/2 and 1/2 in  $wk_4$  which level. ???????.

The discretized equation can be written as

$$\mathbf{P}_k \Psi_{k-1}^{t_n+\Delta t} + \mathbf{Q}_k \Psi_k^{t_n+\Delta t} + \mathbf{R}_k \Psi_{k+1}^{t_n+\Delta t} = \mathbf{f}_k \quad (5.226)$$

with

$$P_k = \frac{A(k_m)}{\Delta z} \left( \frac{1}{\Delta z} + \frac{\epsilon(k_m)}{2} \right) - \frac{e^{-z} K(k_m)}{\Delta^2 z} - \frac{e^{-z} W(k)}{2\Delta z} \quad (5.227)$$

$$R_k = \frac{A(k_p)}{\Delta z} \left( \frac{1}{\Delta z} + \frac{\epsilon(k_p)}{2} \right) - \frac{e^{-z} K(k_p)}{\Delta^2 z} + \frac{e^{-z} W(k)}{2\Delta z} \quad (5.228)$$

$$Q_k = - \left[ \frac{A(k_m)}{\Delta z} \left( \frac{1}{\Delta z} - \frac{\epsilon(k_m)}{2} \right) \right. \\ \left. \frac{A(k_p)}{\Delta z} \left( \frac{1}{\Delta z} + \frac{\epsilon(k_p)}{2} \right) - \frac{e^{-z} K(k_m)}{\Delta^2 z} - \frac{e^{-z} K(k_p)}{\Delta^2 z} + JS e^{-z} - \frac{e^{-z}}{2\Delta t} \right] \quad (5.229)$$

$$f_k = e^{-z} \left[ \frac{\Psi^{t_n-\Delta t}(k)}{2\Delta t} - \mathbf{v}_n \cdot \nabla \Psi^{t_n}(k) \right] \quad (5.230)$$

In the source code the values are

$$P_k(i, j) = [A(k_m)(i, j) \left( \frac{1}{\Delta z} + \frac{\epsilon(k_m)(j)}{2} \right) \\ - e^{-(z+\frac{1}{2}\Delta z)} (e^{\frac{1}{2}\Delta z} K(k??z - \frac{1}{2}\Delta z) d_{fac}(\frac{1}{\Delta z} - wk_3) + \\ 0.25(W(z) + W(z + \Delta z))) \Delta(i, j)] \frac{1}{\Delta z} \quad (5.231)$$

$$R_k(i, j) = [A(k_p)(i, j) \left( \frac{1}{\Delta z} - \frac{\epsilon(k_p)(j)}{2} \right) \\ - e^{-(z+\frac{1}{2}\Delta z)} (e^{-\frac{1}{2}\Delta z} K(k + 1/z + \frac{1}{2}\Delta z) d_{fac}(\frac{1}{\Delta z} + wk_4) - \\ 0.25(W(z) + W(z + \Delta z))) \Delta(i, j)] \frac{1}{\Delta z} \quad (5.232)$$

$$\begin{aligned}
Q_k(i, j) = & -\frac{1}{\Delta z} [A(k_m)(i, j) \left( \frac{1}{\Delta z} - \frac{\epsilon(k_m)(j)}{2} \right) + A(k_p)(i, j) \left( \frac{1}{\Delta z} + \frac{\epsilon(k_p)(j)}{2} \right) \\
& + e^{-(z+\frac{1}{2}\Delta z)} (\{e^{\frac{1}{2}\Delta z} K(k+1/z + \frac{1}{2}\Delta z) (\frac{1}{\Delta z} - wk_4) - \\
& e^{-\frac{1}{2}\Delta z} K(k/z - \frac{1}{2}\Delta z) (\frac{1}{\Delta z} + wk_3)\} \frac{d_{fac}}{\Delta z} + \frac{1}{2\Delta t} \\
& ) \Delta(i, j) - fs(i, j)]
\end{aligned} \tag{5.233}$$

The right hand side is assembled in the following

$$f_k(i) = e^{-(z+\frac{1}{2}\Delta z)} \left[ \frac{\Psi_i^{t_n-\Delta t, smo}}{2\Delta t} - \mathbf{v}_n \cdot \nabla \Psi_i + f_{s,0}(i) + h_{d,i} \right] \tag{5.234}$$

for  $i = 1, 2$  corresponding to  $O_2$  and  $O$ , respectively.

At the lower boundary the coefficients are adjusted ??? what's the condition there???

$$Q_k^*(i, j)(z_{bot}) = Q_k(i, j)(z_{bot}) + P_k(i, 1)(z_{bot})b(1, j) + P_k(i, 2)(z_{bot})b(2, j) \tag{5.235}$$

with  $z_{bot} = -6.75$  or  $z_{bot} = z_{LB} + \frac{1}{2}\Delta z$ , and  $i = 1, 2$  and  $j = 1, 2$  corresponding to  $O_2$  and  $O$ , respectively. The updated right hand side is

$$f_k^*(i)(z_{bot}) = f_k(i)(z_{bot}) - P_k(i, 1)(z_{bot})fb(1) - P_k(i, 2)(z_{bot})fb(2) \tag{5.236}$$

with  $i = 1, 2$  corresponding to  $O_2$  and  $O$ , respectively.

At the upper boundary we set  $\frac{\partial}{\partial z} \Psi = \epsilon \Psi$  which leads to

$$\frac{\Psi(k+1) - \Psi(k)}{\Delta z} = \frac{\epsilon(z + \frac{1}{2}\Delta z)}{2} (\Psi(k+1) + \Psi(k)) \tag{5.237}$$

with  $k = nlev1 - 1$  and  $k+1 = nlev$  corresponding to  $z_{ub} - \frac{3}{2}\Delta z = 6.25$  and  $z_{ub} - \frac{1}{2}\Delta z = 6.75$ , respectively. The coefficient equation looks like

$$P_k \Psi(k-1) + [Q_k + R_k \frac{1 + 0.5\epsilon(k+1/2)\Delta z}{1 - 0.5\epsilon(k+1/2)\Delta z}] \Psi(k) = f_k \tag{5.238}$$

??? make matrix out of the equation????

$$Q_k^*(i, j)(z_{ub} - \frac{3}{2}\Delta z) = Q_k(i, j)(z_{ub} - \frac{3}{2}\Delta z) + \frac{1 + 0.5\epsilon(k + 1/2)\Delta z}{1 - 0.5\epsilon(k + 1/2)\Delta z} R_k(i, j)(z_{ub} - \frac{3}{2}\Delta z) \quad (5.239)$$

$$R_k^*(i, j)(z_{ub} - \frac{3}{2}\Delta z) = 0 \quad (5.240)$$

with  $i = 1, 2$  and  $j = 1, 2$  corresponding to  $O_2$  and  $O$ , respectively. For solving the equation the following values are needed ??? is this Newton iteration??? How does it work????

$$Q'_k(i, j) = Q_k(i, j) - P_k(i, 1) * \gamma(1, j)(k) - P_k(i, 2) * \gamma(2, j)(k) \quad (5.241)$$

$$wk_1 = \det|Q'_k| \quad (5.242)$$

$$wk_{m1}(1, j) = \frac{1}{wk_1} [\Delta(1, j)Q_k(2, 2) - (1 - \Delta(1, j))Q_k(1, j)] \quad (5.243)$$

$$wk_{m1}(2, j) = \frac{1}{wk_1} [\Delta(2, j)Q_k(1, 1) - (1 - \Delta(2, j))Q_k(2, j)] \quad (5.244)$$

$$wk_{v1}(i) = f_k(i) - \sum_{j=1}^2 P_k(i, j)zz(k)(j) \quad (5.245)$$

$$\gamma(k+1)(1, j) = \sum_{m=1}^2 wk_{m1}(1, m)R_k(m, j) \quad (5.246)$$

$$\gamma(k+1)(2, j) = \sum_{m=1}^2 wk_{m1}(2, m)R_k(m, j) \quad (5.247)$$

$$zz(k+1)(i) = \sum_{m=1}^2 wk_{m1}(i, m)wk_{v1}(m) \quad (5.248)$$

Hereby end the height loop from the bottom to the top of the model. The values at the top ( $k = nlev + 1$  or  $z_{UB} + \frac{1}{2}\Delta z = 7.25$ ) are set

$$\Psi_i^{t_n + \Delta t}(z_{UB} + \frac{1}{2}\Delta z) = 0 \quad (5.249)$$

with  $i = 1, 2$  corresponding to  $O_2$  and  $O$ , respectively. The updated value is

$$upd_i(z_{UB} + \frac{1}{2}\Delta z) = 0 \quad (5.250)$$

Then the downward sweep begins

$$upd_i(k) = zz(k+1)(i) \quad (5.251)$$

$$upd_i(k) = upd_i(k) - \sum_{j=1}^2 \gamma(k+1)(i, j) upd_j(k+1) \quad (5.252)$$

$$\Psi_i^{t_n+\Delta t}(k) = upd_i(k) \quad (5.253)$$

with  $k$  and  $k+1$  corresponding to  $z - \frac{1}{2}\Delta z$  and  $z + \frac{1}{2}\Delta z$ , respectively, and with  $i = 1, 2$  and  $j = 1, 2$  corresponding to  $O_2$  and  $O$ , respectively.

The upper boundary is set by

$$\Psi_i^{t_n+\Delta t}(lev1) = \frac{1 + 0.5\epsilon_i(k_p)\Delta z}{1 - 0.5\epsilon_i(k_p)\Delta z} \Psi_i^{t_n+\Delta t}(lev1 - 1) \quad (5.254)$$

with  $i = 1, 2$  and corresponding to  $O_2$  and  $O$ , respectively.

The calculated values for the mass mixing ratio  $\Psi_i^{upd,t+\Delta t}$  are smoothed by a Fast Fourier transformation. All the wave numbers larger than a predefined value at each latitude are removed. The wave numbers are defined in the module `cons.F`. The values of the mass mixing ratio at the timestep  $t_n$  are also updated by using

$$\Psi_i^{upd,t_n} = \frac{1}{2}(1 - c_{smo})(\Psi_i^{t_n-\Delta t} + \Psi_{i,smo}^{upd,t_n+\Delta t}) + c_{smo}\Psi_i^{t_n} \quad (5.255)$$

with  $c_{smo} = 0.95$ , and  $i = 1, 2$  and corresponding to  $O_2$  and  $O$ , respectively. Non negative values are assured by

$$\Psi_i^{upd,t_n} < 1 \times 10^{-6} \quad \Psi_i^{upd,t_n} = 1 \times 10^{-6} \quad (5.256)$$

$$\Psi_i^{upd,t_n+\Delta t} < 1 \times 10^{-6} \quad \Psi_i^{upd,t_n+\Delta t} = 1 \times 10^{-6} \quad (5.257)$$

$$1 - \sum_{i=1}^2 \Psi_i^{upd,t_n+\Delta t} < 1 \times 10^{-6} \quad \Psi_i^{upd,t_n+\Delta t} = \Psi_i^{upd,t_n+\Delta t} \frac{1 - 10^{-6}}{\sum_{i=1}^2 \Psi_i^{upd,t_n+\Delta t}} \quad (5.258)$$

$$1 - \sum_{i=1}^2 \Psi_i^{upd,t_n} < 1 \times 10^{-6} \quad \Psi_i^{upd,t_n} = \Psi_i^{upd,t_n} \frac{1 - 10^{-6}}{\sum_{i=1}^2 \Psi_i^{upd,t_n}} \quad (5.259)$$

physical field	variable	unit	module	timestep
inverse of molecular mass $O_2$	$1/m_{O_2}$	<i>mole/g</i>	cons	—
inverse of molecular mass $O$	$1/m_O$	<i>mole/g</i>	cons	—
inverse of molecular mass $N_2$	$1/m_{N_2}$	<i>mole/g</i>	cons	—
reference pressure	$p_0$	???	cons	—
-	$e^z$	—	cons	—
Boltzman constant	$k_B$	—	cons	—
molecular mass $NO$	$m_{NO}$	<i>g/mole</i>	cons	—
molecular mass $N(^4S)$	$m_{N^4S}$	<i>g/mole</i>	cons	—
molecular mass $N(^2D)$	$m_{N^2D}$	<i>g/mole</i>	cons	—
molecular mass $O_2$	$m_{O_2}$	<i>g/mole</i>	cons	—
molecular mass $O$	$m_O$	<i>g/mole</i>	cons	—
total $O_2$ dissociation frequency	$rj$	$1/s$	qrj	<i>interface</i>
$O_2^+$ production rate	$Q(O_2^+)$	??	qrj	<i>interface</i>
$O^+$ production rate	$Q(O^+)$	??	qrj	<i>interface</i>
chemical reaction rates	$k_i$	???	chemrates	—
chemical reaction rates	$\beta_i$	???	chemrates	—
chemical reaction rates	$a_i$	???	chemrates	—
coefficient matrix	$fs$	???	chemrates	—

Table 5.13: Module data used in subroutine `comp_o2o`



physical field	variable	unit	pressure level	timestep
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n$
mass mixing ratio $O_2$	$\Psi(O_2)$	—	midpoints	$t_n - \Delta t$
mass mixing ratio $O$	$\Psi(O)$	—	midpoints	$t_n - \Delta t$
neutral temperature	$T_n$	$K$	midpoints	$t_n$
neutral zonal velocity	$u_n$	$cm/s$	midpoints	$t_n$
neutral meridional velocity	$v_n$	$cm/s$	midpoints	$t_n$
neutral "vertical" velocity	$W$	$1/s$	interfaces	$t_n$
horizontal diffusion of $O_2$	$h_a(O_2)$	??	midpoints ???	$t_n$
horizontal diffusion of $O$	$h_d(O)$	??	midpoints ???	$t_n$

Table 5.14: Input fields to **subroutine comp**

physical field	variable	unit	pressure level	timestep
updated mass mixing ratio $O_2$	$\Psi(O_2)^{upd}$	—	midpoints	$t_n$
updated mass mixing ratio $O$	$\Psi(O)^{upd}$	—	midpoints	$t_n$
updated mass mixing ratio $O_2$	$\Psi(O_2)^{upd}$	—	midpoints	$t_n + \Delta t$
updated mass mixing ratio $O$	$\Psi(O)^{upd}$	—	midpoints	$t_n + \Delta t$

Table 5.15: Output fields of **subroutine comp**

physical field	variable	unit	module	timestep
inverse of molecular mass $O_2$	$1/m_{O_2}$	<i>mole/g</i>	cons	—
inverse of molecular mass $O$	$1/m_O$	<i>mole/g</i>	cons	—
inverse of molecular mass $N_2$	$1/m_{N_2}$	<i>mole/g</i>	cons	—
-	$e^{-z-\frac{1}{2}\Delta z}$	—	cons	—
-	$e^{-\frac{1}{2}\Delta z}$	—	cons	—
-	$e^{\frac{1}{2}\Delta z}$	—	cons	—
molecular mass $O_2$	$m_{O_2}$	<i>g/mole</i>	cons	—
molecular mass $O$	$m_O$	<i>g/mole</i>	cons	—
	$\Pi$	—	cons	—
	$\frac{1}{2\Delta t}$		cons	—
smoothing factor	$f_{smo} = 0.95$		cons	—
	$\frac{1}{2}(1 - 0.95)$		cons	—
background eddy diffusion	$d_k$		cons	—
wave filtering	$k_{ut5}$		cons	—
matrix coefficients with source and sinks	<b>fs</b>		chemrates	—

Table 5.16: Module data used in subroutine `comp`



## Chapter 6

# Ionospheric precesses

## 6.1 Joule heating calculation

For the Joule heating calculation we assume that the energy transfer  $\mathbf{J} \cdot \mathbf{E}$  is almost equal to  $\mathbf{J}_\perp \cdot \mathbf{E}$  since the electric field along the geomagnetic field  $\mathbf{B}$  is much smaller than the perpendicular component.  $\mathbf{J}_\perp$  is the current component perpendicular to the geomagnetic field. We neglect the work done by the Ampère Force, and focus on the Joule heating term  $\mathbf{J}_\perp \cdot \mathbf{E}'$ , with  $\mathbf{E}'$  the electric field in the frame of the neutral wind  $\mathbf{v}_n$ . We can substitute

$$\mathbf{J}_\perp \cdot \mathbf{E}' = \sigma_P \mathbf{E}'^2 \quad (6.1)$$

with  $\sigma_P$  denoting the Pederson conductivity. The square of the electric field can be written as

$$\mathbf{E}'^2 = B^2 \left( \frac{\mathbf{E} \times \mathbf{B}}{B^2} - \mathbf{v}_{n\perp} \right)^2 \quad (6.2)$$

with the electrodynamic drift velocity  $\mathbf{v}_{ExB}$  which is  $\frac{\mathbf{E} \times \mathbf{B}}{B^2}$ , and  $\mathbf{v}_{n\perp}$  is the neutral component perpendicular to the geomagnetic field. In the code we substitute  $\sigma_P B^2$  by  $\lambda_1 = \frac{\sigma_P B^2}{\rho}$  with  $\rho$  the atmospheric mass density, therefore we calculate

$$Q_J = \frac{\mathbf{J}_\perp \cdot \mathbf{E}'}{\rho} = \lambda_1 (\mathbf{v}_{ExB} - \mathbf{v}_{n\perp})^2 \quad (6.3)$$

with  $Q_J$  the energy rate per mass [erg/s/g] from Joule heating.

The Joule heating is added to the equation to solve for the ion and neutral temperature, see chapter 4.2 and 6.3.

In the heat equation for the neutrals there is no explicit term for the energy transfer from the ion to the neutrals, since we assume that eventually the whole Joule heating will go into the neutral temperature.

$$Q_J^{T_n} = \lambda_1 (\mathbf{v}_{ExB} - \mathbf{v}_{n\perp})^2 \quad (6.4)$$

We refer to [18] eq. 5.48d, which is part of the transport equation for the high latitude E-region

$$0 = \sum_n \frac{\nu_{in}}{m_i + m_n} [3k(T_n - T_i) + m_n(\mathbf{v}_i - \mathbf{v}_n)^2] \quad (6.5)$$

??? check with book what the values are Sum over what n???? This equation assumes that we have monotonic particles, such that we only have kinetic, and no rotational, energy. In the above equation the collision frequency  $\nu_{in}$  instead of the ion drag coefficient is used, since it also uses the difference in velocity between the ion and neutrals  $\mathbf{v}_i - \mathbf{v}_n$ , instead of only the  $\mathbf{E} \times \mathbf{B}$  drift velocity.

According to [18] only part of the Joule heating contributes to the ion temperature

$$Q_J^{T_i} = \frac{\overline{m}_n}{\overline{m}_n + \overline{m}_i} \lambda_1 (\mathbf{v}_{ExB} - \mathbf{v}_{n\perp})^2 \quad (6.6)$$

This approximation is valid above approx. 100 km where the contributions from the electron neutral collisions to the Pedersen conductivity  $\sigma_P$  is small. Only around 75 km we would have to consider also the Joule heating part which goes into the electron temperature. However, since the contribution from the electrons is small, we can justify using  $\lambda_1$  which is based on the Pedersen conductivity including the electron neutral collisions.

### 6.1.1 Joule heating calculation for ion temperature

The input to subroutine `qjoule_ti` is summarized in table 6.1. The output of subroutine `qjoule_ti` is summarized in table 6.2. The mean molecular mass of the ions  $\overline{m}_{ion}$  at the midpoints in [g/mol] is calculated by

$$\overline{m}_{ion} = \frac{N_{O^+}m_O + N_{O_2^+}m_{O_2} + N_{N^+}m_{N^{4s}} + N_{N_2^+}m_{N_2} + N_{NO^+}m_{NO}}{N_{O^+} + N_{O_2^+} + N_{N^+} + N_{N_2^+} + N_{NO^+}} \quad (6.7)$$

and the mean molecular mass of the neutrals  $\overline{m}_n$  at the midpoints in [g/mol] is

$$\overline{m}_n(z + \frac{1}{2}\Delta z) = 0.5 * (\overline{m}_n(z) + \overline{m}_n(z + \Delta z)) \quad (6.8)$$

with  $\overline{m}_n$  on the interface level with  $z$  correspond to the height index  $k$ ,  $z + \Delta z$  to  $k + 1$ , and on the midpoint level  $z + \frac{1}{2}\Delta z$  correspond to the height index  $k$ . The scale height  $H$  [cm] at midpoints is

$$H = \frac{R^*T_n}{\overline{m}_ng} \quad (6.9)$$

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoint	$t_n$
mean molecular mass	$\overline{m}$	$\frac{g}{mole}$	interface	$t_{n+1}$
mass mixing ration of $O_2$	$\Psi_{O_2}$	mmr	midpoint	$t_n$
number density of ions	$N_{O_2^+}$	$1/cm^3$	midpoint	$t_n$
	$N_{O^+}$	$1/cm^3$	midpoint	$t_n$
	$N_{NO^+}$	$1/cm^3$	midpoint	$t_n$
	$N_{N^+}$	$1/cm^3$	midpoint	$t_n$
ion drag coefficient (mag.east.)	$\lambda_1$	$1/s$	interface	$t_n$
$\mathbf{E} \times \mathbf{B}$ velocity	$\mathbf{v}_{ExB}$	$cm/s$	interface	$t_n$
dimensionless vertical velocity	$W$	$1/s$	interface	$t_n$
neutral velocity	$\mathbf{v}_n$	$cm/s$	midpoints	$t_n$

Table 6.1: Input fields to subroutine `qjoule_ti`

physical field	variable	unit	pressure level	timestep
Joule heating of ion temperature	$Q_J^{T_i}$	$\frac{ergs}{sg}$	midpoints	$t_n$ $t_{n+1}$

Table 6.2: Output fields of subroutine `qjoule_ti`

since  $T_n$  and  $\overline{m}_n$  are on the midpoint level. Note that the gas constant  $R^*$  is in units of [erg/K/mol] and the mean molecular mass in units of [g/mol]. The vertical neutral velocity  $w$  in [cm/s] is

$$w = WH \quad (6.10)$$

with the dimensionless vertical velocity  $W$ . The dimensionless vertical velocity at the midpoints is determined by averaging the values at the height level  $k$  and  $k+1$  to get the midpoint level  $k$ , i.e.  $W(z+\frac{1}{2}) = 0.5[W(z)+W(z+\Delta z)]$ . The  $\mathbf{E} \times \mathbf{B}$  drift velocity  $\mathbf{v}_{ExB}$  in [cm/s] at the midpoints is  $\mathbf{v}_{ExB}(z+\frac{1}{2}\Delta z) = 0.5(\mathbf{v}_{ExB}(z) + \mathbf{v}_{ExB}(z + \Delta z))$ , and the ion drag coefficient in magnetic eastward direction  $\lambda_1$  in [1/s] is averaged in the same way to get the midpoint

variable	physical name	value
$N_A$	Avogadro number	$6.023 \times 10^{23} \# / mol$
$g$	gravitational acceleration at lower boundary	$cm^2 / s$
$R^*$	gas constant	$8.314 \times 10^7 erg / K / mol$
$m_i$	molecular weight species i	$g / mol$

Table 6.3: Global parameters used in subroutine `qjoule_ti`

values.

The Joule heating in [ergs/s/g] which goes into the ion temperature is

$$Q_J^{T_i} = \frac{\bar{m}_n}{\bar{m}_n + \bar{m}_{ion}} \lambda_1 (\mathbf{v}_{ExB} - \mathbf{v}_n)^2 \quad (6.11)$$

In subroutine `qjoule_tn` the Joule heating for the neutral temperature is calculated. Since the calculation is the same as for the Joule heating for the ion temperature we refer to the previous subsection. The Joule heating for the neutral temperature doesn't have the ratio of the mean molecular mass of ion to ion plus neutral. Since we have no explicit heating term for the energy transfer from ions to neutrals.

$$Q_J^{T_n} = \lambda_1 (\mathbf{v}_{ExB} - \mathbf{v}_n)^2 \quad (6.12)$$



physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoint	$t_n$
mean molecular mass	$\overline{m}$	$\frac{g}{mole}$	interface	$t_{n+1}$
mass mixing ration of molecular oxygen	$\Psi_{O_2}$	-	midpoint	$t_n$
mass mixing ration of atomic oxygen	$\Psi_O$	-	midpoint	$t_n$
ion temperature	$T_i$	K	midpoint	$t_n$
electron temperature	$T_e$	K	midpoint	$t_n$
number density of ions	$N_{O_2^+}$	$1/cm^3$	midpoint	$t_n$
	$N_{O^+}$	$1/cm^3$	midpoint	$t_n$
	$N_{NO^+}$	$1/cm^3$	midpoint	$t_n$

Table 6.4: Input fields to subroutine lamdas

## 6.2 Ion drag calculation /

The input to subroutine lamdas is summarized in table 6.4.

The output of subroutine lamdas is summarized in table 6.5. First the factor

$$\frac{q_e}{B} \text{ in } \left[ \frac{C}{T} \frac{cm^3}{m^3} \right] \quad (6.13)$$

is calculated. The gyro frequencies  $\Omega$  in units of  $[\frac{CT}{kg}]$  are

$$\Omega_{O^+} = \frac{q_e B}{N_a m_{O^+}} \quad (6.14)$$

$$\Omega_{O_2^+} = \frac{q_e B}{N_a m_{O_2^+}} \quad (6.15)$$

$$\Omega_{NO^+} = \frac{q_e B}{N_a m_{NO^+}} \quad (6.16)$$

$$\Omega_e = \frac{q_e B}{m_e} \quad (6.17)$$

physical field	variable	unit	pressure level	timestep
ion drag coefficients				
geographic direction	$\lambda_{xx}, \lambda_{yy}, \lambda_{xy}, \lambda_{yx}$	$1/s$	interface	$t_n$
magnetic east. direction	$\lambda_1$	$1/s$	interface	$t_n$
conductivities	$\sigma_H, \sigma_P$	$S/m$	midpoint	$t_n$

Table 6.5: Output fields of subroutine `lamdas`

variable	physical name	value
$q_e$	electron charge	$1.602 \times 10^{-19}C$
$\frac{q_e}{10m_e}$		$1.7588028 \times 10^7 C/g$
$\frac{q_e}{10N_a}$		$9.6489 \times 10^3 C/mol$
$m_{NO^+}$	molecular weight of $NO^+$	$30g/mol$

Table 6.6: Local parameters used in subroutine `lamdas`

The collision frequencies  $\nu$  in units of  $[s^{-1}]$  are determined by, e.g. [18]

$$\frac{1}{N_{O_2}}\nu_{O_2^+-O_2} = 2.59 \times 10^{-11} \sqrt{\frac{T_i + T_e}{2}} \left[ 1 - 0.73 \log_{10} \sqrt{\frac{T_i + T_e}{2}} \right]^2 \quad (6.18)$$

$$\frac{1}{N_{O_2}}\nu_{O^+-O_2} = 6.64 \times 10^{-10} \quad (6.19)$$

$$\frac{1}{N_{O_2}}\nu_{NO^+-O_2} = 4.27 \times 10^{-10} \quad (6.20)$$

$$\frac{1}{N_O}\nu_{O^+-O} = 3.67 \times 10^{-11} \sqrt{\frac{T_i + T_e}{2}} \left[ 1 - 0.73 \log_{10} \sqrt{\frac{T_i + T_e}{2}} \right]^2 f_{cor} \quad (6.21)$$

$$\frac{1}{N_O}\nu_{NO^+-O} = 2.44 \times 10^{-10} \quad (6.22)$$

$$\frac{1}{N_O}\nu_{O_2^+-O} = 2.31 \times 10^{-10} \quad (6.23)$$

$$\frac{1}{N_{N_2}}\nu_{O_2^+-N_2} = 4.13 \times 10^{-10} \quad (6.24)$$

$$\frac{1}{N_{N_2}}\nu_{NO^+-N_2} = 4.34 \times 10^{-10} \quad (6.25)$$

$$\frac{1}{N_{N_2}}\nu_{O^+-N_2} = 6.82 \times 10^{-10} \quad (6.26)$$

with  $N_n$  the number density for the neutral n in units of  $[1/cm^3]$ , and the temperature in  $[K]$ . The collisions frequencies for  $\nu_{O_2^+-O_2}$  and  $\nu_{O^+-O}$  are resonant, all other are nonresonant. The Burnsideactor  $f_{cor}$  multiplies the  $\nu_{O^+-O}$  collision frequency and is set to  $f_{cor} = 1.5$  which has been found to improve agreement between calculated winds and electron densities in the upper thermosphere in other models. The mean mass  $\bar{m}_{mid}$  in  $[g/mole]$  at the midpoints of the height level is calculated by

$$N\bar{m}_{mid} = \frac{p_o e^{-Z} \bar{m}_{mid}}{k_B T_n} \quad (6.27)$$

The total number density  $N$  is in units of  $[1/cm^3]$ ,  $p_o e^{-Z}$  is the pressure at the midpoints in  $[dyn/cm^2]$  with  $Z$  the dimensionless variable at midpoints. The mean molecular weight at midpoints is averaged by  $\bar{m}_{mid}(z + \frac{1}{2}\Delta z) = 0.5 * (\bar{m}(z) + \bar{m}(z + \Delta z))$  with the height index on the interface level  $k$  corresponds to  $z$ ,  $k + 1$  to  $z + \Delta z$ , and on the midpoint level corresponds  $z + \frac{1}{2}\Delta z$  to the  $k$  index level. The Boltzmann constant is denoted by  $k_B$  in  $[erg/K]$  and the neutral temperature  $T_n$  is in units of  $[K]$ .

The number densities in  $[1/cm^3]$  are

$$N_{O_2} = \frac{N\bar{m}_{mid}\Psi_{O_2}}{m_{O_2}} \quad (6.28)$$

$$N_O = \frac{N\bar{m}_{mid}\Psi_O}{m_O} \quad (6.29)$$

$$N_{N_2} = \frac{N\bar{m}_{mid}\Psi_{N_2}}{m_{N_2}} \quad (6.30)$$

with  $\Psi$  the mass mixing ration. The mass mixing ratio of  $N_2$  is determined by  $\Psi_{N_2} = 1 - \Psi_{O_2} - \Psi_O$  with  $\frac{\Psi_{N_2}}{m_{N_2}} \geq 1. \times 10^{-20} \frac{mol}{g}$ .

The collision frequencies in  $[1/s]$  are

$$\nu_{O_2^+} = \nu_{O_2^+-O_2} + \nu_{O_2^+-O} + \nu_{O_2^+-N_2} \quad (6.31)$$

$$\nu_{O^+} = \nu_{O^+-O_2} + \nu_{O^+-O} + \nu_{O^+-N_2} \quad (6.32)$$

$$\nu_{NO^+} = \nu_{NO^+-O_2} + \nu_{NO^+-O} + \nu_{NO^+-N_2} \quad (6.33)$$

$$\begin{aligned} \nu_{en} = & 2.33 \times 10^{-11} N_{N_2} T_e (1 - 1.21 \times 10^{-4} T_e) + \\ & 1.82 \times 10^{-10} N_{O_2} \sqrt{T_e} (1 + 3.6 \times 10^{-2} \sqrt{T_e}) + \\ & 8.9 \times 10^{-11} N_O \sqrt{T_e} (1 + 5.7 \times 10^{-4} T_e) \end{aligned} \quad (6.34)$$

The ratios  $r$  between collision frequency  $\nu$  and gyro frequency  $\Omega$  are

$$r_{O_2^+} = \frac{\nu_{O_2^+}}{\Omega_{O_2^+}} \quad (6.35)$$

$$r_{O^+} = \frac{\nu_{O^+}}{\Omega_{O^+}} \quad (6.36)$$

$$r_{NO^+} = \frac{\nu_{NO^+}}{\Omega_{NO^+}} \quad (6.37)$$

$$r_e = \frac{\nu_{en}}{\Omega_e} \quad (6.38)$$

with the gyro frequency for ions  $\Omega_i = eB/m_i$  and for electrons  $\Omega_e = eB/m_e$ . The Pedersen conductivity in  $[S/m]$  is

$$\begin{aligned} \sigma_P = \frac{e}{B} [ & N_{O^+} \frac{r_{O^+}}{1 + r_{O^+}^2} + N_{O_2^+} \frac{r_{O_2^+}}{1 + r_{O_2^+}^2} + \\ & N_{NO^+} \frac{r_{NO^+}}{1 + r_{NO^+}^2} + N_e \frac{r_e}{1 + r_e^2} ] \end{aligned} \quad (6.39)$$

The Hall conductivity in  $[S/m]$  is

$$\begin{aligned} \sigma_H = \frac{e}{B} [ & -N_{O^+} \frac{1}{1 + r_{O^+}^2} - N_{O_2^+} \frac{1}{1 + r_{O_2^+}^2} - \\ & N_{NO^+} \frac{1}{1 + r_{NO^+}^2} + N_e \frac{1}{1 + r_e^2} ] \end{aligned} \quad (6.40)$$

with  $N_e = N_{O^+} + N_{O_2^+} + N_{NO^+}$  assuming charge equilibrium. The ion drag coefficients are in magnetic eastward and magnetic northward direction

$$\lambda_1 = \frac{\sigma_P B^2}{\rho} \quad (6.41)$$

$$\lambda_2 = \frac{\sigma_H B^2}{\rho} \quad (6.42)$$

with  $\rho = \frac{\bar{m}}{N_A}$ , and  $N_A$  the Avagadro number. The ion drag coefficients are transferred to interfaces by

$$\lambda_1(z) = \sqrt{\lambda_1(z + \frac{1}{2}\Delta z) * \lambda_1(z - \frac{1}{2}\Delta z)} \quad (6.43)$$

$$\lambda_2(z) = \sqrt{\lambda_2(z + \frac{1}{2}\Delta z) * \lambda_2(z - \frac{1}{2}\Delta z)} \quad (6.44)$$

with the height index  $k$  at the  $z$  interface level, and  $k + 1$  at  $z + \Delta z$ . On the midpoint level the index  $k$  corresponds to  $z + \frac{1}{2}\Delta z$ . For the top and bottom boundary the values are calculated by

$$\lambda_1(z_{top}) = \sqrt{\lambda_1^3(z_{top} - \frac{1}{2}\Delta z) / \lambda_1(z_{top} - \frac{3}{2}\Delta z)} \quad (6.45)$$

$$\lambda_2(z_{top}) = \sqrt{\lambda_2^3(z_{top} - \frac{1}{2}\Delta z) / \lambda_2(z_{top} - \frac{3}{2}\Delta z)} \quad (6.46)$$

$$\lambda_1(z_{bot}) = \sqrt{\lambda_1^3(z_{bot} + \frac{1}{2}\Delta z) / \lambda_1(z_{bot} + \frac{3}{2}\Delta z)} \quad (6.47)$$

$$\lambda_2(z_{bot}) = \sqrt{\lambda_2^3(z_{bot} + \frac{1}{2}\Delta z) / \lambda_2(z_{bot} + \frac{3}{2}\Delta z)} \quad (6.48)$$

with  $z_{top}$  on the interface level corresponds to the index  $nlev$ , and  $z_{top} - \frac{1}{2}\Delta z$  is on the midpoint level and has the index  $nlev - 1$ . At the bottom boundary  $z_{bot}$  corresponds to the index 1 on the interface level, and  $z_{bot} + \frac{1}{2}\Delta z$  corresponds to the index 1 on the midpoint level. The ion drag tensor in magnetic direction  $\underline{\lambda}^{mag}$  is

$$\underline{\lambda}^{mag} = \begin{pmatrix} \lambda_{xx}^{mag} & \lambda_{xy}^{mag} \\ \lambda_{yx}^{mag} & \lambda_{yy}^{mag} \end{pmatrix} = \begin{pmatrix} \lambda_1 & \lambda_2 \sin I \\ -\lambda_2 \sin I & \lambda_1 \sin^2 I \end{pmatrix} \quad (6.49)$$

with the x-direction in magnetic east, and y-direction magnetic south in the northern hemisphere. The inclination of the geomagnetic field lines is  $I$ . Note that in the code the value of  $\lambda_{yx}$  has a sign change, however the value is not used. The ion drag tensor can be rotated in geographic direction by using the rotation matrix  $\mathbf{R}$

$$\mathbf{R} = \begin{pmatrix} \cos D & \sin D \\ -\sin D & \cos D \end{pmatrix} \quad (6.50)$$

with the declination  $D$  of the geomagnetic field. Applying the rotation to the ion drag tensor  $\mathbf{R}\underline{\lambda}^{mag}\mathbf{R}^{-1}$  leads to

$$\Lambda = \begin{pmatrix} \lambda_{xx} & \lambda_{xy} \\ \lambda_{yx} & \lambda_{yy} \end{pmatrix} = \quad (6.51)$$

$$\begin{pmatrix} \lambda_{xx}^{mag} \cos^2 D + \lambda_{yy}^{mag} \sin^2 D & \lambda_{xy}^{mag} + (\lambda_{yy}^{mag} - \lambda_{xx}^{mag}) \sin D \cos D \\ -\lambda_{xy}^{mag} + (\lambda_{yy}^{mag} - \lambda_{xx}^{mag}) \sin D \cos D & \lambda_{yy}^{mag} \cos^2 D + \lambda_{xx}^{mag} \sin^2 D \end{pmatrix} \quad (6.52)$$

Note that in the code  $\lambda_{yx}$  has a reversed sign, and is later, in the Joule heating calculation, used in the code as  $-\lambda_{yx}^{code}$ .

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
mass mixing ratio $O_2$	$\Psi_{O_2}$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi_O$	—	midpoints	$t_n$
mean molecular mass	$\overline{m}$	$g/mol$	interfaces	$t_n + \Delta t$
Joule heating of ions	$Q_{J,T_i}$	$\frac{erg}{K\ s}$	midpoints	$t_n$
electron density	$N_e$	$\#/cm^3$	interfaces	$t_n$
electron temperature	$T_e$	$K$	midpoints	$t_n$
ion temperature	$T_i$	$K$	midpoints	$t_n$
number density $O^+$	$N_{O^+}$	$\#/cm^3$	interfaces	$t_n?$
number density $O_2^+$	$N_{O_2^+}$	$\#/cm^3$	interfaces	$t_n?$
number density $NO^+$	$N_{NO^+}$	$\#/cm^3$	interfaces	$t_n?$

Table 6.7: Input fields to subroutine `setei`

## 6.3 Calculation of electron and ion temperature /

The input to subroutine `settei` is summarized in table 6.7. The output of subroutine `settei` is summarized in table 6.8. The module data of subroutine `settei` is summarized in table 6.9. The general energy conservation equation without chemical and viscous heating of electron gas

$$\frac{3}{2}N_e k_B \frac{\partial T_e}{\partial t} = -N_e k_B T_e \nabla \cdot \mathbf{u}_e - \frac{3}{2}N_e k_B \mathbf{u}_e \cdot T_e - \nabla \cdot q_e + \sum Q_e - \sum L_e \quad (6.53)$$

with the electron bulk velocity  $\mathbf{u}_e$ , the electron heat flow vector  $q_e$ , the sum of all local electron heating rates are  $\sum Q_e$ , and the sum of all local cooling

physical field	variable	unit	pressure level	timestep
electron temperature	$T_e^{t_n+\Delta t}$	$K$	midpoints	$t_n + \Delta t$
ion temperature	$T_i^{t_n+\Delta t}$	$K$	midpoints	$t_n + \Delta t$

Table 6.8: Output fields of subroutine `settei`

physical field	variable	unit	pressure level	timestep

Table 6.9: Module data of subroutine `settei`

rates are  $\sum L_e$ . The electron heat vector is

$$q_e = -\beta_e \mathbf{J} - K^e \nabla T_e \quad (6.54)$$

with  $\beta_e$  is the thermalelectric transport coefficient,  $\mathbf{J}$  is the electric current, and  $K^e$  is the electron thermal conductivity which is

$$K^e = \frac{7.5 \cdot 10^5 T_e^{2.5}}{1 + 3.22 \cdot 10^4 \frac{T_e^2}{N_e} (d_1 N_{N_2} + d_2 N_{O_2} + d_3 N_O)} \quad (6.55)$$

we assume that  $\mathbf{J}$  and  $q_e$  are parallel to the magnetic field and  $T_e$  and  $N_e$  vary only in vertical direction. In addition it's assumed that field aligned current is not present so that adiabatic expansion and heat advection can be omitted. With these assumptions the general electron energy conservation equation is simplified to

$$\frac{3}{2} N_e k_B \frac{\partial T_e}{\partial t} = \sin^2 I \frac{\partial}{\partial Z} \left( K^e \frac{\partial T_e}{\partial Z} \right) + \sum Q_e - \sum L_e \quad (6.56)$$

In the high range of the model the time scales are very short such that the time derivative can be neglected and a thermal quasi steady state can be assumed

$$\sin^2 I \frac{\partial}{\partial Z} \left( K^e \frac{\partial T_e}{\partial Z} \right) + \sum Q_e - \sum L_e = 0 \quad (6.57)$$

The heating sources are solar EUV radiation, deactivation of excited neutral and ion species, dissociative recombination of electrons with ions, energetic

particle precipitation, and Joule heating. Only the solar EUV radiation and the energetic particle precipitation are considered, all other contributions are neglectable small.

We substitute

$$K^e = K^0 T_e^{5/2} \quad (6.58)$$

$$L_e = L_{on}(T_e - T_n) + L_{oi}(T_e - T_i) \quad (6.59)$$

with  $G = T_e^{7/2}$  the derivative is

$$\frac{\partial G}{\partial Z} = \frac{7}{2} T_e^{5/2} \frac{\partial T_e}{\partial Z} \quad (6.60)$$

and, therefore

$$\frac{K^e}{H} \frac{\partial T_e}{\partial Z} = \frac{2}{7} \frac{K^0}{H} \frac{\partial G}{\partial Z} \quad (6.61)$$

and the loss terms are

$$L_e = \frac{L_{on} + L_{oi}}{T_e^{5/2}} G - L_{on} T_n - L_{oi} T_i \quad (6.62)$$

The energy conservation equation reads

$$\sin^2 I \frac{\partial}{\partial Z} \left( \frac{2}{7} \frac{K^0}{H} \frac{\partial G}{\partial Z} \right) - \left( \frac{L_{on} + L_{oi}}{T_e^{5/2}} \right) G = -L_{on} T_n - L_{oi} T_i - Q_e \quad (6.63)$$

The heat flux from the topside ionosphere is  $F_e$  with

$$F_{eD} = F_{10.7}^* 1.2 [-5 \cdot 10^7 A - 4 \cdot 10^7] \quad (6.64)$$

for the daytime, and for the nighttime

$$F_{eD} = \frac{F_e D}{2} \quad (6.65)$$

with  $F_{10.7}^* = F_{10.7}$  and  $F_{10.7}^* \leq 235$ . The factor A is set to

$$\text{for } |\lambda_m| \geq 40^\circ \quad A = 1 \quad (6.66)$$

$$\text{for } |\lambda_m| < 40^\circ \quad A = \frac{1}{2} [1 + \sin(\Pi \frac{|\lambda_m| - 20}{40})] \quad (6.67)$$



The aurora contribution is added

$$F_{eDA} = F_{eD} + Q_{aurora} \quad (6.68)$$

$$F_{eNA} = F_{eN} + Q_{aurora} \quad (6.69)$$

For solar zenith angles  $\psi \geq 90^\circ$  the flux is  $F_e = F_{eNA}$ , and for  $\psi < 90^\circ$  the flux is  $F_e = F_{eDA}$

$$\text{for } 80^\circ < \psi < 100 \quad F_e = \frac{1}{2}(F_{eDA} + F_{eNA}) + \frac{1}{2}(F_{eDA} - F_{eNA}) \cos\left(\Pi \frac{\psi - 80}{20}\right) \quad (6.70)$$

$$\text{for } \psi \leq 80 \text{ or } \psi \geq 100 \quad F_e \quad (6.71)$$

For  $|\lambda_m| > 60^\circ$  a polar contribution is added  $Q_{aurora} = 3 \cdot 10^9$ . The values of the neutral temperature  $T_n$ , the mass mixing ratio  $\Psi_{O_2}$  and  $\Psi_O$ , and the electron temperature  $T_e$  at the interfaces are calculated by averaging the values from the height level  $z + \frac{1}{2}\Delta z$  and  $z - \frac{1}{2}\Delta z$  to get the value at the level  $z$ , with the height index  $k$  corresponding to  $z$ , and  $k$  and  $k+1$  corresponding to  $z - \frac{1}{2}\Delta z$  and  $z + \frac{1}{2}\Delta z$  respectively on the midpoint level; e.g. for the electron temperature

$$T_e(z) = \frac{1}{2}(T_e(z + \frac{1}{2}\Delta z) + T_e(z - \frac{1}{2}\Delta z)) \quad (6.72)$$

The bottom value is extrapolated for  $T_e$ ,  $T_n$ ,  $\Psi_O$ , and  $\Psi_{O_2}$ , as shown for the electron temperature

$$T_e(z_{bot}) = \frac{1}{2}(3T_e(z_{bot} + \frac{1}{2}\Delta z) - T_e(z_{bot} + \frac{3}{2}\Delta z)) \quad (6.73)$$

with the height index  $k = 1$  for the midpoint level  $z_{bot} + \frac{1}{2}\Delta z$ , and the interface height index  $k = 1$  for  $z_{bot}$ . Note that even for the neutral temperature the values are extrapolated although a lower boundary value exist. The value at the top are also extrapolated for  $T_e$ ,  $T_n$ ,  $\Psi_O$ , and  $\Psi_{O_2}$ , as shown for the electron temperature

$$T_e(z_{top}) = \frac{1}{2}(3T_e(z_{top} - \frac{1}{2}\Delta z) - T_e(z_{top} - \frac{3}{2}\Delta z)) \quad (6.74)$$

The mass mixing ratio of  $N_2$  is calculated by

$$\Psi_{N_2} = 1 - \Psi_O - \Psi_{O_2} \quad \text{with} \quad \Psi_{N_2} \geq 0 \quad (6.75)$$

The mass mixing ratios  $\Psi_i$  are converted to number densities  $N_i$ . First the exponentials  $e^{-z}$  are set

$$e^{-Z} = e^{\frac{1}{2}\Delta Z} e^{-Z-\frac{1}{2}\Delta Z} \quad (6.76)$$

$$e^{-Z_{top}} = e^{\frac{1}{2}\Delta Z} e^{-Z_{top}-\frac{1}{2}\Delta Z} \quad (6.77)$$

For the conversion from mass mixing ratio to number density the following factor  $N\bar{m}$  is calculated

$$N\bar{m} = \frac{p_0 e^{-Z\bar{m}}(z)}{k_B T_n(z)} = \frac{p\bar{m}(z)}{k_B T_n(z)} \quad (6.78)$$

The number densities at the interface level are

$$N_{O_2} = N\bar{m} \frac{\Psi_{O_2}}{m_{O_2}} \quad (6.79)$$

$$N_O = N\bar{m} \frac{\Psi_O}{m_O} N_{N_2} = N\bar{m} \frac{\Psi_{N_2}}{m_{N_2}} \quad (6.80)$$

The thermal conductivity  $K^e$  in  $[\frac{ergs}{cm\ s\ K}]$  is calculated according to [Rees & Roble 1975]

$$K^e = \frac{7.5 \cdot 10^5}{1 + 3.22 \cdot 10^4 \frac{T_e^2}{N_e} [\sqrt{T_e} d_1 N_{N_2} + d_2 N_{O_2} + d_3 N_O]} \quad (6.81)$$

with

$$d_1 = 2.82 \cdot 10^{-17} - 3.41 \cdot 10^{-21} T_e \quad (6.82)$$

$$d_2 = 2.2 \cdot 10^{-16} - 7.92 \cdot 10^{-18} \sqrt{T_e} \quad (6.83)$$

$$d_3 = 1.1 \cdot 10^{-16} (1 + 5.7 \cdot 10^{-4} T_e) \quad (6.84)$$

The scale height  $H$  in  $[cm]$  is determined on midpoint level and interface level

$$H = \frac{R^* T_n}{g} \quad (6.85)$$

with  $R^*$  the gas constant,  $g$  the gravitational acceleration, and  $T_n$  the neutral temperature either on midpoint or interface level. A minimum inclination of  $I_{min} = 0.17$  is assumed.

$$\text{for } |I| \geq I_{min} \quad \sin I^* = \sin^2 I \quad (6.86)$$

$$\text{for } |I| < I_{min} \quad \sin I^* = \sin^2 I_{min} \quad (6.87)$$

with  $\sin I^* \geq 0.1$ . ???  $\sin^2 I_{min} \leq 0.1$  ?????

The term  $\sin^2 I \frac{\partial}{\partial Z} \left( \frac{2}{7} \frac{K^o}{H} \frac{\partial G}{\partial Z} \right)$  of the electron energy conservation equation is first determined. The derivative is calculated by

$$\begin{aligned} \frac{\partial}{\partial Z} \left( f \frac{\partial Y}{\partial Z} \right) (z + \frac{1}{2} \Delta z) &= \frac{1}{\Delta z} \left[ f(z + \Delta z) \frac{\partial Y}{\partial Z}(z + \Delta z) - f(z) \frac{\partial Y}{\partial Z}(z) \right] = \\ \frac{1}{\Delta z^2} [f(z)Y(z - \frac{1}{2} \Delta z) + Y(z + \frac{1}{2} \Delta z)(-f(z + \Delta z) - f(z)) + & \\ f(z + \Delta z)Y(z + \frac{3}{2} \Delta z)] & \end{aligned} \quad (6.88)$$

with  $f = \frac{2K^o}{7H}$  and  $Y = G$ . The solver needs the equation in the following form

$$\begin{aligned} P(z + \frac{1}{2} \Delta z)G(z - \frac{1}{2} \Delta z) + Q(z + \frac{1}{2} \Delta z)G(z + \frac{1}{2} \Delta z) + \\ R(z + \frac{1}{2} \Delta z)G(z + \frac{3}{2} \Delta z) = RHS(z + \frac{1}{2} \Delta z) \end{aligned} \quad (6.89)$$

Therefore, from the derivative the following values can be set

$$P(z + \frac{1}{2} \Delta z) = \frac{2 \sin^2 I^*}{7 \Delta^2 z H(z + \frac{1}{2} \Delta z)} \frac{K^o(z)}{H(z)} \quad (6.90)$$

$$R((z + \frac{1}{2} \Delta z) = \frac{2 \sin^2 I^*}{7 \Delta^2 z H(z + \frac{1}{2} \Delta z)} \frac{K^o(z + \Delta z)}{H(z + \Delta z)} \quad (6.91)$$

$$Q((z + \frac{1}{2} \Delta z) = \frac{2 \sin^2 I^*}{7 \Delta^2 z H(z + \frac{1}{2} \Delta z)} \left[ -\frac{K^o(z + \Delta z)}{H(z + \Delta z)} - \frac{K^o(z)}{H(z)} \right] \quad (6.92)$$

At the bottom of the model we set  $T_e(z_{bot}) = T_n(z_{bot})$  which leads to  $G = T_n^{7/2}$ . The boundary is then

$$G(z_{bot}) = T_n^{7/2}(z_{bot}) = \frac{1}{2} [G(z_{bot} - \frac{1}{2} \Delta z) + G(z_{bot} + \frac{1}{2} \Delta z)] \quad (6.93)$$

which leads to

$$G(z_{bot} - \frac{1}{2} \Delta z) = 2T_n^{7/2}(z_{bot}) - G(z_{bot} + \frac{1}{2} \Delta z) \quad (6.94)$$

and is inserted into

$$P(z_{bot} + \frac{1}{2}\Delta z)G(z_{bot} - \frac{1}{2}\Delta z) + Q(z_{bot} + \frac{1}{2}\Delta z)G(z_{bot} + \frac{1}{2}\Delta z) + \\ R(z_{bot} + \frac{1}{2}\Delta z)G(z_{bot} + \frac{3}{2}\Delta z) = RHS(z_{bot} + \frac{1}{2}\Delta z) \quad (6.95)$$

and gives

$$P(z_{bot} + \frac{1}{2}\Delta z) \left[ 2T_n^{7/2}(z_{bot}) - G(z_{bot} + \frac{1}{2}\Delta z) \right] + \\ Q(z_{bot} + \frac{1}{2}\Delta z)G(z_{bot} + \frac{1}{2}\Delta z) + R(z_{bot} + \frac{1}{2}\Delta z)G(z_{bot} + \frac{3}{2}\Delta z) = \\ RHS(z_{bot} + \frac{1}{2}\Delta z) \quad (6.96)$$

Therefore at the lower boundary the coefficients are

$$Q^*(z_{bot} + \frac{1}{2}\Delta z) = Q(z_{bot} + \frac{1}{2}\Delta z) - P(z_{bot} + \frac{1}{2}\Delta z) \quad (6.97)$$

$$RHS^*(z_{bot} + \frac{1}{2}\Delta z) = RHS(z_{bot} + \frac{1}{2}\Delta z) - 2P(z_{bot} + \frac{1}{2}\Delta z)T_n^{7/2}(z_{bot}) \quad (6.98)$$

$$P^*(z_{bot} + \frac{1}{2}\Delta z) = 0 \quad (6.99)$$

At the upper boundary the flux is set

$$\frac{2K^o}{7H} \frac{\partial G}{\partial Z} = F_e \quad (6.100)$$

which leads to  $\frac{\partial G}{\partial Z} = \frac{7H}{2K^o} F_e$ . So the top level value can be set by using

$$\frac{G(z_{bot} + \frac{1}{2}\Delta z) - G(z_{bot} - \frac{1}{2}\Delta z)}{\Delta z} = \left( \frac{7H}{2K^o} F_e \right) (z_{top}) \quad (6.101)$$

and solving for  $G(z_{bot} + \frac{1}{2}\Delta z)$ . Inserting it into

$$P(z_{top} - \frac{1}{2}\Delta z)G(z_{top} - \frac{3}{2}\Delta z) + Q(z_{top} - \frac{1}{2}\Delta z)G(z_{top} - \frac{1}{2}\Delta z) + \\ R(z_{top} - \frac{1}{2}\Delta z)G(z_{top} + \frac{1}{2}\Delta z) = RHS(z_{top} - \frac{1}{2}\Delta z) \quad (6.102)$$

leads to

$$\begin{aligned}
& P(z_{top} - \frac{1}{2}\Delta z)G(z_{top} - \frac{3}{2}\Delta z) + Q(z_{top} - \frac{1}{2}\Delta z)G(z_{top} - \frac{1}{2}\Delta z) + \\
& R(z_{top} - \frac{1}{2}\Delta z) \left[ \left( \frac{7H}{2K_o} F_e \right) (z_{top}) \Delta z + G(z_{bot} - \frac{1}{2}\Delta z) \right] = \quad (6.103) \\
& RHS(z_{top} - \frac{1}{2}\Delta z)
\end{aligned}$$

Therefore at the upper boundary the coefficients are

$$Q^*(z_{top} - \frac{1}{2}\Delta z) = Q(z_{top} + \frac{1}{2}\Delta z) + R(z_{top} - \frac{1}{2}\Delta z) \quad (6.104)$$

$$\begin{aligned}
RHS^*(z_{top} - \frac{1}{2}\Delta z) = & RHS(z_{top} - \frac{1}{2}\Delta z) - \\
& R(z_{top} + \frac{1}{2}\Delta z) \left( \frac{7H}{2K_o} F_e \right) (z_{top}) \Delta z \quad (6.105)
\end{aligned}$$

$$R^*(z_{top} - \frac{1}{2}\Delta z) = 0 \quad (6.106)$$

The flux  $F_e$  was set before see eq. (6.64)

The heating rate is

$$\sum Q_e = \left[ Q_{O_2^+} + Q_{O^+} + Q_{N_2^+} + Q_{NO^+} + Q_{N^+} + Q_{O^+(2D)} + Q_{O^+(2p)} \right] \epsilon \quad (6.107)$$

with  $\epsilon$  the heat efficiency. In the code first  $\sum Q_e/\epsilon$  is calculated at the interface level. The values of  $\sum Q_e/\epsilon$  at the midpoint level are calculated by

$$\frac{\sum Q_e}{\epsilon}(z + \frac{1}{2}\Delta z) = \sqrt{\frac{\sum Q_e}{\epsilon}(z) \frac{\sum Q_e}{\epsilon}(z + \Delta z)} \quad (6.108)$$

In the same way the electron density is determined at the midpoint level

$$N_e(z + \frac{1}{2}\Delta z) = \sqrt{N_e(z)N_e(z + \Delta z)} \quad \text{with } N_e \geq 100. \quad (6.109)$$

For the conversion from mass mixing ratio to number density  $N\overline{m}$  at the midpoint level is determined

$$N\overline{m}(z + \frac{1}{2}\Delta z) = \frac{p_0 e^{-z - \frac{1}{2}\Delta z} \overline{m}(z + \frac{1}{2}\Delta z)}{k_B T_n(z + \frac{1}{2}\Delta z)} \quad (6.110)$$

The number densities  $N_i$  at the midpoint level are

$$N_{O_2}(z + \frac{1}{2}\Delta z) = N\bar{m}(z + \frac{1}{2}\Delta z) \frac{\Psi_{O_2}(z + \frac{1}{2}\Delta z)}{m_{O_2}} \quad (6.111)$$

$$N_O(z + \frac{1}{2}\Delta z) = N\bar{m}(z + \frac{1}{2}\Delta z) \frac{\Psi_O(z + \frac{1}{2}\Delta z)}{m_O} \quad (6.112)$$

$$N_{N_2}(z + \frac{1}{2}\Delta z) = N\bar{m}(z + \frac{1}{2}\Delta z) \frac{\Psi_{N_2}(z + \frac{1}{2}\Delta z)}{m_{N_2}} \quad (6.113)$$

with  $\Psi_{N_2} = 1 - \Psi_{O_2} - \Psi_O$  and  $\Psi_{N_2} \geq 0$ . The heat efficiency  $\epsilon$  at the midpoint level is then

$$\epsilon = \exp \left[ - \left( 12.75 + 6.941R + 1.166R^2 + 0.08043R^3 + 0.001996R^4 \right) \right] \quad (6.114)$$

with

$$R = \ln \frac{N_e}{N_{O_2} + 0.1 \cdot N_O + N_{N_2}} \quad (6.115)$$

Therefore, the following term is added to the right hand side

$$RHS = \frac{\sum Q_e}{\epsilon} (z + \frac{1}{2}\Delta z) \quad (6.116)$$

The cooling term due to vibrational excitation  $L(e, N_2)_{vib}$  of  $N_2$  is given by

$$\frac{L(e, N_2)_{vib}}{N_e} = N_{N_2} 1.3 \cdot 10^{-4} A \frac{-3200}{T_e T_n} \frac{1 - \exp \left[ 3200 \left( \frac{1}{T_e} - \frac{1}{T_n} \right) \right]}{3200 \left( \frac{1}{T_e} - \frac{1}{T_n} \right)} \quad (6.117)$$

with the value of  $A$

$$\begin{aligned} A &= 5.7 \cdot 10^{-8} \exp\left(\frac{-3352.6}{T_e}\right) \quad \text{for } T_e < 1000K \\ A &= 2. \cdot 10^{-7} \exp\left(\frac{-4605.2}{T_e}\right) \quad \text{for } 1000K \leq T_e \leq 2000K \\ A &= 2.53 \cdot 10^{-6} \sqrt{T_e} \exp\left(\frac{-17620}{T_e}\right) \quad \text{for } 2000K < T_e < \end{aligned}$$

The rotational excitation of  $N_2$  and the cooling rates due to elastic electron-neutral collisions are  $L(e, N_2)_{elast} + L(e, N_2)_{rot}$

$$\frac{L(e, N_2)_{elast} + L(e, N_2)_{rot}}{N_e} = N_{N_2} \left[ 1.77 \cdot 10^{-19} \{1 - 1.21 \cdot 10^{-4} T_e\} T_e + 2.9 \cdot 10^{-14} \frac{1}{\sqrt{T_e}} \right] \quad (6.118)$$

The elastic, vibrational and rotational excitation of  $O_2$  is

$$\frac{L(e, O_2)_{elast} + L(e, O_2)_{vib} + L(e, O_2)_{rot}}{N_e} = N_{O_2} \left[ 1.21 \cdot 10^{-18} \left( 1 + 3.6 \cdot 10^{-2} \sqrt{T_e} \right) \sqrt{T_e} + 3.125 \cdot 10^{-21} T_e^2 + 6.9 \cdot 10^{-14} \frac{1}{\sqrt{T_e}} \right] \quad (6.119)$$

due to elastic electron neutral collision and due to fine structure excitation of  $O$  is

$$\frac{L(e, O)_{elast} + L(e, O)_{fs}}{N_e} = N_O \left[ 7.9 \cdot 10^{-19} (1 + 5.7 \cdot 10^{-4} T_e) \sqrt{T_e} + 3.4 \cdot 10^{-12} \frac{1 - 7 \cdot 10^{-5} T_e}{T_n} \left( \frac{150}{T_e} + 0.4 \right) \right] \quad (6.120)$$

All the loss terms together are  $L(e, n)$

$$\frac{L(e, n)}{N_e} = \frac{L(e, N_2)_{vib}}{N_e} + \frac{L(e, O_2)_{elast} + L(e, O_2)_{vib} + L(e, O_2)_{rot}}{N_e} + \frac{L(e, O)_{elast} + L(e, O)_{fs}}{N_e} \quad (6.121)$$

and is multiplied by the electron density on the midpoint level. The cooling rate due to mixture of the electrons with ions is  $L(e, i)$

$$L(e, i) = 3.2 \cdot 10^{-8} \frac{N_e}{T_e^{3/2}} 15 (N_{O^+} + 0.5 N_{O_2} + 0.53 N_{NO^+}) \quad (6.122)$$

The cooling due to ion neutral collision is  $L(i, n)$  in  $[\frac{erg}{s cm^3}]$

$$L(i, n) = N_{O^+} \left( 6.6 \cdot 10^{-14} N_{N_2} + 5.8 \cdot 10^{-14} N_{O_2} + 0.21 \cdot 10^{-14} N_O \sqrt{2T_n} \right) + N_{O_2^+} \left( 5.45 \cdot 10^{-14} N_{O_2} + 5.9 \cdot 10^{-14} N_{N_2} + 4.5 \cdot 10^{-14} N_O \right) + N_{O_2^+} \left( 5.8 \cdot 10^{-14} N_{N_2} + 4.4 \cdot 10^{-14} N_O + 0.14 \cdot 10^{-14} N_{O_2} \sqrt{2T_n} \right) \quad (6.123)$$

The coefficients are updated by

$$Q^* = Q - \frac{L(e, n) + L(e, i)}{T_e^{5/2}} \quad (6.124)$$

$$RHS^* = RHS - L(e, n)T_n - L(e, i)T_i \quad (6.125)$$

Note that the temperatures  $T_n$ ,  $T_i$  and  $T_e$  are at timestep  $t_n$  and midpoints height level. The tridiagonal solver solve eq. (6.97) which gives  $G$  and the updated electron temperatures

$$T_e(t_n + \Delta t) = G^{2/7} \quad \text{with} \quad T_e(t_n + \Delta t) \geq T_n(t_n) \quad (6.126)$$

The ion temperature  $T_i$  at timestep  $t_n + \Delta t$  is determined from

$$L(e, i)(T_e - T_i) + \rho Q_J^{T_i} = L(i, n)(T_i - T_n) \quad (6.127)$$

which leads to

$$T_i = \frac{L(e, i)T_e(t_n + \Delta t) + L(i, n)T_n(t_n) + \rho Q_J^{T_i}}{L(e, i) + L(i, n)} \quad (6.128)$$

with  $\rho = \frac{N\bar{m}}{N_A}$  in  $[g/cm^3]$ , and  $N_A$  is the Avogadro number. The ion temperature has to be larger than the neutral temperature  $T_i \geq T_n$ .

For the thermodynamic equation an addition to the heating term is determined.

$$Q(en, ei) = Q(e, n) + Q(e, i) = \frac{N_A}{N\bar{m}} [L(e, n)(T_e^{t_n} - T_n^{t_n}) + L^*(e, i)(T_e^{t_n} - T_i^{t_n})] \quad (6.129)$$

with

$$L^*(e, i) = L(e, i)(T_e^{t_n} - T_i^{t_n}) \quad \text{for } T_e^{t_n} - T_i^{t_n} > 0 \quad (6.130)$$

$$L^*(e, i) = 0 \quad \text{for } T_e^{t_n} - T_i^{t_n} \leq 0 \quad (6.131)$$

with  $L^*(e, i)$  in  $[eV/s/g]$ . The term is added to the total heating term  $Q_{tot}$  at the interface level

$$Q_{tot}^*(z) = Q_{tot}(z) + \frac{1}{2}(Q(en, ei)(z + \frac{1}{2}\Delta z) + Q(en, ei)(z - \frac{1}{2}\Delta z)) \quad (6.132)$$



The upper and lower boundary are extrapolated

$$\begin{aligned}
 Q_{tot}^*(z_{bot}) = & Q_{tot}(z_{bot}) + \frac{3}{2}Q(en, ei)(z + \frac{1}{2}\Delta z) \\
 & - Q(en, ei)(z_{bot} + \frac{3}{2}\Delta z))
 \end{aligned} \tag{6.133}$$

$$\begin{aligned}
 Q_{tot}^*(z_{top}) = & Q_{tot}(z_{top}) + \frac{3}{2}Q(en, ei)(z_{top} - \frac{1}{2}\Delta z) \\
 & - Q(en, ei)(z_{top} - \frac{3}{2}\Delta z))
 \end{aligned} \tag{6.134}$$

## 6.4 Calculation of $O^+$ number density /

The input to subroutine `oplus` is summarized in table 6.10. The output of subroutine `oplus` is summarized in table 6.11. The module data of subroutine `oplus` is summarized in table 6.12. Most major species are in photochemical equilibrium below  $1000km$ , and can be simply calculated by balancing the production and loss rates. However,  $O^+$  is determined by considering diffusion, along the magnetic field line and the  $\mathbf{E} \times \mathbf{B}$  transport. In the following for simplicity the variable  $n$  is used for the  $O^+$  number density  $n(O^+)$ .

$$\frac{\partial n}{\partial t} - Q + Ln = -\nabla \cdot (n\mathbf{v}_i) \quad (6.135)$$

with  $n$  the  $O^+$  number density,  $Q$  the production rate of  $O^+$ ,  $L$  the loss rate of  $O^+$ . The right hand side is the transport due  $\mathbf{E} \times \mathbf{B}$  drift and the field aligned ambipolar diffusion. The ion velocity  $\mathbf{v}_i$  is given by

$$\mathbf{v}_i = \mathbf{v}_{i,\parallel} + \mathbf{v}_{i,\perp} \quad (6.136)$$

with the parallel and perpendicular velocity with respect to the geomagnetic field

$$\mathbf{v}_{i,\parallel} = \left[ \mathbf{b} \cdot \frac{1}{\nu_{in}} \left( \mathbf{g} - \frac{1}{\rho_i} \nabla (P_i + P_e) \right) + \mathbf{b} \cdot \mathbf{v}_n \right] \mathbf{b} \quad (6.137)$$

$$\mathbf{v}_{i,\perp} = \frac{\mathbf{E} \times \mathbf{B}}{|B|} \quad (6.138)$$

The parallel velocity is caused by ambipolar diffusion and the perpendicular velocity by  $\mathbf{E} \times \mathbf{B}$  drift velocity. The unit vector along the geomagnetic field line is  $\mathbf{b}$ ,  $\nu_{in}$  is the  $O^+$  ion-neutral collision frequency,  $\mathbf{g}$  the gravitational acceleration due to gravity,  $\rho_i$  is the ion mass density,  $P_i$  and  $P_e$  are the ion and electron pressure,  $\mathbf{v}_n$  is the neutral velocity,  $|B|$  is the geomagnetic field strength, and  $\mathbf{E}$  is the electric field.

Inserting the parallel (6.137) and perpendicular (6.138) velocity into the  $O^+$

transport equation (6.135) leads to

$$\begin{aligned}
& \frac{\partial n}{\partial t} - Q + Ln + [(\mathbf{b}_h \cdot \nabla_h) K b_z] \left[ \left( \frac{1}{H} \frac{\partial}{\partial Z} (2T_p n) + \frac{mg}{k_B} n \right) \right] \\
& - (\mathbf{b}_h \cdot \nabla_h) (\mathbf{b} \cdot v_n n) + \left( b_z \frac{1}{H} \frac{\partial}{\partial Z} + \nabla \cdot \mathbf{b} \right) K b_z \left( \frac{1}{H} \frac{\partial}{\partial Z} (2T_p n) + \frac{mg}{k_B} n \right) - \\
& \left( b_z \frac{1}{H} \frac{\partial}{\partial Z} + \nabla \cdot \mathbf{b} \right) (\mathbf{b} \cdot v_n n) - \left[ B^2 \mathbf{v}_{ExB,h} \cdot \nabla \left( \frac{n}{B^2} \right) \right]_H - \\
& B^2 \mathbf{v}_{ExB,z} \frac{1}{H} \frac{\partial}{\partial Z} \left( \frac{n}{B^2} \right) + (\mathbf{b}_H \cdot \nabla_H) K (\mathbf{b}_H \cdot \nabla_H) (2nT_p) + \\
& K b_z (\mathbf{b}_H \cdot \nabla_H) \left( \frac{1}{H} \frac{\partial}{\partial Z} (2T_p n) + \frac{mg}{k_B} n \right) + \\
& \left( b_z \frac{1}{H} \frac{\partial}{\partial Z} + \nabla \cdot \mathbf{b} \right) K (\mathbf{b}_H \cdot \nabla_H (2nT_p)) = 0
\end{aligned} \tag{6.139}$$

where the ambipolar diffusion coefficient is  $K = D_A + K_E$  with  $K_E$  the eddy diffusion coefficient in the lower thermosphere, and  $D_A$  the molecular diffusion coefficient. The geomagnetic unit vector, the horizontal vector and vertical component are  $\mathbf{b}$ ,  $\mathbf{b}_H$  and  $b_z$  respectively. The scale height is denoted by  $H$ ,  $\mathbf{v}_{ExB,h}$  is the horizontal drift vector, and  $\mathbf{v}_{ExB,z}$  the vertical component. The horizontal derivative of  $\nabla$  is  $\nabla_H$ . The plasma pressure is  $T_p = \frac{1}{2}(T_e + T_i)$ .

The fourth, eleventh, and sixth term are the contributions of the vertical component of ambipolar diffusion to the plasma transport due to respectively, the horizontal variation of the diffusion coefficient and  $b_z$ , the horizontal variation of the vertical ambipolar diffusion, and the vertical variation of the vertical ambipolar diffusion. The tenth term is the contribution of the horizontal component of the ambipolar diffusion due to variations in the vertical and horizontal direction. The fifth and seventh term are the neutral wind effects on the  $O^+$  distribution, and the eight and ninth terms are the effects of the  $\mathbf{E} \times \mathbf{B}$  transport.

The flux at the upper boundary is determined in the subroutine `oplus_flux`. The transport from and to the plasmasphere is specified by the flux  $\Phi$ . The

latitudinal variation of the flux is specified by the factor  $A$

$$\begin{aligned}
 A &= 1 && \text{for } |\lambda_m| \geq \frac{\Pi}{24} \\
 A &= \frac{1}{2} \left( 1 + \sin \Pi \frac{|\lambda_m| - \frac{\Pi}{48}}{\Pi/24} \right) && \text{for } |\lambda_m| < \frac{\Pi}{24}
 \end{aligned} \tag{6.140}$$

with  $A \geq 0.05$ , and  $\lambda_m$  the geomagnetic latitude. The daytime flux is  $\Phi_D^o$  and upward, and the nighttime flux  $\Phi_N^o$  which is downward

$$\begin{aligned}
 \Phi_D^o &= 2 \cdot 10^8 \\
 \Phi_N^o &= -2 \cdot 10^8
 \end{aligned} \tag{6.141}$$

and the flux variation during the day- and nighttime is given by

$$\begin{aligned}
 F_{eD} &= \Phi_D^o A \\
 F_{eN} &= \Phi_N^o A
 \end{aligned} \tag{6.142}$$

The solar zenith angle  $\psi$  determines which flux  $F^{O^+}$  is used

$$\begin{aligned}
 F^{O^+} &= F_{eN} \quad \text{for } \psi \geq 80^\circ \\
 F^{O^+} &= F_{eD} \quad \text{for } \psi < 100^\circ
 \end{aligned} \tag{6.143}$$

with

$$F^{O^+} = \frac{1}{2} [F_{eD} + F_{eN}] + \frac{1}{2} [F_{eD} - F_{eN}] \cos \left( \Pi \frac{\psi - 80}{20} \right) \quad \text{for } 80^\circ < \psi < 100^\circ \tag{6.144}$$

The divergence of the geomagnetic field vector  $\mathbf{b}$  is determined in **subroutine divb**. Since variation in height of the geomagnetic field is neglected the divergence also varies only with latitude and longitude.

$$\begin{aligned}
 \nabla \cdot \mathbf{b} &= \frac{b_x(\phi + \Delta\phi, \lambda) - b_x(\phi - \Delta\phi, \lambda)}{2\Delta\phi R_E \cos \lambda} + \\
 &\quad \frac{\cos \lambda + \Delta\lambda b_y(\phi, \lambda + \Delta\lambda) - \cos \lambda - \Delta\lambda b_y(\phi, \lambda - \Delta\lambda)}{2\Delta\lambda R_E \cos \lambda} + \\
 &\quad \frac{2b_z(\phi, \lambda)}{R_E}
 \end{aligned} \tag{6.145}$$

with  $b_y$  the northward,  $b_x$  the eastward, and  $b_z$  the upward component of the unit geomagnetic field vector  $\frac{\mathbf{B}}{|\mathbf{B}|}$ . The divergence is stored in the value **dvb**.

In the first latitudinal scan the plasma pressure is determined at  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ , e.g. at  $\lambda$

$$T_p(\phi, \lambda, z + \frac{1}{2}\Delta z) = \frac{1}{2}(T_i + T_e) \quad (6.146)$$

The values in the code are stored in the variable **tpj**.

In **subroutine rrk** the diffusion coefficient are determined. The values are stored in the variable **dj** in the source code at  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ .

$$D_A = \frac{1.42 \cdot 10^{17} k_B T_n}{p \bar{m} \left[ \frac{\Psi_O}{m_O} \sqrt{T_p} (1 - 0.064 \log_{10} T_p)^2 C_f + 18.6 \frac{\Psi_{N_2}}{m_{N_2}} + 18.1 \frac{\Psi_{O_2}}{m_{O_2}} \right]} \quad (6.147)$$

with the pressure  $p(z + \frac{1}{2}\Delta z) = p_0 e^{-z - \frac{1}{2}\Delta z}$ , the number density of  $N_2$  is  $\Psi_{N_2} = 1 - \Psi_{O_2} - \Psi_O$ , the factor is  $C_f = 1.5$ , and  $N = \frac{p_0 e^{-z - \frac{1}{2}\Delta z}}{k_B T_n}$ . The value  $D_A$  is determined at half pressure levels e.g.  $z + \frac{1}{2}\Delta z$ . The variable **tpj** holds  $2T_p$  at the midpoint pressure level  $z + \frac{1}{2}\Delta z$  and at the latitudes  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ . The scale height is also determined at the midpoint pressure level, and the latitudes  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ .

$$H = \frac{R^* T_n}{\bar{m} g} \quad (6.148)$$

The scale height is stored in the variable **hj**. The dot product  $\mathbf{b} \cdot \mathbf{v}_n n$  is stored in **bvel** and calculated also on the midpoint pressure level, and the latitudes  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ .

$$\mathbf{b} \cdot \mathbf{v}_n n = \left[ b_x u_n + b_y v_n + b_z \frac{W(z) + W(z + \frac{1}{2}\Delta z)}{2} H(z + \frac{1}{2}\Delta z) \right] n \quad (6.149)$$

In **subroutine diffus** the term  $\left[ 2 \frac{\partial T_p n}{H \partial z} + \frac{m_{O+g}}{R^*} n \right]$  at the midpoint pressure level is determined

$$F(z + \frac{1}{2}\Delta z) = \frac{1}{2H(z + \frac{1}{2}\Delta z)\Delta z} [2T_p(z + \frac{3}{2}\Delta z)n(z + \frac{3}{2}\Delta z) - 2T_p(z - \frac{1}{2}\Delta z)n(z - \frac{1}{2}\Delta z)] + \frac{m_{O+g}}{R^*} n(z + \frac{1}{2}\Delta z) \quad (6.150)$$

The term is stored in the variable **diffj**. The upper and lower boundary values are set by

$$F(z_{bot} + \frac{1}{2}\Delta z) = \frac{1}{H(z_{bot} + \frac{1}{2}\Delta z)\Delta z} [2T_p(z_{bot} + \frac{3}{2}\Delta z)n(z_{bot} + \frac{3}{2}\Delta z) -$$

$$(6.151)$$

$$2T_p(z_{bot} + \frac{1}{2}\Delta z)n(z_{bot} + \frac{1}{2}\Delta z)] + \frac{m_{O+g}}{R^*}n(z_{bot} + \frac{1}{2}\Delta z)$$

$$F(z_{top} - \frac{1}{2}\Delta z) = \frac{1}{H(z_{top} - \frac{1}{2}\Delta z)\Delta z} [2T_p(z_{top} - \frac{1}{2}\Delta z)n(z_{top} - \frac{1}{2}\Delta z) -$$

$$(6.152)$$

$$2T_p(z_{top} - \frac{3}{2}\Delta z)n(z_{top} - \frac{3}{2}\Delta z)] + \frac{m_{O+g}}{R^*}n(z_{top} - \frac{1}{2}\Delta z)$$

The value  $2nT_p$  is determined at midpoint level, and the latitudes  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ . The value overwrites the variable **tpj**. The latitudinal smoothed value of  $n(O^+)^{t_n-\Delta t}$  are determined by

$$n(O^+)^{smo\lambda, t_n-\Delta t} = n(O^+)^{t_n-\Delta t} - f_{smo}[n(O^+)^{t_n-\Delta t}(\lambda + 2\Delta\lambda) +$$

$$n(O^+)^{t_n-\Delta t}(\lambda - 2\Delta\lambda) - 4(n(O^+)^{t_n-\Delta t}(\lambda + \Delta\lambda) +$$

$$n(O^+)^{t_n-\Delta t}(\lambda - \Delta\lambda)) + 6n(O^+)^{t_n-\Delta t}(\lambda)] \quad (6.153)$$

and stored in **optm1\_smooth**, and  $f_{smo} = 0.003$ .

The second latitudinal scan starts with calculating the value of  $\mathbf{b} \cdot \nabla_H$  in **subroutine bdotdh** at the midpoint level. The output variable is **bdotdh\_op**. The input is the term from eq. (6.150)  $F = \left[ 2\frac{\partial T_p n}{H\partial Z} + \frac{m_{O+g}}{R^*}n \right]$ , which leads to  $(\mathbf{b} \cdot \nabla_H) \left[ 2\frac{\partial T_p n}{H\partial Z} + \frac{m_{O+g}n}{R^*} \right]$

$$T1 = \frac{1}{R_E} \left[ \frac{b_x}{2\Delta\phi \cos \lambda} \{F(\phi + \Delta\phi, \lambda) - F(\phi - \Delta\phi, \lambda)\} + \right.$$

$$\left. b_y \frac{F(\phi, \lambda + \Delta\lambda) - F(\phi, \lambda - \Delta\lambda)}{2\Delta\lambda} \right] \quad (6.154)$$

The term is multiplied by the diffusion coefficient  $D_A$  from **subroutine rrk**, which leads to

$$D_A(z + \frac{1}{2}\Delta z)b_z(\mathbf{b} \cdot \nabla_H) \left[ 2\frac{\partial T_p n}{H\partial Z} + \frac{m_{O+g}}{R^*}n \right] \quad (6.155)$$

The same **subroutine** `bdotdh` is used to calculate  $\mathbf{b} \cdot \nabla_H [2T_p n]$ . Using eq. (6.154) with  $F = 2T_p n$ . The values are determined at the midpoint pressure level, and at the latitudes  $\lambda - \Delta\lambda$ ,  $\lambda$  and  $\lambda + \Delta\lambda$ . Afterwards the value is multiplied by

$$D_A(z + \frac{1}{2}\Delta z) \mathbf{b} \cdot \nabla_H [2T_p n] \quad (6.156)$$

and stored in the variable `bdotdh_opj`.

The third latitudinal scan starts with calling the **subroutine** `bdotdh` for the term in eq. (6.156)  $F = D_A \mathbf{b} \cdot \nabla_H [2T_p n]$ , which leads to (see eq. (6.154))

$$\mathbf{b} \cdot \nabla_H (D_A \mathbf{b} \cdot \nabla_H [2T_p n]) \quad (6.157)$$

evaluated at the midpoint pressure level, and stored in the variable `bdotdh_diff`.

The **subroutine** `bdzdvb` calculates the term  $(b_z \frac{1}{H} \frac{\partial}{\partial z} + \nabla \cdot \mathbf{b}) G$ , with the input into the subroutine  $\nabla \cdot \mathbf{B}$ , and  $G = D_A \mathbf{b} \cdot \nabla_H [2T_p n]$ .

$$T3(z + \frac{1}{2}\Delta z) = \frac{b_z}{2H(z + \frac{1}{2}\Delta z)\delta z} \left\{ G(z + \frac{3}{2}\Delta z) - G(z - \frac{1}{2}\Delta z) \right\} + \nabla \cdot \mathbf{b} G(z + \frac{1}{2}\Delta z) \quad (6.158)$$

At the upper and lower boundary the values are set to

$$T3(z_{top} - \frac{1}{2}\Delta z) = \frac{b_z}{2H(z_{top} - \frac{1}{2}\Delta z)\delta z} \left\{ G(z_{top} - \frac{1}{2}\Delta z) - G(z_{top} - \frac{3}{2}\Delta z) \right\} + \nabla \cdot \mathbf{b} G(z_{top} - \frac{1}{2}\Delta z) \quad (6.159)$$

$$T3(z_{bot} + \frac{1}{2}\Delta z) = \frac{b_z}{2H(z_{bot} + \frac{1}{2}\Delta z)\delta z} \left\{ G(z_{bot} + \frac{3}{2}\Delta z) - G(z_{bot} + \frac{1}{2}\Delta z) \right\} + \nabla \cdot \mathbf{b} G(z_{bot} + \frac{1}{2}\Delta z) \quad (6.160)$$

All the explicit terms are added together from eq. (6.155), (6.156), and

(6.158) which leads to

$$\begin{aligned}
T_{1,explicit} = & -D_A(z + \frac{1}{2}\Delta z)b_z(\mathbf{b} \cdot \nabla_H) \left[ 2\frac{\partial T_p n}{H\partial Z} + \frac{m_{O^+}g}{R^*}n \right] \\
& - \mathbf{b} \cdot \nabla_H (D_A \mathbf{b} \cdot \nabla_H [2T_p n]) \\
& - \left( b_z \frac{1}{H} \frac{\partial}{\partial Z} + \nabla \cdot \mathbf{b} \right) (D_A \mathbf{b} \cdot \nabla_H [2T_p n]) \quad (6.161)
\end{aligned}$$

In addition the term  $(\mathbf{b}_H \cdot \nabla_H)(\mathbf{b} \cdot \mathbf{v}_{n,H})$  and  $[b^2 v_{ExB,H} \cdot \nabla(\frac{n}{B^2})]_H$  are treated as explicit terms which leads to

$$\begin{aligned}
T_{2,explicit} = & T_{1,explicit} + \frac{1}{2R_E} \left[ \frac{b_x}{\Delta\phi \cos\lambda} (\mathbf{b} \cdot \mathbf{v}_n(\phi + \Delta\phi, \lambda) - \mathbf{b} \cdot \mathbf{v}_n(\phi - \Delta\phi, \lambda)) + \right. \\
& v_{ExB,x}(z + \frac{1}{2}\Delta z)B^2(\phi, \lambda) \left( \frac{n(\phi + \Delta\phi, \lambda)}{B^2(\phi + \Delta\phi, \lambda)} - \frac{n(\phi - \Delta\phi, \lambda)}{B^2(\phi - \Delta\phi, \lambda)} \right) \\
& + \frac{1}{\Delta\lambda} (b_y (\mathbf{b} \cdot \mathbf{v}_n(\phi, \lambda + \Delta\lambda) - \mathbf{b} \cdot \mathbf{v}_n(\phi, \lambda - \Delta\lambda)) + \\
& \left. v_{ExB,y}(z + \frac{1}{2}\Delta z)B^2(\phi, \lambda) \left( \frac{n(\phi, \lambda + \Delta\lambda)}{B^2(\phi, \lambda + \Delta\lambda)} - \frac{n(\phi, \lambda - \Delta\lambda)}{B^2(\phi, \lambda - \Delta\lambda)} \right) \right] \quad (6.162)
\end{aligned}$$

Afterwards the following values are set

$$\frac{\nabla \cdot \mathbf{b}}{b_z} \quad (6.163)$$

$$\frac{1}{\Delta z H} \quad (6.164)$$

$$T_p = \frac{1}{2}(T_e + T_i) \quad (6.165)$$

at the midpoint pressure level and stored in the variables `dvb`, `srchdz`, and `tp` respectively.

The term  $2T_p \frac{1}{H\Delta z} \pm \frac{gm}{2R^*}$  are determined

$$S_p(z + \frac{3}{2}\Delta z) = 2T_p(z + \frac{3}{2}\Delta z) \frac{1}{H(z + \Delta z)\Delta z} + \frac{gm}{2R^*} \quad (6.166)$$

$$S_m(z + \frac{3}{2}\Delta z) = 2T_p(z + \frac{1}{2}\Delta z) \frac{1}{H(z + \Delta z)\Delta z} - \frac{gm}{2R^*} \quad (6.167)$$



and stored in the variable **tphdz1** for  $S_p$  and **tphdz0** for  $S_m$  respectively. The lower boundaries are set by

$$S_p(z_{bot} + \frac{1}{2}\Delta z) = 2T_p(z_{bot} + \frac{1}{2}\Delta z) \left[ \frac{1.5}{H(z_{bot} + \frac{1}{2}\Delta z)\Delta z} - \frac{0.5}{H(z_{bot} + \frac{3}{2}\Delta z)\Delta z} \right] + \frac{gm}{2R^*} \quad (6.168)$$

$$S_m(z_{bot} + \frac{1}{2}\Delta z) = 2 \cdot \left[ 2T_p(z_{bot} + \frac{1}{2}\Delta z) - T_p(z_{bot} + \frac{3}{2}\Delta z) \right] \left[ \frac{1.5}{H(z_{bot} + \frac{1}{2}\Delta z)\Delta z} - \frac{0.5}{H(z_{bot} + \frac{3}{2}\Delta z)\Delta z} \right] - \frac{gm}{2R^*} \quad (6.169)$$

and stored in **tphdz1(lev0)** and **tphdz0(lev0)**, respectively, with *lev0* corresponding to  $z_{bot} + \frac{1}{2}\Delta z$  on the midpoint pressure level. The upper boundary values are

$$S_p(z_{top} + \frac{1}{2}\Delta z) = 2 \cdot \left[ 2T_p(z_{top} - \frac{1}{2}\Delta z) - T_p(z_{top} - \frac{3}{2}\Delta z) \right] \left[ \frac{1.5}{H(z_{top} - \frac{1}{2}\Delta z)\Delta z} - \frac{0.5}{H(z_{top} - \frac{3}{2}\Delta z)\Delta z} \right] + \frac{gm}{2R^*} \quad (6.170)$$

$$S_m(z_{top} + \frac{1}{2}\Delta z) = 2T_p(z_{top} - \frac{1}{2}\Delta z) \left[ \frac{1.5}{H(z_{top} - \frac{1}{2}\Delta z)\Delta z} - \frac{0.5}{H(z_{top} - \frac{3}{2}\Delta z)\Delta z} \right] - \frac{gm}{2R^*} \quad (6.171)$$

and stored in **tphdz1(lev1)** and **tphdz0(lev1)**, respectively, with the index *lev1* = *nlev* + 1 corresponding to  $z_{top} + \frac{1}{2}\Delta z$ .

The diffusion coefficient  $D_A$  are calculated at the interface pressure level  $z, z + \Delta z, \dots$  by averaging

$$D_A(z) = \frac{1}{2} \left( D_A(z + \frac{1}{2}\Delta z) + D_A(z - \frac{1}{2}\Delta z) \right) \quad (6.172)$$

and stored in the variable **djint**. The upper and lower boundary values are

determined by extrapolation

$$D_A(z_{bot}) = \frac{1}{2} \left( 3D_A(z_{bot} + \frac{1}{2}\Delta z) - D_A(z_{bot} + \frac{3}{2}\Delta z) \right) \quad (6.173)$$

$$D_A(z_{top}) = \frac{1}{2} \left( 3D_A(z_{top} - \frac{1}{2}\Delta z) - D_A(z_{top} - \frac{3}{2}\Delta z) \right) \quad (6.174)$$

The term  $T_4 = \frac{\nabla \cdot \mathbf{b}}{b_z} + \frac{\mathbf{b}_H \cdot \nabla_H(D_A b_z)}{R_E D_A b_z^2}$  is determined at the midpoint pressure level, and stored in the variable `divbz`

$$\begin{aligned} T_4(z + \frac{1}{2}\Delta z) = & \frac{\nabla \cdot \mathbf{b}}{b_z}(\phi, \lambda) + \frac{1}{R_E D_A(\phi, \lambda, z + \frac{1}{2}\Delta z) b_z^2} [ \\ & \frac{b_x(\phi, \lambda)}{\cos \lambda} \left( \frac{D_A(\phi + \Delta\phi, \lambda, z + \frac{1}{2}\Delta z) b_z(\phi + \Delta\phi, \lambda)}{2\Delta\phi} - \right. \\ & \left. \frac{D_A(\phi - \Delta\phi, \lambda, z + \frac{1}{2}\Delta z) b_z(\phi - \Delta\phi, \lambda)}{2\Delta\phi} \right) + \\ & b_y(\phi, \lambda) \left( \frac{D_A(\phi, \lambda + \Delta\lambda, z + \frac{1}{2}\Delta z) b_z(\phi, \lambda + \Delta\lambda)}{2\Delta\lambda} - \right. \\ & \left. \frac{D_A(\phi, \lambda - \Delta\lambda, z + \frac{1}{2}\Delta z) b_z(\phi, \lambda - \Delta\lambda)}{2\Delta\lambda} \right) ] \end{aligned} \quad (6.175)$$

The periodic points for  $T_4$  are set to zero.

The term  $T_5 = b_z^2(\frac{1}{H\Delta z} \pm \frac{1}{2}T_4)$  are calculated, with  $T_4 = \frac{\nabla \cdot \mathbf{b}}{b_z} + \frac{\mathbf{b}_H \cdot \nabla_H(D_A b_z)}{R_E D_A b_z^2}$ , see above in eq.(6.175)

$$T_{5p}(z + \frac{1}{2}\Delta z) = b_z^2 \left[ \frac{1}{H\Delta z} + \frac{1}{2} \left( \frac{\nabla \cdot \mathbf{b}}{b_z} + \frac{\mathbf{b}_H \cdot \nabla_H(D_A b_z)}{R_E D_A b_z^2} (z + \frac{1}{2}\Delta z) \right) \right] \quad (6.176)$$

$$T_{5m}(z + \frac{1}{2}\Delta z) = b_z^2 \left[ \frac{1}{H\Delta z} - \frac{1}{2} \left( \frac{\nabla \cdot \mathbf{b}}{b_z} + \frac{\mathbf{b}_H \cdot \nabla_H(D_A b_z)}{R_E D_A b_z^2} (z + \frac{1}{2}\Delta z) \right) \right] \quad (6.177)$$

and stored in the variables `hdzpbz` and `hdzmdz` respectively.

The smoothing of  $n(O^+)^{t_n - \Delta t}$  is finished with a longitudinal smoothing.

See eq. (6.153) for the latitudinal smoothing

$$\begin{aligned} n(O^+)^{smo,t_n-\Delta t} = & n(O^+)^{smo\lambda,t_n-\Delta t} - f_{smo}[n(O^+)^{smo\lambda,t_n-\Delta t}(\phi + 2\Delta\phi, \lambda) + \\ & n(O^+)^{smo\lambda,t_n-\Delta t}(\phi - 2\Delta\phi, \lambda) - 4(n(O^+)^{smo\lambda,t_n-\Delta t}(\phi + \Delta\phi, \lambda) + \\ & n(O^+)^{smo\lambda,t_n-\Delta t}(\phi - \Delta\phi, \lambda)) + 6n(O^+)^{t_n-\Delta t}(\phi + \Delta\phi, \lambda)] \end{aligned} \quad (6.178)$$

with  $f_{smo} = 0.003$ . The smoothed number density is added to the explicit term  $T_{2,explicit}$

$$T_{3,explicit} = T_{2,explicit} - \frac{n(O^+)^{smo,t_n-\Delta t}}{2\Delta t} \quad (6.179)$$

The tridiagonal solver need the equation in the following form:

$$\begin{aligned} P(k, i)n^{t+\Delta t}(k-1, i) + Q(k, i)n^{t+\Delta t}(k, i) + \\ R(k, i)n^{t+\Delta t}(k+1, i) = T_{explicit}(k, i) \end{aligned} \quad (6.180)$$

with the height index  $k$  for  $z + \frac{1}{2}\Delta z$ ,  $k+1$  for  $z + \frac{3}{2}\Delta z$ , and  $k-1$  for  $z - \frac{1}{2}\Delta z$ . The longitude index is denoted by  $i$ . Note that the equation is solved at each latitude  $\lambda$  with the index  $j$ .

The fourth and sixth term of the  $O^+$  transport equation eq.(6.139) are treated implicit with the fourth term being

$$[(\mathbf{b}_h \cdot \nabla_h)Kb_z] \left[ \left( \frac{1}{H} \frac{\partial}{\partial Z} (2T_p n) + \frac{mg}{k_B} n \right) \right]$$

and the sixth term

$$\left( b_z \frac{1}{H} \frac{\partial}{\partial Z} + \nabla \cdot \mathbf{b} \right) Kb_z \left( \frac{1}{H} \frac{\partial}{\partial Z} (2T_p n) + \frac{mg}{k_B} n \right)$$

$$P_1((z + \frac{1}{2}\Delta z), \phi) = T_{5m}(z + \frac{1}{2}\Delta z, \phi) D_A(z, \phi) S_m(z + \frac{1}{2}\Delta z, \phi) \quad (6.181)$$

$$\begin{aligned} Q_1((z + \frac{1}{2}\Delta z), \phi) = & - (T_{5p}(z + \frac{1}{2}\Delta z, \phi) D_A(z + \Delta z, \phi) S_m(z + \frac{3}{2}\Delta z, \phi) + \\ & T_{5m}(z + \frac{1}{2}\Delta z, \phi) D_A(z, \phi) S_p(z + \frac{1}{2}\Delta z, \phi)) \end{aligned} \quad (6.182)$$

$$R_1((z + \frac{1}{2}\Delta z), \phi) = T_{5p}(z + \frac{1}{2}\Delta z, \phi) D_A(z + \Delta z, \phi) S_p(z + \frac{3}{2}\Delta z, \phi) \quad (6.183)$$

for the terms please see equations (6.167),(6.166), (6.172),(6.177),and (6.176).  
The term  $\mathbf{b} \cdot \mathbf{v}_n$  is determined

$$\begin{aligned} T_6(z + \frac{1}{2}\Delta z) = & b_x u_n(z + \frac{1}{2}\Delta z) + b_y v_n(z + \frac{1}{2}\Delta z) + \\ & H(z + \frac{1}{2}\Delta z) b_z W(z + \frac{1}{2}\Delta z) \end{aligned} \quad (6.184)$$

Note that the dimensionless vertical velocity  $W$  is on the interface level  $z, z + \Delta z, \dots$

Part of the seventh term in eq. (6.139) which is

$$(b_z \frac{1}{H} \frac{\partial}{\partial Z})(\mathbf{b} \cdot \mathbf{v}_n)$$

and the ninth term

$$B^2 \mathbf{v}_{ExB,z} \frac{1}{H} \frac{\partial}{\partial Z} \left( \frac{n}{B^2} \right)$$

are treated implicit leading to ??? who is this done???

$$\begin{aligned} P_2((z + \frac{1}{2}\Delta z), \phi) = & P_1 + b_z \mathbf{b} \cdot \mathbf{v}_n((z + \frac{1}{2}\Delta z), \phi) + \\ & \mathbf{v}_{ExB,z}((z + \frac{3}{2}\Delta z), \phi) \frac{1}{2H(z + \frac{3}{2}\Delta z), \phi) \Delta z} \end{aligned} \quad (6.185)$$

$$Q_2((z + \frac{1}{2}\Delta z), \phi) = Q_1 - \mathbf{v}_{ExB,z}((z + \frac{1}{2}\Delta z), \phi) \frac{6}{R_E} \quad (6.186)$$

$$\begin{aligned} R_2((z + \frac{1}{2}\Delta z), \phi) = & R_1 - b_z \mathbf{b} \cdot \mathbf{v}_n((z + \frac{3}{2}\Delta z), \phi) + \\ & \mathbf{v}_{ExB,z}((z + \frac{1}{2}\Delta z), \phi) \frac{1}{2H(z + \frac{1}{2}\Delta z), \phi) \Delta z} \end{aligned} \quad (6.187)$$

The coefficients at the upper and lower boundary are set to

$$\begin{aligned}
 P_2^*((z_{bot} + \frac{1}{2}\Delta z), \phi) &= P_2((z_{bot} + \frac{1}{2}\Delta z), \phi) + b_z[2\mathbf{b} \cdot \mathbf{v}_n((z_{bot} + \frac{1}{2}\Delta z), \phi) \\
 &\quad - \mathbf{b} \cdot \mathbf{v}_n((z_{bot} + \frac{3}{2}\Delta z), \phi)] \\
 &\quad + \mathbf{v}_{ExB,z}((z_{bot} + \frac{1}{2}\Delta z), \phi) \frac{1}{2H(z_{bot} + \frac{1}{2}\Delta z), \phi) \Delta z}
 \end{aligned} \tag{6.188}$$

$$\begin{aligned}
 Q_2^*((z_{top} - \frac{1}{2}\Delta z), \phi) &= Q_2((z_{top} - \frac{1}{2}\Delta z), \phi) \\
 &\quad - \mathbf{v}_{ExB,z}((z_{top} - \frac{1}{2}\Delta z), \phi) \frac{6}{R_E}
 \end{aligned} \tag{6.189}$$

$$\begin{aligned}
 R_2^*((z_{top} - \frac{1}{2}\Delta z), \phi) &= R_2((z_{top} - \frac{1}{2}\Delta z), \phi) - b_z[2\mathbf{b} \cdot \mathbf{v}_n((z_{top} - \frac{1}{2}\Delta z), \phi) \\
 &\quad - \mathbf{b} \cdot \mathbf{v}_n((z_{top} - \frac{3}{2}\Delta z), \phi)] \\
 &\quad + \mathbf{v}_{ExB,z}((z_{top} - \frac{1}{2}\Delta z), \phi) \frac{1}{2H(z_{top} - \frac{1}{2}\Delta z), \phi) \Delta z}
 \end{aligned} \tag{6.190}$$

We add the other part of the seventh term in the transport equation (6.139)??  
check  $b_z$  where does it come from???

$$(\nabla \cdot \mathbf{b})(\mathbf{b} \cdot \mathbf{v}_n n)$$

and the time derivative of the number density of  $n(O^+)$  to the Q-coefficient

$$Q_3((z + \frac{1}{2}\Delta z), \phi) = Q_2 - (b_z \nabla \cdot \mathbf{b}(\phi))(\mathbf{b} \cdot \mathbf{v}_n((z + \frac{1}{2}\Delta z), \phi)) - \frac{1}{2\Delta t} \tag{6.191}$$

The upper boundary condition is defined by

$$-b_z^2 D_a \left( T_p \frac{\partial}{H \partial Z} + \frac{mg}{R^*} \right) n = F^{O^+} \tag{6.192}$$

with  $F^{O^+}$  the flux of  $O^+$  from and to the plasmasphere, which was defined in eq. (6.143) and (6.144).

$$B = -b_z^2 D_a(z_{top}) S_m(z_{top} + \frac{1}{2}\Delta z) \tag{6.193}$$

$$A = -b_z^2 D_a(z_{top}) S_p(z_{top} + \frac{1}{2}\Delta z) \tag{6.194}$$

with  $S_m = 2T_p \frac{\partial}{\partial Z} + \frac{mg}{R^*}$  from eq. (6.171) leading to

$$Q_3^*((z_{top} - \frac{1}{2}\Delta z), \phi) = Q_3((z_{top} - \frac{1}{2}\Delta z), \phi) + \frac{B}{A}R_2^*((z_{top} - \frac{1}{2}\Delta z), \phi) \quad (6.195)$$

and for the right hand side

$$T_{3,explicit}^*((z_{top} - \frac{1}{2}\Delta z), \phi) = T_{3,explicit}((z_{top} - \frac{1}{2}\Delta z), \phi) - F^{O^+} R_2^*((z_{top} - \frac{1}{2}\Delta z), \phi) \frac{1}{A} \quad (6.196)$$

The source and sink terms are calculated

$$n(XIO^+(^2P)) = \frac{1}{2} \left( Q(O^+(^2P))(z) + Q(O^+(^2P))(z + \frac{1}{2}\Delta z) \right) \frac{1}{(k_{16} + k_{17})n(N_2) + k_{18}n(O) + (k_{19} + k_{20})N_e(z??) + k_{21} + k_{22}} \quad (6.197)$$

$$n(XIO^+(^2D)) = \frac{1}{2} \left( Q(O^+(^2D))(z) + Q(O^+(^2D))(z + \frac{1}{2}\Delta z) \right) + \frac{(k_{20}N_e(z??) + k_{22})n(XIO^+(^2P))}{k_{23}n(N_2) + k_{24}n(O) + k_{26}n(O_2)} \quad (6.198)$$

$$L^{O^+} = k_1n(O_2) + k_2n(N_2) + k_{10}n(N(^2D)) \quad (6.199)$$

The loss term  $L^{O^+}$  is added to the left hand side

$$Q_4((z + \frac{1}{2}\Delta z), \phi) = Q_3((z + \frac{1}{2}\Delta z), \phi) - L^{O^+} \quad (6.200)$$

The right hand side is updated by

$$T_{4,explicit}((z + \frac{1}{2}\Delta z), \phi) = T_{3,explicit}((z + \frac{1}{2}\Delta z), \phi) - Q(O^+) - (k_{19}N_e(z) + k_{21})n(XIO^+(^2P)) - (k_{25}N_e(z) + k_{27})n(XIO^+(^2D)) - (k_{18}n(XIO^+(^2P)) + k_{24}n(XIO^+(^2D)))n(O) \quad (6.201)$$

The lower boundary condition is specified by photochemical equilibrium  $n = \frac{Q}{L}$  leading to

$$Q_4^*((z_{bot} + \frac{1}{2}\Delta z), \phi) = Q_4((z_{bot} + \frac{1}{2}\Delta z), \phi) - P_2((z_{bot} + \frac{1}{2}\Delta z), \phi) \quad (6.202)$$

$$T_{4,explicit}^*((z_{bot} + \frac{1}{2}\Delta z), \phi) = T_{4,explicit}((z_{bot} + \frac{1}{2}\Delta z), \phi) - 2P_2((z_{bot} + \frac{1}{2}\Delta z), \phi) \frac{Q(O^+)}{1.5L^{O^+}(z_{bot} + \frac{1}{2}\Delta z) - 0.5L^{O^+}(z_{bot} + \frac{3}{2}\Delta z)} \quad (6.203)$$

$$P_2^*((z_{bot} + \frac{1}{2}\Delta z), \phi) = 0 \quad (6.204)$$

Solving for the number density of  $O^+$  at each latitude leads to the updated number densities  $n(O^+)_{upd,t_n+\Delta t}$  at the midpoints. The calculated values for the number density of  $n(O^+)_{upd,t+\Delta t}$  are smoothed by a Fast Fourier transformation leading to  $n(O^+)_{smo}^{upd,t+\Delta t}$ . All the wave numbers larger than a predefined value at each latitude are removed. The wave numbers are defined in the module `cons.F???`. The values of the number densities at the timestep  $t_n$  are also updated by using

$$n(O^+)_{upd,t} = \frac{1}{2}(1 - c_{smo})(n(O^+)^{t-\Delta t} + n(O^+)_{smo}^{upd,t+\Delta t}) + c_{smo}n(O^+)^{t_n} \quad (6.205)$$

with  $c_{smo} = 0.95$  The upper boundary values are set to zero

$$n(O^+)_{upd,t_n}(z_{top} - \frac{1}{2}\Delta z) = 0 \quad (6.206)$$

$$n(O^+)_{smo}^{upd,t_n}(z_{top} - \frac{1}{2}\Delta z) = 0 \quad (6.207)$$

and the number density is set such that it has a minimum value of  $1 \cdot 10^{-5}$ .

$$n(O^+)_{upd,t_n}(z + \frac{1}{2}\Delta z) \geq 1 \cdot 10^{-5} \quad (6.208)$$

$$n(O^+)_{smo}^{upd,t_n}(z + \frac{1}{2}\Delta z) \geq 1 \cdot 10^{-5} \quad (6.209)$$

physical field	variable	unit	pressure level	timestep
neutral temperature	$T_n$	$K$	midpoints	$t_n$
neutral zonal velocity	$u_n$	$cm/s$	midpoints	$t_n$
neutral meridional velocity	$v_n$	$cm/s$	midpoints	$t_n$
dimensionless vertical velocity	$W^{t+\Delta t}$	$1/s$	interfaces	$t + \Delta t$
mass mixing ratio $O_2$	$\Psi_{O_2}$	—	midpoints	$t_n$
mass mixing ratio $O$	$\Psi_O$	—	midpoints	$t_n$
mean molecular mass	$\bar{m}$	$g/mol$	interfaces	$t_n + \Delta t$
electron temperature	$T_e$	$K$	midpoints	$t_n$
ion temperature	$T_i$	$K$	midpoints	$t_n$
electron density	$N_e$	$\#/cm^3$	interfaces	$t_n$
number density of $N_2(D)??$	$n(N_2(D))??$	$\#/cm^3$	midpoints	$t_n$
electrodynamic drift velocity	$v_{ExB,x}$	$cm/s$	interface	$t_n$
electrodynamic drift velocity	$v_{ExB,y}$	$cm/s$	interfaces	$t_n$
electrodynamic drift velocity	$v_{ExB,z}$	$cm/s$	interfaces	$t_n$
conversion factor $mmr$ to $\#/cm^3$	$N\bar{m}$	$\frac{\#g}{cm^3mole}$	midpoints???	$t_n$
number density of $O^+$	$n(O^+)^{t_n}$	$\#/cm^3$	midpoints???	$t_n$
number density of $O^+$	$n(O^+)^{t_n-\Delta t}$	$\#/cm^3$	midpoints???	$t_n - \Delta t$

Table 6.10: Input fields to subroutine oplus



physical field	variable	unit	pressure level	timestep
number density of $O^+$	$n(O^+)^{upd,t_n}$	$\#/cm^3$	midpoints???	$t_n$
number density of $O^+$	$n(O^+)^{upd,t_n+\Delta t}$	$\#/cm^3$	midpoints???	$t_n + \Delta t$

Table 6.11: Output fields of subroutine oplus

physical field	variable	unit	pressure level	timestep
heating from solar radiation ???	$Q(^2P)$	$\frac{erg}{Ks} ???$	interfaces	$t_n$
heating from solar radiation	$Q(O^+(^2D))$	$\frac{erg}{Ks} ???$	interfaces	$t_n$
heating from solar radiation ????	$Q(O^+)$	$\frac{erg}{Ks} ???$	interfaces	$t_n$
chemical reaction rates	$k_i$	??	-	-???

Table 6.12: Module data of subroutine oplus

# Chapter 7

## Electrodynamics

## 7.1 Introduction

This report presents the governing equations, physical parameterizations and numerical algorithms used in the NCAR Thermosphere-Ionosphere-Electrodynamics GCM version 1.8. The model description provides help on the major model component, numerics and coding implementation.

The electrodynamic part of TIEGCM is a serial code, which uses finite differencing to discretize the stationary electrostatic equation. We assume that the field-lines are equipotential which reduces the 3D equation to 2D. In addition, at low- and mid-latitude hemispheric symmetry of the electric potential is assumed and therefore the electrodynamic equation is only solved in one hemisphere. At high latitudes the electric potential is prescribed from empirical models e.g. Heelis or Weimer [literature].

Conventions	
<b>command</b>	bold
<i>template filenames</i>	italics
flags	medium bold
<i>directories, files</i>	slanted
<b>source code</b>	typewrite
<i>keywords</i>	emphasize

## 7.2 Steady-State Electrodynamic Equations

The basic equations of the steady state electrodynamics are shown in this chapter. If an equation is taken from [14], then the additional equation number refers to the equation number in [14]. In the following the presentation of the equations is based on the coding in the source code and might not look straight forward in many places. For the location in the source code of the equations it is referred to the `subroutine names`.

For longer time scales it is valid to assume steady state electrodynamics with a divergence free current density  $\mathbf{J}$ . It is also assumed that the conductivity along the magnetic field line is very high, thus there is no electric field component in this direction. Therefore the electrodynamics equation can be reduced to a two dimensional equation.

The current density is divergence free

$$\nabla \cdot \mathbf{J} = 0 \quad (7.1)$$

The current density has an ohmic component transverse to the magnetic field and parallel to the magnetic field line  $\mathbf{J}_{\parallel}$  and a non-ohmic magnetospheric component  $\mathbf{J}_M$ . In the TIEGCM only the ohmic component transverse to the magnetic field is considered by default. The other two components can be added by the user which is discussed later in chapter 7.7.3 and 7.7.3. The total current density is expressed by (eq. 2.1 in [14])

$$\mathbf{J} = \sigma_P(\mathbf{E} + \mathbf{u} \times \mathbf{B}) + \sigma_H \mathbf{b} \times (\mathbf{E} + \mathbf{u} \times \mathbf{B}) + \mathbf{J}_{\parallel} + \mathbf{J}_M \quad (7.2)$$

with  $\sigma_P$  and  $\sigma_H$  the Pedersen and Hall conductivities. The neutral wind is denoted by  $\mathbf{u}$ , the electric field by  $\mathbf{E}$  and the geomagnetic field by  $\mathbf{B}$  with  $\mathbf{b}$  the unit vector parallel to  $\mathbf{B}$ .

The following relations are used to derive the electrodynamics equation. For details it is referred to [14]. Apex coordinates are used with two sets of base vectors  $\mathbf{e}_i$  and  $\mathbf{d}_j$  which are calculated in `subroutine apxparm` (see chapter 7.4). The directions of  $\mathbf{e}_1$  and  $\mathbf{d}_1$  are more or less in magnetic eastward,  $\mathbf{e}_2$  and  $\mathbf{d}_2$  in downward or equatorward, and  $\mathbf{e}_3$  and  $\mathbf{d}_3$  in field line

direction. (eq. 3.11- 3.13 in [14])

$$\mathbf{e}_1 = \mathbf{d}_2 \times \mathbf{d}_3 \quad (7.3)$$

$$\mathbf{e}_2 = \mathbf{d}_3 \times \mathbf{d}_1 \quad (7.4)$$

$$\mathbf{e}_3 = \mathbf{d}_1 \times \mathbf{d}_2 \quad (7.5)$$

with (eq. 3.8- 3.10 in [14])

$$\mathbf{d}_1 = R_0 \cos \lambda_m \nabla \phi_m \quad (7.6)$$

$$\mathbf{d}_2 = -R_0 \sin I_m \nabla \lambda_m \quad (7.7)$$

$$\mathbf{d}_3 = \frac{\mathbf{b}_0}{|\mathbf{d}_1 \times \mathbf{d}_2|} \quad (7.8)$$

The geomagnetic longitude and apex latitude are  $\phi_m$  and  $\lambda_m$ ,  $I_m$  is the inclination of the geomagnetic field,  $R_0$  the radius to the reference height  $R_E + h_0$ , and  $\mathbf{b}_0$  the unit vector in the direction of the geomagnetic field. The neutral wind  $\mathbf{u}$  and the electric field  $\mathbf{E}$  can be expressed in terms of the base vectors which has the advantage that the components are constant along a magnetic field line (eq. 4.5 in [14]).

$$\mathbf{u} = u_{e1}\mathbf{e}_1 + u_{e2}\mathbf{e}_2 \quad \text{with} \quad u_{ei} = \mathbf{u} \cdot \mathbf{d}_i \quad (7.9)$$

$$\mathbf{E} = E_{d1}\mathbf{d}_1 + E_{d2}\mathbf{d}_2 \quad \text{with} \quad E_{di} = \mathbf{E} \cdot \mathbf{e}_i \quad (7.10)$$

The geomagnetic field  $\mathbf{B}$  is approximated by the main field  $\mathbf{B}_0$ . We are using the International Geomagnetic Reference Field (IGRF2000) in TIEGCM and ignore the magnetic perturbation  $\Delta\mathbf{B}$  due to the external currents (eq. 3.10, 3.15, 4.4 in [14]).

$$\mathbf{B}_0 = B_{e3}\mathbf{e}_3 \quad (7.11)$$

$$\mathbf{b}_0 = \mathbf{d}_3 D \quad \text{with} \quad D = |\mathbf{d}_1 \times \mathbf{d}_2| \quad (7.12)$$

The current density can be expressed by

$$\mathbf{J} = \sum_{i=1}^3 J_{ei}\mathbf{e}_i \quad \text{with} \quad J_{ei} = \mathbf{J} \cdot \mathbf{d}_i \quad (7.13)$$

Using all the equations from above leads to the current density components  $J_{e1}$  and  $J_{e2}$  (eq. 5.7, 5.8 in [14])

$$J_{e1} = \sigma_P d_1^2 (E_{d1} + u_{e2} B_{e3}) + (\sigma_H \mathbf{d}_1 \cdot \mathbf{d}_2 - \sigma_H D) (E_{d2} - u_{e1} B_{e3}) \quad (7.14)$$

$$J_{e2} = (\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2 + \sigma_H D) (E_{d1} + u_{e2} B_{e3}) + \sigma_P d_2^2 (E_{d2} - u_{e1} B_{e3}) \quad (7.15)$$

The height integrated current density in magnetic eastward and downward/equatorward direction are  $K_{m\phi}$  and  $K_{m\lambda}$ . Knowing the current density  $\mathbf{J}$  the height integrated components can be calculated by (eq. 5.1, 5.2 in [14])

$$K_{m\phi} = |\sin I_m| \int_{s_L}^{s_U} \frac{J_{e1}}{D} ds \quad (7.16)$$

$$K_{m\lambda} = \mp \int_{s_L}^{s_U} \frac{J_{e2}}{D} ds \quad (7.17)$$

with the index  $(\cdot)_m$  standing for modified apex (see chapter 7.4). The integration is done along the field line and  $s_L$  and  $s_U$  are the lower and upper boundary of the ionosphere, i.e. in the TIEGCM v 1.7 model 90 km to the top of the model. The electrostatic field is the gradient of the electric potential. Therefore the component of the electric field are (eq. 5.9, 5.10 in [14])

$$E_{m\phi} = E_{d1} = -\frac{1}{R \cos \lambda_m} \frac{\partial \Phi}{\partial \phi_m} \quad (7.18)$$

$$E_{m\lambda} = -E_{d2} \sin I_m = -\frac{1}{R} \frac{\partial \Phi}{\partial \lambda_m} \quad (7.19)$$

Inserting equations (7.18) and (7.19) into the current density component expressions (7.14) and (7.15), which then can be used to calculate the height integrated current density in equations (7.16) and (7.17). This leads to (eq. 5.11, 5.12 in [14])

$$K_{m\phi} = \Sigma_{\phi\phi} E_{m\phi} + \Sigma_{\phi\lambda} E_{m\lambda} + K_{m\phi}^D \quad (7.20)$$

$$K_{m\lambda} = \Sigma_{\lambda\phi} E_{m\phi} + \Sigma_{\lambda\lambda} E_{m\lambda} + K_{m\lambda}^D \quad (7.21)$$

The terms  $K_{m\phi}^D$  and  $K_{m\lambda}^D$  are the wind driven height integrated current densities which are the driving forces (eq. 5.19, 5.20 in [14]).

$$K_{m\phi}^D = B_{e3} |\sin I_m| \int_{s_L}^{s_U} \left[ \frac{\sigma_P d_1^2}{D} u_{e2} + \left( \sigma_H - \frac{\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2}{D} \right) u_{e1} \right] ds \quad (7.22)$$

$$K_{m\lambda}^D = \mp B_{e3} \int_{s_L}^{s_U} \left[ \left( \sigma_H + \frac{\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2}{D} \right) u_{e2} - \frac{\sigma_P d_2^2}{D} u_{e1} \right] ds \quad (7.23)$$

The conductances in the equations (7.20) and (7.21) are (eq. 5.13–5.18 in

[14])

$$\Sigma_{\phi\phi} = |\sin I_m| \int_{s_L}^{s_U} \frac{\sigma_P d_1^2}{D} ds \quad (7.24)$$

$$\Sigma_{\lambda\lambda} = \frac{1}{|\sin I_m|} \int_{s_L}^{s_U} \frac{\sigma_P d_2^2}{D} ds \quad (7.25)$$

$$\Sigma_H = \int_{s_L}^{s_U} \sigma_H ds \quad (7.26)$$

$$\Sigma_C = \int_{s_L}^{s_U} \frac{\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2}{D} ds \quad (7.27)$$

$$\Sigma_{\phi\lambda} = \pm(\Sigma_H - \Sigma_C) \quad (7.28)$$

$$\Sigma_{\lambda\phi} = \mp(\Sigma_H + \Sigma_C) \quad (7.29)$$

$$(7.30)$$

Since current continuity applies, the divergence of the horizontal current  $K_{m\phi}$  and  $K_{m\lambda}$  has to be balanced by an upward current density  $J_{mr}$  at the top of the ionospheric current sheet layer. (eq. 5.3 in [14])

$$J_{mr} = \frac{-1}{R \cos \lambda_m} \left( \frac{\partial K_{m\phi}}{\partial \phi_m} + \frac{\partial K_{m\lambda} \cos \lambda_m}{\partial \lambda_m} \right) \quad (7.31)$$

Inserting the height integrated current densities (7.20) and (7.21) into equation (7.31) and assuming that in the closed field line region the field lines are equipotential leads to (eq. 5.23 in [14])

$$\begin{aligned} & \frac{\partial}{\partial \phi_m} \left( \frac{\Sigma_{\phi\phi}^T}{\cos \lambda_m} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\phi\lambda}^T \frac{\partial \Phi}{\partial |\lambda_m|} \right) + \frac{\partial}{\partial |\lambda_m|} \left( \Sigma_{\lambda\phi}^T \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\lambda\lambda}^T \cos \lambda_m \frac{\partial \Phi}{\partial |\lambda_m|} \right) \\ &= R \frac{\partial K_{m\phi}^{DT}}{\partial \phi_m} + R \frac{\partial K_{m\lambda \cos \lambda_m}^{DT}}{\partial |\lambda_m|} + R^2 \cos \lambda_m J_{Mr} \end{aligned} \quad (7.32)$$

with  $\frac{\partial}{\partial |\lambda_m|} = -\frac{\partial^{SH}}{\partial \lambda_m} = \frac{\partial^{NH}}{\partial \lambda_m}$  and  $J_{Mr} = J_{mr}^{SH} + J_{mr}^{NH}$ . The values  $(\cdot)^T$  denote the sum of the values from northern  $(\cdot)^{NH}$  and southern  $(\cdot)^{SH}$  hemisphere

(eq. 5.24–5.29 [14])

$$\Sigma_{\phi\phi}^T = \Sigma_{\phi\phi}^{NH} + \Sigma_{\phi\phi}^{SH} \quad (7.33)$$

$$\Sigma_{\lambda\lambda}^T = \Sigma_{\lambda\lambda}^{NH} + \Sigma_{\lambda\lambda}^{SH} \quad (7.34)$$

$$\Sigma_{\lambda\phi}^T = \Sigma_{\lambda\phi}^{NH} - \Sigma_{\lambda\phi}^{SH} \quad (7.35)$$

$$\Sigma_{\phi\lambda}^T = \Sigma_{\phi\lambda}^{NH} - \Sigma_{\phi\lambda}^{SH} \quad (7.36)$$

$$K_{m\phi}^{DT} = K_{m\phi}^{D,NH} + K_{m\phi}^{D,SH} \quad (7.37)$$

$$K_{m\lambda}^{DT} = K_{m\lambda}^{D,NH} - K_{m\lambda}^{D,SH} \quad (7.38)$$

In the source code the electrodynamic equation (7.32) is divided by  $\frac{\partial\lambda_m}{\cos\lambda_0\partial\lambda_0}$  with  $\lambda_0$  the equally spaced distribution in modified apex latitudes  $\lambda_m$  which is irregular spaced. The latitudinal distribution is explained in more detail in section 7.5.



physical field	variable	unit	pressure level	timestep
neutral zonal wind	$u_n$	$\frac{cm}{s}$	half	$t_n$
neutral meridional wind	$v_n$	$\frac{cm}{s}$	half	$t_n$
dimensionless vertical wind	$W$	$\frac{1}{s}$	full	$t_n$
geopotential height	$z$	cm	full	$t_n + \Delta t$
Pedersen conductivity	$\sigma_P$	S/m	half	$t_n$
Hall conductivity	$\sigma_H$	S/m	half	$t_n$
mean molecular mass	$\overline{m}$	$\frac{g}{mole}$	full	$t_n + \Delta t$
neutral temperature	$T_n$	$K$	half	$t_n$

Table 7.1: Input fields to subroutine `prep-dynamo`

### 7.3 Input to the Electrodynamo

In subroutine `prep-dynamo` fields are prepared for the electrodynamo calculation. The preparation includes reversing the order of the indexing, as well as gathering the fields from the different processors to the master processor. The electrodynamo part is still serial and therefore a gathering of all the subdomains at the beginning and a distribution of the fields to all the subdomains at the end has to be done.

The input to subroutine `prep-dynamo` is summarized in table 7.1. To calculate the vertical neutral velocity  $w_n$  the pressure scale height  $H$  in  $[cm]$  is determined at first, assuming hydrostatic equilibrium for timescales longer than a few minutes.

$$H = \frac{R^* T_n}{\overline{m} g} \quad (7.39)$$

with  $R^*$  the gas constant in  $[\frac{erg}{mole K}]$ ,  $T_n$  the neutral temperature in  $[K]$ ,  $\overline{m}$  the mean molecular mass in  $[\frac{g}{mole}]$  and  $g$  acceleration of gravity in  $[\frac{cm}{s^2}]$ . The dimensionless vertical wind  $W$  is

$$W = -\frac{1}{p} \frac{dp}{dt} \quad (7.40)$$

which is used to get the vertical wind at a constant pressure level by

$$w_n = HW \quad (7.41)$$

with the pressure  $p$  and  $\frac{dp}{dt}$  the time rate of change following the fluid motion.

## 7.4 Apex Coordinates

The apex and modified apex coordinate system is described in [14]. The apex latitude  $\lambda_A$  is constant along a field line with an apex height  $h_A$ .

$$\lambda_A = \pm \cos^{-1} \left( 1 + \frac{h_A}{R_{eq}} \right)^{-1/2} \quad (7.42)$$

with  $R_{eq}$  denoting the Earth radius at the equator and the  $\pm$  sign for the location of the field line foot point in the northern / southern geomagnetic hemisphere. In the electrodynamic part of TIEGCM modified apex coordinates are used. Modified apex coordinates  $\lambda_m$  have a reference height  $h_R$  associated with them.

$$\lambda_m = \pm \cos^{-1} \left( \frac{R_E + h_R}{R_E + h_A} \right)^{-1/2} \quad (7.43)$$

The mean Earth radius is denoted by  $R_E$  assuming a spherical Earth. The reference height  $h_R$  is assumed to be the bottom boundary of the ionosphere at  $h_R = h_0 = 90\text{km}$ . One of the advantages for using modified apex latitudes  $\lambda_m$  is that the field line foot point latitudes are continuous at the 90 km (for TIEGCM) lower boundary of the model. Apex latitudes, in contrast, would have a gap at low latitudes since only field line with an apex of at least 90 km could be used for the field line integration. The apex longitude  $\phi_A$  and the modified apex longitude  $\phi_m$  are the same. The apex routines are called once per model run from **program** `tgcm`. The only input to the calculation of the apex coordinate system in **subroutine** `apxparm` is the model year. If the electric potential is not calculated in TIEGCM (input flag `dynamo==0`) the magnetic field information as well as the information needed for the mapping to and from the geographic to the geomagnetic grid is read from an existing NetCDF-file. Note that even if the electric potential is not calculated a potential pattern at high latitude can be prescribed.

In the **subroutine** `apxparm` the apex coordinates as well as the geomagnetic main field and the base vectors are determined which are summarized in table 7.2 and later used for the electrodynamic calculation. For each geographic grid point  $\lambda_g, \phi_g$  the modified apex latitude and longitude  $\lambda_m, \phi_m$  is calculated. The north-, east- and downward component, respectively,  $B_x$ ,  $B_y$  and  $B_z$ , of the main field  $\mathbf{B}_0$  and the components of the base vector  $\mathbf{d}_1$  and  $\mathbf{d}_2$  are determined. The base vectors  $\mathbf{d}_1$  and  $\mathbf{d}_2$  are more or less in

variable	description	unit
$\lambda_m, \phi_m$	modified apex coordinates	radian
$B_{e3}(h_0)$	magnetic field component in $\mathbf{e}_3$ direction	nT
$B_z(h_0)$	downward magnetic field component	Gauss
$B_0(h_0)$	main magnetic field strength	Gauss
$\mathbf{d}_1(h_0)$	base vector approx. mag. eastward	-
$\mathbf{d}_2(h_0)$	base vector approx. mag. down-/equatorward	-
$D(h_0)$	$ \mathbf{d}_1 \times \mathbf{d}_2 $	-

Table 7.2: Apex quantities calculated in `subroutine apxparm` and used for the calculation of the electric potential

magnetic eastward and down-/equatorward direction.  $B_{e3}$  is the main field component in  $\mathbf{e}_3$  direction. The vector  $\mathbf{e}_3$  is in the direction of the magnetic field line and decreases with increasing altitude. In addition the quantity  $D$  is calculated with  $D = |\mathbf{d}_1 \times \mathbf{d}_2|$ .

The magnetic field quantities  $B_z(h_0)$  and  $B_0(h_0)$  are in units of [Gauss],  $B_{e3}(h_0)$  is in [nT] and the coordinates  $\lambda_m$  and  $\phi_m$  in [rad] with  $h_0$  the reference height (90 km). The mapping from the geographic to the geomagnetic grid and vice versa is done by bilinear interpolation. For each grid point the surrounding grid points of the other grid are determined and the weighting factor for each of these corner grid points are calculated.

## 7.5 Latitudinal modified apex grid

Within TIEGCM the distribution of the geomagnetic latitudinal grid points is expressed in two different ways. One is the irregular distribution of modified apex latitudes  $\lambda_m^*$  which gives a better distribution of the latitudinal grid points by having more grid points close to the geomagnetic equator and therefore resolves the equatorial electrojet better. The second expression of latitudinal grid point distribution is equally spaced in modified apex latitude  $\lambda_m^*$  and is denoted by  $\lambda_0$ . The relation between the two is expressed by

$$\tan \lambda_m^* = \frac{r_1}{R_0} \tan \lambda_0 + \frac{\tan \lambda_0^{2(\alpha+1)}}{(1 + \tan^2 \lambda_0)^\alpha}^{1/2} \quad (7.44)$$

with  $\alpha = 1.668$  and  $r_1 = 1.06e7$ . The radius  $R_0$  is the radius to the lower boundary of the model at height  $h_0$ . For each equally spaced  $\lambda_0$  the latitude

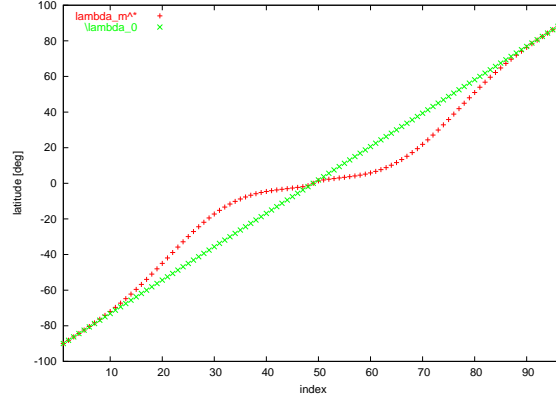


Figure 7.1: Distribution of modified apex latitude points for  $\lambda_0$  (crosses) and  $\lambda_m^*$  (pluses)

$\lambda_m^*$  is calculated. In addition a look up table is set up for equally one degree spaced latitudes  $\lambda_m^*$  with the corresponding  $\lambda_0$  determined by using Newton's methods. All the arrays are set up in `subroutine consdyn`. Figure 7.1 shows the distribution of the grid points for  $\lambda_0$  and  $\lambda_m^*$  for 97 latitudinal grid points.

## 7.6 Mapping from and to the geomagnetic grid

The fields in table 7.3 are mapped from the geographic grid to the geomagnetic grid in `subroutine transf`. `Subroutine transf` is called from `subroutine dynamo` once per timestep. The lower boundary of the TIEGCM model (up to version 1.8) is at 97 km, however the field line integration starts at  $h_0 = 90$  km altitude, where the lower boundary of the ionosphere is assumed to lie. Therefore the fields in table 7.3 needed for the field line integration have to be extended downward. Three additional height levels ( $k=-2$  to 0) are introduced with  $k$  being the height index. The geopotential height  $z$  is linearly extrapolated and the conductivities are assumed to vary

variable	description	unit	dimension
$\sigma_P$	Pedersen conductivity	S/m	3D
$\sigma_H$	Hall conductivity	S/m	3D
$z$	geopotential height	cm	3D
$\sin I_m(h_0)$	inclination angle	-	2D
$B_{e3}(h_0)$	magnetic field component	T	2D
$\frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}(h_0)$	base vector quantity	-	2D
$\frac{\mathbf{d}_1 \cdot \mathbf{d}_1}{D}(h_0)$	base vector quantity	-	2D
$\frac{\mathbf{d}_2 \cdot \mathbf{d}_2}{D}(h_0)$	base vector quantity	-	2D
$u_{e1}, u_{e2}$	neutral wind components	$\frac{m}{s}$	3D

Table 7.3: Mapped fields in subroutine `transf`

exponentially.

$$z(k) = h_0 + (k + 2) \left( \frac{z(k = 1) - h_0}{3} \right) \quad \text{for } k=0 \text{ to } -2 \text{ by } -1 \quad (7.45)$$

$$\sigma_P(k') = \sigma_P(k' = 1) \exp \left( \frac{z(k + \frac{1}{2}) - z(k = 1\frac{1}{2})}{fac_{ped}} \right) \quad \text{for } k' = 0 \text{ to } -2 \text{ by } -1 \quad (7.46)$$

$$\sigma_H(k') = \sigma_H(k' = 1) \exp \left( \frac{z(k + \frac{1}{2}) - z(k = 1\frac{1}{2})}{fac_{hall}} \right) \quad \text{for } k' = 0 \text{ to } -2 \text{ by } -1 \quad (7.47)$$

Note that the geopotential height is saved on full pressure levels ( $k$ ) and the conductivities on half pressure levels ( $k' = k + \frac{1}{2}$ ). Therefore the geopotential height  $z$  for the conductivity extension (eq. 7.46 and 7.47) is calculated at half pressure levels denoted by e.g.  $k' = k + \frac{1}{2}$ . The factors at which the conductivities are assumed to decay below the lower boundary of the model are  $fac_{ped} = 5. \times 10^5$  and  $fac_{hall} = 3. \times 10^5$

The neutral winds  $\mathbf{u}$  are assumed to be constant between  $h_0=90$  to 97 km and can be expressed by

$$\mathbf{u} = \mathbf{e}_1 u_{e1} + \mathbf{e}_2 u_{e2} \quad (7.48)$$

with the base vectors  $\mathbf{e}_i$  (see [14]). The base vectors  $\mathbf{d}_i$  and  $\mathbf{e}_i$  satisfy  $\mathbf{d}_i \mathbf{e}_j = \delta_{ij}$  with  $\delta_{ij}$  the Kronecker delta. The components  $u_{e1}$  in magnetic eastward

and  $u_{e2}$  in down-/equatorward direction at altitude  $h$  are calculated by

$$u_{e1}(h) = \mathbf{d}_1(h) \cdot \mathbf{u}(h) \quad (7.49)$$

$$u_{e2}(h) = \mathbf{d}_2(h) \cdot \mathbf{u}(h) \quad (7.50)$$

The height variation of  $\mathbf{d}_1(h)$  and  $\mathbf{d}_2(h)$  is determined by

$$\mathbf{d}_1(h) = \left[ \frac{R_E + h_0}{R_E + h} \right]^{3/2} \mathbf{d}_1(h_0) \quad (7.51)$$

$$\mathbf{d}_2(h) = \left[ \frac{R_E + h_0}{R_E + h} \right]^{3/2} \sqrt{\frac{4. - 3.\cos^2 \lambda_m(h_0)}{(4. - 3.\frac{R_E + h_0}{R_E + h} \cos^2 \lambda_m(h_0))}} \mathbf{d}_2(h_0) \quad (7.52)$$

with  $\lambda_m(h_0)$  the modified apex value at height  $h_0$  which is kept constant vertically and thus representing the quasi-dipole latitude. In addition the following quantities are calculated

$$\frac{\mathbf{d}_1 \cdot \mathbf{d}_1}{D} \quad (7.53)$$

$$\frac{\mathbf{d}_2 \cdot \mathbf{d}_2}{D} \quad (7.54)$$

$$\frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D} \quad (7.55)$$

These values are calculated at height  $h_0$ . The values at the pole need special treatment since we have different longitudinal grid points for one spatial point. Therefore the pole values are extrapolated from the longitudinal averaged values next to the pole.

$$x(l_{pole}) = \frac{9 \sum_{lon} x(l_{pole} \pm 1) - \sum_{lon} x(l_{pole} \pm 2)}{8 nlon} \quad (7.56)$$

with the latitudinal index of the pole  $l_{pole}$  and  $x(l_{pole} \pm 1)$  denoting the values one grid point off the south- and northpole respectively. The number of geographic longitudinal grid points is  $nlon$  and  $\sum_{lon}$  denotes the sum over all longitudinal grid points. The following fields are processed:  $z(h)$ ,  $\sigma_P(h)$ ,  $\sigma_H(h)$ ,  $u_{e1}(h)$ ,  $u_{e2}(h)$ ,  $\frac{\mathbf{d}_1 \cdot \mathbf{d}_1}{D}$ ,  $\frac{\mathbf{d}_2 \cdot \mathbf{d}_2}{D}$ ,  $\frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}$ ,  $\sin I_m$ ,  $B_{e3}$ . In addition, periodic points for these fields are added.

The mapping from the geographic to the geomagnetic grid is done for each latitude separately right before the integration along the field line which foot point at this latitude. The field line integration is described in section 7.8.

The geomagnetic equatorial values  $\sigma_{P,eq}(h)$ ,  $\sigma_{H,eq}(h)$ ,  $u_{e1,eq}(h)$ ,  $u_{e2,eq}(h)$  have to be known at each geomagnetic latitude and therefore are calculated before the field line integration is done. The mapping from the geographic to the geomagnetic grid is done by a bilinear interpolation. The surrounding geographic grid points for each geomagnetic grid point and the weighting factors for each of the geographic points are determined in **subroutine** `apxparm`.



## 7.7 High Latitude Input

### 7.7.1 Weimer

To use the high latitude potential as defined by Weimer the flag `POTENTIAL_MODEL = WEIMER` in the input file of a TIEGCM has to be set. However the Weimer high latitude potential is not working in the version 1.7 and 1.8 of TIEGCM. Please check newer version carefully.

### 7.7.2 Heelis

At high latitude the electric potential pattern can be prescribed as determined by Heelis. The calculation of the electric potential due to Heelis is not described since we didn't work on this part of the code. The Heelis potential pattern is the default if the flag `POTENTIAL_MODEL` is not specified. The Heelis model is also the basis for the high latitude modifications described in the following sections. Therefore when using these modifications the flag `POTENTIAL_MODEL = HEELIS` should be set in the input file.

### 7.7.3 Modification of the high latitude input

In the electrodynamic equation (7.32) we neglected so far the current part  $J_{Mr}$  between the ionosphere and magnetosphere. The current from the magnetosphere can be influenced by the electric field distribution, however the mechanism is not fully understood. The total field-aligned current between ionosphere and magnetosphere can be described as the divergence of a magnetospheric current  $\mathbf{K}^M$

$$J_{Mr} = \frac{1}{R_0 \cos \lambda_m} \left( \frac{\partial K_\phi^M}{\partial \phi_m} + \frac{\partial K_{|\lambda|}^M \cos \lambda_m}{\partial |\lambda_m|} \right) \quad (7.57)$$

The height integrated current density  $\mathbf{K}^M$  doesn't have to be realistic, but the divergence, i.e. the current  $J_{Mr}$ , should be. Using the divergence assures that the integrated field-aligned current over both hemispheres vanishes, and therefore there is no net current into the ionosphere. The two components of the field-aligned current  $K_\phi^M$  and  $K_{|\lambda|}^M$ , eastward and poleward/ upward, can be differently defined depending on the acting region and the mimicking mechanism. The different contributions are described in the following three subsections. Note that in the default code none of these options is used. To

use them one or all of the flags `mod_heelis`, `J_rR` and `eqMgCnd` have to be set to `.true.` in the `dynamo_module`.

### Field-aligned current

This part has not been tested yet, however the source code can be found in subroutine `calrhs_jrr`. To use the field-aligned part the flag `J_rR = .true.` in `dynamo_module` has to be set. The magnetospheric current components  $K_\phi^M$  and  $K_{|\lambda|}^M$  for the field-aligned current can be derived from a reference potential  $\Phi_R$  which we assume is the Heelis potential for now. Using the Heelis potential leads to realistic magnitudes and directions in the current, but might not represent correctly the field-aligned current in the region 1.

$$K_\phi^M = \frac{f_\lambda}{R_0} \left( \frac{\Sigma_{\phi\phi}^T}{\cos\lambda_m} \frac{\partial\Phi_R}{\partial\phi_m} + \Sigma_{\phi\lambda}^T \frac{\partial\Phi_R}{\partial|\lambda_m|} \right) \quad (7.58)$$

$$K_{|\lambda|}^M = \frac{f_\lambda}{R_0 \cos\lambda_m} \left( \Sigma_{\lambda\phi}^T \frac{\partial\Phi_R}{\partial\phi_m} + \Sigma_{\lambda\lambda}^T \cos\lambda_m \frac{\partial\Phi_R}{\partial|\lambda_m|} \right) \quad (7.59)$$

The factor  $f_\lambda$  is set such that it's 1 poleward of the the convection reversal boundary  $\lambda_m^{crb}$  and zero equatorward. Thus, the current represents region 1 current and is zero in the region 2.

$$f_\lambda = 1 \quad \text{for} \quad |\lambda_m| \geq \lambda_m^{crb} \quad (7.60)$$

$$f_\lambda = 0 \quad \text{for} \quad |\lambda_m| < \lambda_m^{crb} \quad (7.61)$$

In TIEGCM the value for the convection reversal boundary  $\lambda_m^{crb}$  is set to  $75^\circ$  in the module `cons`. Note that this is not a physical meaningful value since the convection reversal boundary is fixed. For the modified reference potential in section 7.7.3 a variable value for the convection reversal boundary will be used which is set in the `aurora module`. The current components in equations (7.58) and (7.59) are calculated in a similar way as the left hand side of the electrodynamo equation, which is described in section 7.10. The conductance expressions in equation (7.153)–(7.156) are used to calculate the current components in equations (7.58) and (7.59), and therefore these conductances are input to the subroutine `calrhs_jrr` where the current components eq. (7.153)–(7.156) are calculated. The finite difference stencil for the partial derivatives in equations (7.58) and (7.59) is set up in subroutine `nsstencil`. In comparison to the set up of the finite difference stencil in

section 7.10 for the left hand side of the electrodynamic equation, here, it's done for both hemispheres and without upwinding technique. Once the finite difference stencil is calculated the electric potential  $\Phi_R$  is inserted, which is done in `subroutine insert_pot`, to calculate the current components. Although the calculation is done for both hemisphere, it is not necessary since the used Heelis potential is symmetric about the equator and the coefficients of the conductances in equations (7.153)–(7.156) are already the sum of the two hemispheres. After calculating the current it is added to the right hand side of the electrodynamic equation (7.32).

### Equivalent magnetospheric conductances

The magnetospheric field-aligned current can be influenced by the electric field distribution in the ionosphere, and therefore depend on the electric potential. The region 2 current with the shielding effect of strong electric fields from high to low latitude is an example of this magnetosphere–ionosphere interaction. The region 2 current can be approximated by a Hall conductor. In addition, the magnetospheric ion loss can be simulated by adding a zonal Pedersen conductance. In TIEGCM we adopt the concept from [11] by using equivalent magnetospheric conductances  $\Sigma_{\phi\phi}^M$  and  $\Sigma_H^M$ . The magnetospheric current in eq. (7.57) can be replaced by

$$K_{\phi}^M = \frac{-1}{R_0} \left( \frac{\Sigma_{\phi\phi}^M}{\cos\lambda_m} \frac{\partial\Phi}{\partial\phi_m} + \Sigma_H^M \frac{\partial\Phi}{\partial|\lambda_m|} \right) \quad (7.62)$$

$$K_{|\lambda|}^M = \frac{\Sigma_H^M}{R_0 \cos\lambda_m} \frac{\partial\Phi_R}{\partial\phi_m} \quad (7.63)$$

with  $\Sigma_{\phi\phi}^M$  and  $\Sigma_H^M$  being the equivalent magnetospheric zonal Pedersen and Hall conductances. The values of  $\Sigma_{\phi\phi}^M$  and  $\Sigma_H^M$  are taken from figure 4 in [11] and plotted in figure 7.2. In `subroutine set_cicr` the equivalent magnetospheric conductances are set up and added to the conductances due to solar ionization and particle precipitation in `subroutine add_cicr`. In figure 7.2 the equivalent magnetospheric conductances start at  $72^\circ$  magnetic latitude which is the convection reversal boundary for this specific case. However, the convection reversal boundary varies with the geomagnetic conditions and the location is determined in the `aurora module`. The contributions to the electrodynamic equation due to the equivalent magnetospheric conductances are calculated in a similar way as described in section 7.8 for the left hand side

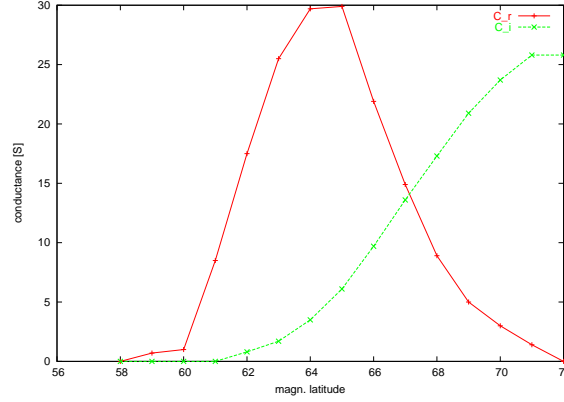


Figure 7.2: Latitudinal variation of equivalent magnetospheric conductances  $\Sigma_{\phi\phi}^M (C_r)$  and  $\Sigma_H^M (C_i)$  for the convection reversal boundary at  $72^\circ$ .

of the electrodynamo equation. The conductances are calculated on the irregular spaced grid  $\lambda_m^*$ , but for the finite differencing the regular grid  $\lambda_0$  in  $\lambda_m^*$  is used. Therefore, the difference in the partial derivatives due to the change from  $\lambda_m^*$  to  $\lambda_0$  have to be taken into account, as described in table 7.5. The conductance quantities are then prepared for the finite differencing as shown in eq. (7.153) and (7.155) and added to the conductances due to solar ionization and particle precipitation. To use the equivalent magnetospheric conductances, the flag `eqMgCnd` has to be set to `.true.` in the `dynamo_module`.

### Modified reference potential

In the region 1 the magnetospheric current in eq.(7.57) can be represented by the combination of a field-aligned current described in section 7.7.3 and a reference electric potential distribution  $\Phi^R$ . The later is described in the following. The contribution to the magnetospheric current from a reference potential can be specified by

$$K_\phi^M = \frac{\Sigma^R}{R_0 \cos \lambda_m} \frac{\partial(\Phi^R - \Phi)}{\partial \phi_m} \quad (7.64)$$

$$K_{|\lambda|}^M = \frac{\Sigma^R}{R_0} \frac{\partial(\Phi^R - \Phi)}{\partial \phi_m} \quad (7.65)$$

The reference conductance  $\Sigma^R$  is not a physical conductance, but determines how strongly the calculated electric potential  $\Phi$  reflects the reference poten-

tial  $\Phi^R$ . The reference conductance is set to

$$\Sigma^R = \min(\Sigma_{max}^R, \Sigma_b [e^{|\lambda_m - \lambda_m^{crb}| \frac{2}{\alpha_t}} - 1]) \quad \text{for } |\lambda_m| \geq \lambda_m^{crb} \quad (7.66)$$

$$\Sigma^R = 0 \quad \text{for } |\lambda_m| < \lambda_m^{crb} \quad (7.67)$$

with  $\alpha_t$  being the width of the transition zone, here  $3^\circ$ , equatorward of the convection reversal boundary  $\lambda_m^{crb}$ . The maximum reference conductance  $\Sigma_{max}^R$  is set to 10,000 S and the base conductance  $\Sigma_b$  is 5 S. In the polar cap region the electric potential should be the reference potential. In the source code the Heelis potential is used for the reference potential  $\Phi^R$ . The convection reversal boundary is denoted by  $\lambda_m^{crb}$ , which varies with the geomagnetic conditions, and is set in the `aurora module`. In figure 7.3 the latitudinal variation of the reference conductance  $\Sigma^R$  is shown for  $\lambda_m^{crb} = 72^\circ$ .

In the source code the calling tree is the following

```
subroutine dynamo
...
if (mod_heelis) then
  if(istep = 1 ) then call set_zigmar
  call add_zigmar
  call diff_rimr
  call add_rimr
endif
...
```

To use the modified reference potential the flag `mod_heelis` in the `dynamo_module` has to be set to `.true..` The current in the equations (7.64) and (7.65) are calculated like the left hand side of the electrodynamo equation which is described in section 7.10. The reference conductances  $\Sigma^R$  are calculated according to eq. (7.66) and (7.67) in subroutine `set_zigmar`. The coefficients of the reference conductance are added in subroutine `add_zigmar` to the conductances  $\Sigma_{\phi\phi}$  and  $\Sigma_{\lambda\lambda}$  of the electrodynamo equation. The finite difference stencil is set up in subroutine `diff_rimr` by subroutine `nsstencil`. In comparison to the set up of the stencil for the left hand side of the electrodynamo equation, in section 7.10, the stencil is calculated for both hemispheres and no upwinding technique are used. Once the finite difference stencil is calculated the electric potential  $\Phi_R$  is inserted to calculate the additional current for the right hand side of the electrodynamo equation in subroutine

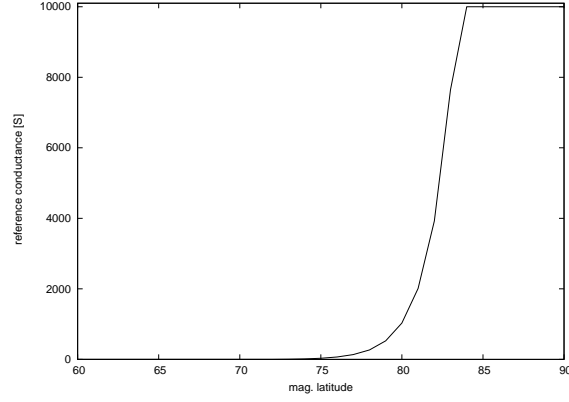


Figure 7.3: Latitudinal variation of reference conductance  $\Sigma^R$  for  $\lambda_m^{crb} = 72^\circ$

`insert_pot`. Although the additional current is determined for both hemisphere separately, this is not necessary since the reference potential and the coefficients of  $\Sigma^R$  are symmetric about the equator.

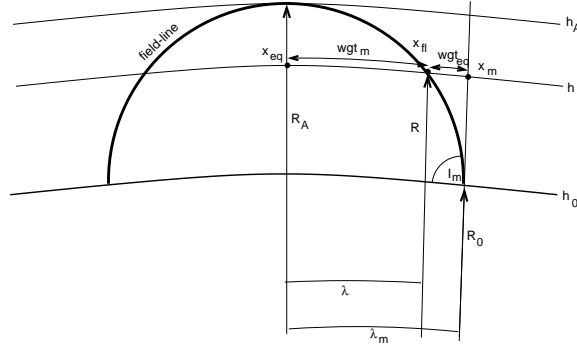


Figure 7.4: Sketch of geometry for the field-line integration

## 7.8 Field line Integration

This section refers to the subroutine `fieldline_integrals` in TIEGCM.

The electrodynamic equation is reduced to two dimensions assuming that the field-lines are equipotential due to the high conductivity along the field-line. The variable along the field line is  $s$ , and  $s_L$  and  $s_U$  are the lower and upper boundary of the line-integration. The inclination of the geomagnetic field-line at the reference height  $h_0$  on an assumed spherical Earth is  $I_m$ , and  $B_{e3}$  is the component of the geomagnetic field along the field-line. Note that all values except the geopotential height  $z$ , are stored on half pressure levels to make the integration more convenient.

**Approximation of field line values** The correct way to do the field line integration would be to trace points along the field line. However, the geomagnetic grid in TIEGCM is not oriented along the field line, and therefore the tracking would involve a two dimensional search and an interpolation to calculate the value on the field line. This can be computationally expensive and therefore an approximation, which should be close to the true field line integration, is used. The field line integration is approximated by a height integration combined with an interpolation between the height-varying values at the foot point of the field line  $(\lambda_m, h)$  and the magnetic equator  $(\lambda_m = 0, h)$  (see. figure 7.4). Hence, only the height varying values at the foot point location  $(\lambda_m, h)$  are needed. Figure 7.4 shows schematically a field

line with the foot point latitude  $\lambda_m$  at the reference height  $h_0$ . The value  $x_{fl}$  at height  $h$  on the field line is approximated by the value  $x_{eq}$  at the equator and height  $h$  and the value  $x_m$  at foot point latitude  $\lambda_m$  and height  $h$ .

$$x_{fl} = wgt_{eq}x_{eq} + wgt_mx_m \quad (7.68)$$

with the weights  $wgt_{eq}$  for the equator value and  $wgt_m$  for the foot point value. From figure 7.4 the weight can be found as

$$wgt_{eq} = \frac{\lambda_m - \lambda}{\lambda_m} \approx \frac{\sin(\lambda_m - \lambda)}{\lambda_m} \quad (7.69)$$

assuming that the difference  $\lambda_m - \lambda$  is small, which is true close to the foot point of the field line. Note that determining  $\lambda$  would involve searching for the point on the field line at height  $h$  which is time consuming, thus the sinus is used. For field lines which foot point is at mid- and height latitude the value on the field line is essentially the height-varying value at the foot point, since the field line is almost vertical. Close to the magnetic equator the approximation is not so good anymore but the inaccuracy can be neglected when compared to the total field line integration. The term  $\sin(\lambda_m - \lambda)$  can be substituted by

$$\sin(\lambda_m - \lambda) = \sin\lambda_m \cos\lambda - \cos\lambda_m \sin\lambda \quad (7.70)$$

and since for a dipolar field  $R = R_A \cos^2\lambda$  the  $\cos\lambda$  and  $\sin\lambda$  in equation (7.70) can be substituted by

$$\cos\lambda = \sqrt{\frac{R}{R_A}}; \quad \sin\lambda = \sqrt{1 - \frac{R}{R_A}}; \quad (7.71)$$

$$\cos\lambda_m = \sqrt{\frac{R_0}{R_A}}; \quad \sin\lambda_m = \sqrt{1 - \frac{R_0}{R_A}}; \quad (7.72)$$

with  $R_A$  the radius of the field-line apex (see figure 7.4). The weighting factors are

$$wgt_{eq} \approx \frac{1}{\lambda_m} \sqrt{1 - \frac{R_0}{R_A}} \sqrt{\frac{R}{R_A}} - \sqrt{\frac{R_0}{R_A}} \sqrt{1 - \frac{R}{R_A}} \quad (7.73)$$

$$wgt_m = 1 - wgt_{eq} \quad (7.74)$$



The quantities on the field-line at  $(h, \lambda)$  are therefore approximated by

$$\sigma_P(h, \lambda) = wgt_{eq}(h, \lambda_{eq})\sigma_P(h, \lambda_{eq}) + wgt_m(h, \lambda_m)\sigma_P(h, \lambda_m) \quad (7.75)$$

$$\sigma_H(h, \lambda) = wgt_{eq}(h, \lambda_{eq})\sigma_H(h, \lambda_{eq}) + wgt_m(h, \lambda_m)\sigma_H(h, \lambda_m) \quad (7.76)$$

$$u_{e1}(h, \lambda) = wgt_{eq}u_{e1}(h, \lambda_{eq})(h, \lambda_{eq}) + wgt_m(h, \lambda_m)u_{e1}(h, \lambda_m) \quad (7.77)$$

$$u_{e2}(h, \lambda) = wgt_{eq}u_{e2}(h, \lambda_{eq})(h, \lambda_{eq}) + wgt_m(h, \lambda_m)u_{e2}(h, \lambda_m) \quad (7.78)$$

**Height variation of  $\mathbf{d}_1$  and  $\mathbf{d}_2$**  The apex values  $\frac{d_1^2}{D}$ ,  $\frac{d_2^2}{D}$  and  $\frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}$  are referenced to height  $h_0$  (see section 7.4). The height variation of these values are small, but should be taken into account. The values  $\mathbf{d}_1$ ,  $\mathbf{d}_2$  and  $D$  vary with height like

$$\mathbf{d}_1^2(h) = \left[\frac{R_0}{R}\right]^3 \mathbf{d}_1^2(h_0) \quad (7.79)$$

$$\mathbf{d}_2^2(h) = \left[\frac{R_0}{R}\right]^3 \left[\frac{4 - 3\cos^2\lambda}{4 - 3\frac{R_0}{R}\cos^2\lambda}\right] \mathbf{d}_2^2(h_0) \quad (7.80)$$

$$D(h) = \mathbf{d}_1 \cdot \mathbf{d}_2 = \left(\frac{R_0}{R}\right)^3 \left(\frac{4 - 3\cos^2\lambda}{4 - 3\frac{R_0}{R}\cos^2\lambda}\right)^{1/2} D(h_0) \quad (7.81)$$

Using the dipole approximation  $\cos^2\lambda = \frac{R}{R_A}$  we can approximate the height variation by

$$\frac{\mathbf{d}_1^2(h)}{D(h)} = \left(\frac{R_A - \frac{3}{4}R_0}{R_A - \frac{3}{4}R}\right)^{1/2} \frac{\mathbf{d}_1^2(h_0)}{D(h_0)} = \frac{1}{h_{fac}} \frac{\mathbf{d}_1^2(h_0)}{D(h_0)} \quad (7.82)$$

$$\frac{\mathbf{d}_2^2(h)}{D(h)} = \left(\frac{R_A - \frac{3}{4}R}{R_A - \frac{3}{4}R_0}\right)^{1/2} \frac{\mathbf{d}_2^2(h_0)}{D(h_0)} = h_{fac} \frac{\mathbf{d}_2^2(h_0)}{D(h_0)} \quad (7.83)$$

**Approximation of  $ds$  along the field line** Since the integration is done in height rather than along the field-line  $ds$  in equations (7.24)–(7.29) is expressed in terms of height  $h$ .

$$ds = \frac{dh}{|\sin I|} \quad (7.84)$$

However,  $\sin I$  is going to zero at the magnetic equator and  $ds$  would be infinite. Therefore, we have to approximate the relation in equation (7.84).

Starting from the calculation of  $\sin I$  and using the dipole approximation  $\cos^2 \lambda = \frac{R}{R_A}$  leads to

$$\sin I = \frac{2 \sin \lambda}{\sqrt{4 - 3 \cos^2 \lambda}} = 2 \sqrt{\frac{h_A - h}{R_E + 4h_A - 3h}} \quad (7.85)$$

The numerator  $\sqrt{h_A - h}$  varies more than the denominator. Therefore equation (7.84) is written as

$$ds = \frac{dh}{|\sin I|} = -A(h) d\sqrt{h_A - h} = \frac{A(h) dh}{2\sqrt{h_A - h}} \quad (7.86)$$

with  $A(h)$  is the area at height  $h$ . The minus sign is introduced since  $ds$  should increase with increasing height. From equation (7.86) follows that the area  $A(h)$  and  $A(h_0)$  at the reference height is

$$A(h) = \frac{2\sqrt{h_A - h}}{|\sin I|}; \quad A(h_0) = \frac{2\sqrt{h_A - h_0}}{|\sin I_m|}; \quad (7.87)$$

Thus, the height varying factor is

$$\frac{A(h)}{A(h_0)} = \frac{2\sqrt{h_A - h}}{|\sin I|} \frac{|\sin I_m|}{2\sqrt{h_A - h_0}} = \sqrt{\frac{R_A - \frac{3}{4}R}{R_A - \frac{3}{4}R_0}} \quad (7.88)$$

substituting the inclination angle  $\sin I$  and  $\sin I_m$  from equation (7.85). Inserting equation (7.87) for  $A(h_0)$  in equation (7.86) will give

$$A(h) = \frac{2\sqrt{h_A - h_0}}{|\sin I_m|} \sqrt{\frac{R_A - \frac{3}{4}R}{R_A - \frac{3}{4}R_0}} = A(h_0) h_{fac} \quad (7.89)$$

The height varying factor  $A(h)$  consists of two terms: a height dependent factor  $h_{fac}$  which was already defined in equation (7.83) and a height independent term  $A(h_0)$ .

The factor  $-d\sqrt{h_A - h}$  in equation (7.84) at the pressure level  $k$  can be discretized as follows

$$-d_k \sqrt{h_A - h} = \sqrt{h_A - h_k} - \sqrt{h_A - h_{k+1}} \quad (7.90)$$

with  $k$  being the index of the discrete pressure levels. Note that the geopotential height  $z$  is used for  $h$  which is stored at full pressure levels. The increment along the field line in eq. (7.86) can be written as

$$ds = -A(h_0) h_{fac} d\sqrt{h_A - h} \quad (7.91)$$

quantity	name in source code	unit
$\frac{\Sigma_{\phi\phi}}{ sinI_m }$	zigm11	S
$ sinI_m \Sigma_{\lambda\lambda}$	zigm22	S
$\Sigma_C$	zigmc	S
$\Sigma_H$	zigm2	S
$\frac{K_{m\phi}^D}{ sinI_m }$	rim(1)	A/m
$\pm K_{m\lambda}^D$	rim(2)	A/m

Table 7.4: Field line integrated quantities in subroutine `fieldline_integrals`

**Field line integration** The following fields are calculated (see also equations 7.22, 7.23, 7.24, 7.25, 7.28, 7.29) using the field line integration

$$\frac{\Sigma_{\phi\phi}}{|sinI_m|} = \int_{s_L}^{s_U} \frac{\sigma_P \mathbf{d}_1^2}{D} ds \quad (7.92)$$

$$|sinI_m|\Sigma_{\lambda\lambda} = \int_{s_L}^{s_U} \frac{\sigma_P \mathbf{d}_2^2}{D} ds \quad (7.93)$$

$$\Sigma_C = \int_{s_L}^{s_U} \frac{\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2}{D} ds \quad (7.94)$$

$$\Sigma_H = \int_{s_L}^{s_U} \sigma_H ds \quad (7.95)$$

$$\frac{K_{m\phi}^D}{|sinI_m|} = B_{e3}(h_0) \int_{s_L}^{s_U} \left[ \frac{\sigma_P \mathbf{d}_1^2}{D} u_{e2} + \left( \sigma_H - \frac{\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2}{D} \right) u_{e1} \right] ds \quad (7.96)$$

$$-K_{m\lambda}^D = \pm B_{e3}(h_0) \int_{s_L}^{s_U} \left[ -\frac{\sigma_P \mathbf{d}_2^2}{D} u_{e1} + \left( \sigma_H + \frac{\sigma_P \mathbf{d}_1 \cdot \mathbf{d}_2}{D} \right) u_{e2} \right] ds \quad (7.97)$$

The field line integration is approximated by taking the sum over all pressure level  $k$  ( $k = -2$  to `mlev`, with `mlev` the number of pressure levels). With the approximations of the field line integration in the previous section, the

integrals in equations (7.92)–(7.97) are calculated by

$$\frac{\Sigma_{\phi\phi}}{|\sin I_m|} = -A(h_0) \frac{d_1^2}{D}(h_0) \sum_{k=-2}^{mlev} \sigma_{P,k} d_k \sqrt{h_A - h} \quad (7.98)$$

$$|\sin I_m| \Sigma_{\lambda\lambda} = -A(h_0) \frac{d_2^2}{D}(h_0) \sum_{k=-2}^{mlev} \sigma_{P,k} h_{fac,k}^2 d_k \sqrt{h_A - h} \quad (7.99)$$

$$\Sigma_C = -A(h_0) \frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}(h_0) \sum_{k=-2}^{mlev} \sigma_{P,k} h_{fac,k} d_k \sqrt{h_A - h} \quad (7.100)$$

$$\Sigma_H = -A(h_0) \sum_{k=-2}^{mlev} \sigma_{H,k} h_{fac,k} d_k \sqrt{h_A - h} \quad (7.101)$$

$$\begin{aligned} \frac{K_{m\phi}^D}{|\sin I_m|} &= -B_{e3} A(h_0) \sum_{k=-2}^{mlev} \left[ \sigma_{P,k} \frac{d_1^2}{D}(h_0) u_{e2,k} + \sigma_{H,k} u_{e1,k} h_{fac,k} - \right. \\ &\quad \left. \sigma_{P,k} \frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}(h_0) u_{e1,k} h_{fac,k} \right] d_k \sqrt{h_A - h} \\ -K_{m\lambda}^D &= \pm B_{e3} A(h_0) \sum_{k=-2}^{mlev} \left[ \sigma_{H,k} u_{e2,k} h_{fac,k} + \sigma_{P,k} \frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}(h_0) u_{e2,k} h_{fac,k} - \right. \\ &\quad \left. \sigma_{P,k} \frac{d_2^2}{D}(h_0) u_{e1,k} h_{fac,k}^2 \right] d_k \sqrt{h_A - h} \end{aligned} \quad (7.102)$$

After the field line integration is carried out the equatorial field line integral values are set, as well as the equatorial boundary condition is included. Finally, the coefficients of the partial differential equation are modified to take into account that the finite differencing is done with respect to the equally spaced grid with  $\lambda_0$  which is a function of  $\lambda_m^*$ , although the derivatives are calculated on the irregular grid with  $\lambda_m^*$ . These tasks are carried out in subroutine `transf` of TIEGCM and described in the following.

**Equatorial values** The values at the geomagnetic equator are approximated since no field line integration can be performed. It is assumed that the average along a field line for a quantities which primarily depend on the Pedersen conductivity  $\sigma_P$  increase by a factor of four from one field line to

the next higher one. The average along a field line for quantities mainly dependent on Hall conductivity  $\sigma_H$  vary by 0.83 from one field line to the next higher one. The exact value should not be important for the electric potential calculation, as long as the values are physically reasonable and not too different than those of adjacent field lines. The factor of  $\frac{1}{2}$  is introduced to take the adding of the two hemispheres into account, which is done later.

$$\frac{\Sigma_{\phi\phi,eq}}{|\sin I_m|} = \frac{1}{2} \frac{1}{4} \frac{\Sigma_{\phi\phi,eq+\Delta\lambda_m}}{|\sin I_m|} \quad (7.103)$$

$$|\sin I_m| \Sigma_{\lambda\lambda,eq} = \frac{1}{2} \frac{1}{4} |\sin I_m| \Sigma_{\lambda\lambda,eq+\Delta\lambda_m} \quad (7.104)$$

$$\Sigma_{C,eq} = \frac{1}{2} \frac{1}{4} \Sigma_{C,eq+\Delta\lambda_m} \quad (7.105)$$

$$\Sigma_{H,eq} = \frac{1}{2} 0.12 \Sigma_{H,eq+\Delta\lambda_m} \quad (7.106)$$

$$\frac{K_{m\phi,eq}^D}{|\sin I_m|} = \frac{1}{2} 0.12 \frac{K_{m\phi,eq+\Delta\lambda_m}^D}{|\sin I_m|} \quad (7.107)$$

$$K_{m\lambda,eq}^D = \frac{1}{2} 0.12 K_{m\lambda,eq+\Delta\lambda_m}^D \quad (7.108)$$

**Equatorial boundary condition** At the equator the northward height integrated current density has to vanish (see [14] eq. 5.30 or 5.31).

$$K_{m\lambda} = 0 \quad (7.109)$$

Solving equation (5.31) in [14] for  $\frac{\partial\Phi}{\partial\lambda_m}$  leads to

$$\frac{\partial\Phi}{\partial\lambda_m} = \frac{1}{\Sigma_{\lambda\lambda}} \left[ R_0 K_{m\lambda}^D - \frac{\Sigma_{\lambda\phi}}{\cos\lambda_m} \frac{\partial\Phi}{\partial\phi_m} \right] \quad (7.110)$$

which is substituted into the electrodynamo equation (7.32). Due to the special geometry at the geomagnetic equator with horizontal field lines we can use the Cowling conductivity

$$\Sigma_{Cowling} = \Sigma_{\phi\phi} - \frac{\Sigma_{\phi\lambda}\Sigma_{\lambda\phi}}{\Sigma_{\lambda\lambda}} \quad (7.111)$$

and get

$$\begin{aligned} & \frac{\partial}{\partial\phi_m} \left[ \frac{\Sigma_{Cowling}}{\cos\lambda_m} \frac{\partial\Phi}{\partial\phi_m} \right] + \frac{\partial}{\partial|\lambda_m|} \left[ \Sigma_{\lambda\phi} \frac{\partial\Phi}{\partial\phi_m} + \Sigma_{\lambda\lambda} \cos\lambda_m \frac{\partial\Phi}{\partial|\lambda_m|} \right] = \\ & R_0 \frac{\partial}{\partial\phi_m} \left[ K_{m\phi}^D - \frac{\Sigma_{\phi\lambda}}{\Sigma_{\lambda\lambda}} K_{m\lambda}^D \right] + R_0 \frac{\partial K_{m\lambda}^{DT} \cos\lambda_m}{\partial|\lambda_m|} \end{aligned} \quad (7.112)$$

Therefore the value  $\frac{\Sigma_{\phi\phi}}{|\sin I_m|}$  (see table 7.4) at the geomagnetic equator has to be modified by

$$\frac{\Sigma_{\phi\phi}^{mod}}{|\sin I_m|} = \left[ \frac{\Sigma_{\phi\phi}}{|\sin I_m|} - \frac{\Sigma_{\phi\lambda}\Sigma_{\lambda\phi}}{\Sigma_{\lambda\lambda}|\sin I_m|} \right]_{eq} \quad (7.113)$$

as well as the value  $\frac{K_{m\phi}^D}{|\sin I_m|}$  (see table 7.4) by

$$\frac{K_{m\phi,eq}^{D,mod}}{|\sin I_m|} = \left[ \frac{K_{m\phi}^D}{|\sin I_m|} - \frac{\Sigma_{\phi\lambda}K_{m\lambda}^D}{\Sigma_{\lambda\lambda}|\sin I_m|} \right]_{eq} \quad (7.114)$$

**Transformation from  $\lambda_m^*$  to  $\lambda_0$**  The geomagnetic latitudinal grid  $\lambda_m^*$  is irregular spaced in latitude. For convenience the derivatives are taken with respect to  $\lambda_0$  which is equally spaced in  $\lambda_m^*$ . Therefore, the electrodynamic equation (see also eq. 7.32) can be written with  $\lambda_m = \lambda_m^*$

$$\begin{aligned} & \frac{\partial}{\partial \phi_m} \left( \frac{\Sigma_{\phi\phi}}{\cos \lambda_m^*} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\phi\lambda} \frac{\partial \Phi}{\partial |\lambda_m^*|} \right) + \frac{\partial}{\partial |\lambda_m^*|} \left( \Sigma_{\lambda\phi} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\lambda\lambda} \cos \lambda_m^* \frac{\partial \Phi}{\partial |\lambda_m^*|} \right) \\ &= R \frac{\partial K_{m\phi}^D}{\partial \phi_m} + R \frac{\partial K_{m\lambda}^D \cos \lambda_m^*}{\partial |\lambda_m^*|} + R^2 \cos \lambda_m^* J_{mr} \end{aligned} \quad (7.115)$$

and has to be transformed to account for the change to  $\lambda_0$ . Note that the longitude is not changing. The whole equation is multiplied by  $\frac{\partial \lambda_m^*}{\partial \lambda_0}$  which lead to

$$\begin{aligned} & \frac{\partial \lambda_m^*}{\partial \lambda_0} \frac{\partial}{\partial \phi_m} \left( \frac{\Sigma_{\phi\phi}}{\cos \lambda_0} \frac{\cos \lambda_0}{\cos \lambda_m^*} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\phi\lambda} \frac{\partial \lambda_0}{\partial \lambda_m^*} \frac{\partial \Phi}{\partial \lambda_0} \right) + \\ & \frac{\partial \lambda_m^*}{\partial \lambda_0} \frac{\partial}{\partial \lambda_m^*} \left( \Sigma_{\lambda\phi} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\lambda\lambda} \cos \lambda_0 \frac{\cos \lambda_m^*}{\cos \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_m^*} \frac{\partial \Phi}{\partial \lambda_0} \right) \\ &= R_0 \frac{\partial \lambda_m^*}{\partial \lambda_0} \frac{\partial K_{m\phi}^D}{\partial \phi_m} + R_0 \frac{\partial K_{m\lambda}^D \cos \lambda_0 \frac{\cos \lambda_m^*}{\cos \lambda_0}}{\partial \lambda_0} + R_0^2 \cos \lambda_m^* \frac{\partial \lambda_m^*}{\partial \lambda_0} J_{mr} \end{aligned} \quad (7.116)$$

The electrodynamic equation is multiplied by  $\frac{\partial \lambda_m^*}{\partial \lambda_0}$  to avoid problems at the geomagnetic equator due to  $\frac{1}{\sin I_m}$  which is not defined at the equator, however  $\frac{1}{\sin I_m} \frac{\partial \lambda_0}{\partial \lambda_m^*}$  is defined at the equator. The quantities after the transformation are listed in table (7.5) with  $(\cdot)(0)$  denoting the quantity  $(\cdot)$  referenced to  $\lambda_0$ . The polar values of the conductances are calculated by extrapolated

quantity		name in source code	unit
$\Sigma_{\phi\phi}(0)$	=	zigm11	S
$\Sigma_{\phi\phi} \frac{\cos\lambda_0}{\cos\lambda_m^*} \frac{\partial\lambda_m^*}{\partial\lambda_0}$			
$\Sigma_{\lambda\lambda}(0)$	=	zigm22	S
$\Sigma_{\lambda\lambda} \frac{\cos\lambda_m^*}{\cos\lambda_0} \frac{\partial\lambda_0}{\partial\lambda_m^*}$			
$\Sigma_C(0) = \Sigma_C$		zigmc	S
$\Sigma_H(0) = \Sigma_H$		zigm2	S
$K_{m\phi}^D(0) = K_{m\phi}^D \frac{\partial\lambda_m^*}{\partial\lambda_0}$		rim(1)	A/m
$\pm K_{m\lambda}^D(0)$	=	rim(2)	A/m
$\pm K_{m\lambda}^D \frac{\cos\lambda_m^*}{\cos\lambda_0}$			

Table 7.5: Quantities after the transformation at the end of **subroutine transf**

weighting e.g. for a quantity  $x$  the polar value is determined by

$$x(j_{pole}) = \frac{1}{3nmlon} \left[ 4. \sum_{i=1}^{nmlon} x(i, j_{pole} \mp 1) - \sum_{i=1}^{nmlon} x(i, j_{pole} \mp 2) \right] \quad (7.117)$$

with  $nmlon$  the number of longitudes and  $j_{pole}$  the latitudinal index at the north / south pole and the  $\mp$  sign referring to the poles respectively. The height integrated current densities  $K_{m\phi}^D(0)$  and  $K_{m\lambda}^D(0)$  are averaged over the pole. Note that the electrodynamo equation is not solved at the pole, however the polar values are needed for the finite differencing.

## 7.9 Gravity and plasma pressure driven current

### 7.9.1 Gravity Driven Current

This section refers to the subroutine `magpres_grav` in TIEGCM. Note that the units in this section are the units used in the source code of TIEGCM. By default the gravity driven current is calculated for a model run. To omit the gravity and plasma pressure driven current the flag `j_pg=.false.` in `magpres_g_module` has to be set.

The current driven by gravity can be calculated by

$$\mathbf{J}_g(h) = \frac{1}{\mathbf{B}(h)^2} \rho_{ion} \mathbf{g}(h) \times \mathbf{B}(h) \quad (7.118)$$

with  $\mathbf{B}$  [Gauss] the Earth main magnetic field, the ion density  $\rho_{ion}$  [ $\frac{1}{cm^3}$ ], and  $\mathbf{g}(h)$  [ $\frac{cm}{s^2}$ ] the gravitational acceleration at height  $h$ . The gravitational field gets weaker with height and therefore the gravitational acceleration at reference height  $h_0 = 90 \text{ km}$  is scaled by

$$\mathbf{g}(h) = \left( \frac{R_0}{R} \right)^2 \mathbf{g}(h_0) \quad (7.119)$$

with  $R = R_E + h$  and  $R_E$  the mean Earth radius. The radius of the reference height is  $R_0 = R_E + h_0$ . The ion density is determined by

$$\rho_{ion} = M_i \sum_i n_i m_i \quad \text{with} \quad i = O^+, O^{2+}, N^+, N^{2+}, NO^+ \quad (7.120)$$

with the mass of a unit atomic weight  $M_i$  [g],  $n_i$  [ $\frac{1}{cm^3}$ ] the ion number density of the species  $i$  and  $m_i$  its corresponding atomic weight. Combining equations (7.119) and (7.120) and converting from [ $\frac{g}{s^2 cm^2}$ ] to [ $\frac{kg}{s^2 m^2}$ ] will introduce an additional factor of 10 (see equation 7.122).

The height variation of the Earth main magnetic field is approximated by

$$\mathbf{B}(h) = \left( \frac{R_0}{R} \right)^3 \mathbf{B}(h_0) \quad (7.121)$$

with  $\mathbf{B}(h_0)$  [Gaus] referenced to  $h_0$ . The components of the main field are  $\mathbf{B} = (b_x, b_y, b_z)$  the north-, east- and downward components or  $\mathbf{B} =$



$(b_{\phi_g}, b_{\lambda_g}, b_{z_g})$  with  $\phi_g$ ,  $\lambda_g$  and  $z_g$  the directions in geographic longitude, latitude and upward height respectively. The current in  $[\frac{A}{cm^2}]$  due to the gravitational force is calculated at half pressure levels  $k + \frac{1}{2}$  by

$$\mathbf{J}_{g,k+\frac{1}{2}} = 10 \frac{R}{R_0} \frac{1}{\mathbf{B}_0^2} \rho_{ion} g(h_0)(b_x, -b_y, 0) \quad (7.122)$$

Note that in the TIEGCM code most quantities are evaluated at half levels  $k + \frac{1}{2}$  and stored at level  $k'$  with  $(\cdot)'$  denoting the half levels  $(\cdot) + \frac{1}{2}$  in contrast to  $k$  which is the full pressure level  $k$ . Therefore  $R$  and  $\rho_{ion}$  in equation (7.122) must be evaluated at the half level  $k + \frac{1}{2}$ .

### 7.9.2 Plasma Pressure Gradient Driven Current

This section refers to the subroutine `magpres_grav` in TIEGCM. Note that the units in this section are the units used in the source code of TIEGCM. The plasma pressure gradient driven current is calculated by default for a model run. To omit the gravity and plasma pressure driven current the flag `j_pg=.false.` in `magpres_g_module` has to be set.

The current due to the plasma pressure gradient  $\nabla p_p$  is

$$\mathbf{J}_p = -\frac{1}{\mathbf{B}(h)^2} \nabla p_p \times \mathbf{B}(h) \quad (7.123)$$

with the plasma pressure

$$\nabla p_p = k_B \nabla [(T_i + T_e) N_e] \quad (7.124)$$

The Boltzmann constant is denoted by  $k_B$ ;  $T_i$ ,  $T_e$  and  $N_e$  are the ion temperature [K], the electron temperature [K] and the electron density  $[\frac{1}{cm^3}]$ . The gradient  $\nabla$  is taken in the geographic direction  $(\nabla_{\phi_g}, \nabla_{\lambda_g}, \nabla_{z_g})$ .

The vertical gradient  $\nabla_{z_g} p_p$  is approximated at the half pressure level  $k + \frac{1}{2}$  by

$$\nabla_{z_g} p_{p,k+\frac{1}{2}} = 10 k_B \left[ \frac{N_{e,k+1} - N_{e,k}}{z_{k+1} - z_k} (T_i + T_e)_{k+\frac{1}{2}} + \frac{(T_i + T_e)_{k+1} - (T_i + T_e)_k}{z_{k+1} - z_k} N_{e,k+\frac{1}{2}} \right] \quad (7.125)$$

with the geopotential height  $z$  in [cm]. The factor of 10 takes the conversion from  $[\frac{g}{s^2 cm^2}]$  to  $[\frac{kg}{s^2 m^2}]$  into account.

The plasma pressure gradient in geographic eastward direction at the half pressure level  $k + \frac{1}{2}$  and geographic longitude  $\phi_g$  and geographic latitude  $\lambda_g$  is approximated by

$$\begin{aligned} \nabla_{\phi_g} p_{p,k+\frac{1}{2}} = & 10k_B \frac{1}{2\Delta\phi R_{k+\frac{1}{2}} \cos\lambda_g} \left[ \right. \\ & (N_e(\phi_g + \Delta\phi_g) - N_e(\phi_g - \Delta\phi_g))_{k+\frac{1}{2}} (T_i(\phi_g) + T_e(\phi_g))_{k+\frac{1}{2}} + \\ & \left. ((T_i + T_e)(\phi_g + \Delta\phi_g) - (T_i + T_e)(\phi_g - \Delta\phi_g))_{k+\frac{1}{2}} N(\phi_g)_{e,k+\frac{1}{2}} \right] \end{aligned} \quad (7.126)$$

with  $\Delta\phi_g$  the discrete step size in the eastward direction and the radius  $R_{k+\frac{1}{2}}$  at the half pressure level.

The plasma pressure gradient in geographic north direction at the half pressure level  $k + \frac{1}{2}$  and geographic longitude  $\phi_g$  and geographic latitude  $\lambda_g$  is approximated by

$$\begin{aligned} \nabla_{\lambda_g} p_{p,k+\frac{1}{2}} = & 10k_B \frac{1}{2\Delta\lambda R_{k+\frac{1}{2}}} \left[ \right. \\ & (N_e(\lambda_g + \Delta\lambda_g) - N_e(\lambda_g - \Delta\lambda_g))_{k+\frac{1}{2}} (T_i(\lambda_g) + T_e(\lambda_g))_{k+\frac{1}{2}} + \\ & \left. ((T_i + T_e)(\lambda_g + \Delta\lambda_g) - (T_i + T_e)(\lambda_g - \Delta\lambda_g))_{k+\frac{1}{2}} N(\lambda_g)_{e,k+\frac{1}{2}} \right] \end{aligned} \quad (7.127)$$

with  $\Delta\lambda_g$  the discrete step size in the northward direction. At the geographic poles we set

$$\nabla_{\lambda_g} p_{p,k+\frac{1}{2}}(\lambda_g = \pm 90^\circ) = 0 \quad (7.128)$$

Inserting the derivatives (7.125), (7.126) and (7.127) into equation (7.124) lead to

$$\nabla p_p = 10k_B \begin{pmatrix} \nabla_{\phi_g} \\ \nabla_{\lambda_g} \\ \nabla_{z_g} \end{pmatrix} [(T_i + T_e)N_e]_{\phi_g, \lambda_g, k+\frac{1}{2}} \quad (7.129)$$

with  $\nabla p_p$  in  $[\frac{kg}{s^2m^2}]$ . The cross product with the geomagnetic field vector from equation (7.123) can be written as

$$\begin{aligned} \mathbf{J}_{p,\phi_g,\lambda_g,k+\frac{1}{2}} &= -\frac{10k_B}{\mathbf{B}_0^2} \left(\frac{R}{R_0}\right)^3 \begin{pmatrix} \nabla_{\phi_g} \\ \nabla_{\lambda_g} \\ \nabla_{z_g} \end{pmatrix} \times \begin{pmatrix} b_y \\ b_x \\ -b_z \end{pmatrix} [(T_i + T_e)N_e]_{\phi_g,\lambda_g,k+\frac{1}{2}} \\ &= -\frac{10k_B}{\mathbf{B}_0^2} \left(\frac{R}{R_0}\right)^3 \begin{pmatrix} -\nabla_{\lambda_g} b_z - \nabla_{z_g} b_x \\ \nabla_z b_y + \nabla_{\phi_g} b_z \\ \nabla_{\phi_g} b_x - \nabla_{\lambda_g} b_y \end{pmatrix} [(T_i + T_e)N_e]_{\phi_g,\lambda_g,k+\frac{1}{2}} \end{aligned} \quad (7.130)$$

The height variation of the magnetic field is approximated by the factor  $(\frac{R}{R_0})^3$ . The calculated current vectors  $\mathbf{J}_g$  and  $\mathbf{J}_p$  have to be rotated to point in the geomagnetic direction.

$$\frac{1}{D} J_{e1}^{p,g} = \frac{\mathbf{d}_1}{D} \cdot \mathbf{J}_{pg} \quad (7.131)$$

$$\frac{1}{D} J_{e2}^{p,g} = \frac{\mathbf{d}_2}{D} \cdot \mathbf{J}_{pg} \quad (7.132)$$

with  $\mathbf{d}_1$  and  $\mathbf{d}_2$  denoting the vectors in quasi magnetic eastward and down/equatorward direction. The quantity  $D$  varies with the strength of the geomagnetic field and the distortion of the geomagnetic field from a pure dipole field. The quantity  $D$  can be calculated by using the vectors  $\mathbf{d}_1$  and  $\mathbf{d}_2$

$$D = |\mathbf{d}_1 \times \mathbf{d}_2| \quad (7.133)$$

The vectors  $\mathbf{d}_1(h_0)$  and  $\mathbf{d}_2(h_0)$  as well as  $D(h_0)$  are only calculated at the reference height  $h_0$ . The height variation is approximated by

$$\mathbf{d}_1(h) = \mathbf{d}_1(h_0) \left(\frac{R_0}{R}\right)^{\frac{3}{2}}; \quad \mathbf{d}_2(h) = \mathbf{d}_2(h_0) \left(\frac{R_0}{R}\right)^{\frac{3}{2}} \frac{\sqrt{4 - 3\cos^2\lambda_m}}{\sqrt{4 - 3\frac{R_0}{R}\cos^2\lambda_m}} \quad (7.134)$$

Considering equation (7.133) the quantity  $\frac{\mathbf{d}_1}{D}$  varies like  $\frac{1}{\mathbf{d}_2}$  and  $\frac{\mathbf{d}_2}{D}$  varies like  $\frac{1}{\mathbf{d}_1}$ . The current at top pressure level of the model is extrapolated using

$$J_{e1,k_{max}+\frac{1}{2}}^{p,g} = \frac{3}{2} J_{e1,k_{max}-\frac{1}{2}}^{p,g} - \frac{1}{2} J_{e1,k_{max}-\frac{3}{2}}^{p,g} \quad (7.135)$$

$$J_{e2,k_{max}+\frac{1}{2}}^{p,g} = \frac{3}{2} J_{e2,k_{max}-\frac{1}{2}}^{p,g} - \frac{1}{2} J_{e2,k_{max}-\frac{3}{2}}^{p,g} \quad (7.136)$$

with  $k_{max} + \frac{1}{2}$  the index of the highest pressure level.

### 7.9.3 Field–line Integration

This section describes how the gravity and plasma pressure gradient driven current is added to forcing of the electrodynamic equation. The gravity and plasma pressure gradient driven current is therefore added to the current driven by the neutral wind. The current of the different sources are combined in `subroutine fieldline_integrals`, before the field line integration. The field line integration itself is described in section 7.8.

The height–integrated eastward current density  $K_{m\phi}$ , see eq. (7.22), is calculated and included on the right hand side of the electrodynamic equation (7.32). The current  $J_{e1}^{p,g}$  due to gravity and plasma pressure gradient is added.

$$K_{m\phi} = |\sin I_m| \int_{s_L}^{s_U} \frac{J_{e1}}{D} ds = B_{e3} |\sin I_m| \int_{s_L}^{s_U} \left[ \frac{J_{e1}^D}{D} + \frac{J_{e1}^{p,g}}{B_{e3} D} \right] ds \quad (7.137)$$

with  $s$  the line–integral variable and  $s_L$  and  $s_U$  the lower and upper boundary of the line–integration. The inclination of the geomagnetic field line at the reference height  $h_0$  on an assumed spherical Earth is  $I_m$  and  $B_{e3}$  the component of the geomagnetic field along the field–line. The eastward current  $J_{e1}$  has a contribution from the neutral winds  $J_{e1}^D$  and from the plasma pressure and gravity term  $J_{e1}^{p,g}$ .

The field–line integration is approximated by a height–integration combined with an interpolation between the height–varying values at the foot point of the field line ( $\lambda_m$ ) and at the magnetic equator ( $\lambda = 0$ ) which is described in section 7.8. Figure 7.4 shows schematically that for a field line with the foot point at the reference height  $h_0$  and latitude  $\lambda_m$  the value  $x_{fl}$  at height  $h$  on the field line is approximated by the value  $x_{eq}$  at the equator and value  $x_m$  at foot point  $\lambda_m$  and height  $h$ . The calculation of the weighting factors  $x_{fl}$  and  $wgt_{eq}$  for the interpolation are described in section 7.8 equations (7.68) and (7.69).

Therefore the eastward current at  $(\lambda, h)$  on the field line is approximated by

$$J_{e1}^{p,g}(\lambda, h) = wgt_{eq}(h, \lambda_{eq}) J_{e1,eq}^{p,g}(\lambda_{eq}, h) + wgt_m(\lambda_m, h) J_{e1,m}^{p,g}(\lambda_m, h) \quad (7.138)$$

Since the integration is done in height rather than along the field–line,  $ds$  in equation 7.137 is expressed in terms of height  $h$ . The conversion from field line integration to height is shown in section 7.8. The increment  $ds$  along the field line is substituted by eq. (7.91). The contribution  $K_{m\phi}^{p,g}$  to the height

integrated eastward current is the sum over all pressure level k

$$\frac{K_{m\phi}^{p,g}}{|\sin I_m|} = B_{e3}(h_0)A(h_0) \sum_k \left[ \frac{10^4 J_{e1}^{p,g}(\lambda, h_{k+\frac{1}{2}})}{B_{e3}(h_0)D(h_{k+\frac{1}{2}})} \right] 10^{-2} h_{fac}(-d\sqrt{h_A - h_{k+\frac{1}{2}}}) \quad (7.139)$$

The factor  $10^4$  converts the current from  $[\frac{A}{cm^2}]$  to  $[\frac{A}{m^2}]$  and the factor  $10^{-2}$  converts ds from [cm] to [m]. The north-/upward height integrated current density is

$$K_{m\lambda} = \mp \int_{s_L}^{s_U} \frac{J_{e2}}{D} ds = \mp B_{e3} \int_{s_L}^{s_U} \left[ \frac{J_{e2}^D}{D} + \frac{J_{e2}^{p,g}}{B_{e3}D} \right] ds \quad (7.140)$$

With the above mentioned approximation of the field line integration the contribution from the plasma pressure gradient and the gravity driven current is the sum over all pressure level k

$$K_{m\lambda}^{p,g} = \pm B_{e3}(h_0)A(h_0) \sum_k \left[ \frac{10^4 J_{e2}^{p,g}(\lambda, h_{k+\frac{1}{2}})}{B_{e3}(h_0)D(h_{k+\frac{1}{2}})} \right] 10^{-2} h_{fac}(d\sqrt{h_A - h_{k+\frac{1}{2}}}) \quad (7.141)$$

## 7.10 Finite Differencing

**Hemispheric symmetry** As mentioned in section 7.2 we assume that the conductivity along the magnetic field line is very large, thus conjugate foot points are equipotential. To get a symmetric potential pattern we add the conductances and wind driven current densities of the two hemispheres together and solve for only one. The symmetry of the potential pattern is only valid at low- and mid-latitudes with closed field lines. At high latitudes the electric potential is specially treated as discussed in section 7.7.

The added together values from the northern and southern hemisphere are denoted by  $(\cdot)^T$  (see equation (7.33)–(7.38)). In the source code in subroutine `dynamo` the following values are calculated

$$\Sigma_{\phi\phi}^T(0) = \Sigma_{\phi\phi}^{NH}(0) + \Sigma_{\phi\phi}^{SH}(0) \quad (7.142)$$

$$\Sigma_{\lambda\lambda}^T(0) = \Sigma_{\lambda\lambda}^{NH}(0) + \Sigma_{\lambda\lambda}^{SH}(0) \quad (7.143)$$

$$-\Sigma_C^T(0) = -(\Sigma_C^{NH}(0) - \Sigma_C^{SH}(0)) \quad (7.144)$$

$$\Sigma_H^T(0) = \Sigma_H^{NH}(0) - \Sigma_H^{SH}(0) \quad (7.145)$$

$$K_{m\phi}^{DT}(0) = K_{m\phi}^{D,NH}(0) + K_{m\phi}^{D,SH}(0) \quad (7.146)$$

$$K_{m\lambda}^{DT}(0) = K_{m\lambda}^{D,NH}(0) - K_{m\lambda}^{D,SH}(0) \quad (7.147)$$

Note that in the source code  $-\Sigma_C^T(0)$  is put into ZIGMC, and that  $-K_{m\lambda}^{D,SH}(0)$  was saved in RIM(2). The hemispherically added values are saved in the latitude indices of the northern hemisphere from  $(nmlat + 1)/2$ , which is the index for the equator, to the pole at  $nmlat$ . The number of magnetic latitudes is  $nmlat$ .

**Differencing of the right hand side** In subroutine `rhspde` the right hand side is differentiated.

$$rhs = \frac{R_0}{\cos\lambda_0} \left[ \frac{\partial K_{m\phi}^{DT}(0)}{\partial\phi_0} + \frac{\partial K_{m\lambda}^{DT}(0)\cos\lambda_0}{\partial|\lambda_0|} \right] \quad (7.148)$$

A central differencing scheme is used which leads to the derivative at the location  $\phi(i)$ ,  $\lambda_0(j)$

$$\begin{aligned} rhs(i, j) = & \frac{R_0}{2\Delta\phi\cos\lambda_0(j)} [K_{m\phi}^{DT}(0)(i+1, j) - K_{m\phi}^{DT}(0)(i-1, j)] + \\ & \frac{R_0}{2\Delta\lambda_0\cos\lambda_0(j)} [K_{m\lambda}^{DT}(0)(i, j+1)\cos\lambda_0(j+1) - \\ & K_{m\lambda}^{DT}(0)(i, j-1)\cos\lambda_0(j-1)] \end{aligned} \quad (7.149)$$

with  $i, j$  the longitudinal and latitudinal index and the adjacent grid points  $i \pm 1, j \pm 1$ . The polar derivative is approximated by

$$rhs(i, j_{pole}) = -\frac{2R_0}{\cos\lambda_0(j-1)m_{lon}} \left[ \sum_{i=1}^{m_{lon}} K_{m\lambda}^{DT}(0)(i, j_{pole}-1) \right] \quad (7.150)$$

At the magnetic equator the northward current  $K_{m\lambda}$  has to vanish see equation (7.109) or in [14] eq. (5.30) or (5.31). Therefore the right hand side derivatives are discretized by

$$\begin{aligned} rhs(i, j_{eq}) = & \frac{R_0}{\Delta\phi\cos\lambda_0(j_{eq})} [K_{m\phi}^{D,modT}(0)(i+\frac{1}{2}, j_{eq}) - K_{m\phi}^{D,modT}(0)(i-\frac{1}{2}, j_{eq})] + \\ & \frac{2R_0}{\Delta\lambda_0} [K_{m\lambda}^{DT}(0)(i, j_{eq}+\frac{1}{2})\cos\lambda_0(j_{eq}+\frac{1}{2})] \end{aligned} \quad (7.151)$$

with  $K_{m\phi}^{D,mod}$  the modified height integrated eastward current density due to neutral winds  $K_{m\phi}^D$ , see equation (7.114). It is referred to section 7.10 eq. (7.171)–(7.173) for explanation of the discrete boundary condition at the magnetic equator. At the geomagnetic equator  $\cos\lambda_0(j_{eq}) = 1$  and equation (7.151) can be written as

$$\begin{aligned} rhs(i, j_{eq}) = & \frac{R_0}{2\Delta\phi_0} [K_{m\phi}^{D,modT}(0)(i+1, j_{eq}) - K_{m\phi}^{D,modT}(0)(i-1, j_{eq})] + \\ & \frac{R_0}{\Delta\lambda_0} [K_{m\lambda}^{DT}(0)(i, j_{eq}+1)\cos\lambda_0(j_{eq}+1) + K_{m\lambda}^{DT}(0)(i, j_{eq})] \end{aligned} \quad (7.152)$$

The whole right hand side is multiplied by  $R_0$  in [m] to get eq. (7.148).

**Differencing of the left hand side** In this paragraph the finite differencing of the left hand side of the electrodynamo equation is discussed. In the source code the calling tree for the differencing is the following:

```
subroutine dynamo
...
if (isolve == 2) then
    call stencmd
        call htrpex
        call cnmmmod
        call cnm
else
    call stencil
        call htrpex
        call cnm
endif
...
```

The flag `isolve=2` means that at the finest grid level an additional coefficient matrix is set up without upwinding for terms violating the diagonal dominance (see paragraph further down in this section). The multigrid solver which is discussed in section 7.11 uses the coefficient matrix without upwinding to calculate the residual on the finest grid level. At all other grid levels the coefficient matrix with upwinding is used to solve for the residual. If `isolve`  $\neq$  2 the upwinding method is applied at all grid levels to solve for the electric potential. For more information about the different option with the multigrid solver we refer to section 7.11.



In subroutine **dynamo** the conductances are prepared for the finite differencing. The conductance coefficients represent

$$A = \frac{\Sigma_{\phi\phi}^T(0)}{\cos\lambda_0\Delta\phi^2} \rightarrow \text{zigm11} \quad (7.153)$$

$$B = \frac{\Sigma_{\lambda\lambda}^T(0)\cos\lambda_0}{\Delta\lambda_0^2} \rightarrow \text{zigm22} \quad (7.154)$$

$$C = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi} \rightarrow \text{zigmc} \quad (7.155)$$

$$D = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi} \rightarrow \text{zigm2} \quad (7.156)$$

with **zigm11**, **zigm22**, **zigmc**, **zigm2** the variable names in the source code. Note that the factor of four is introduced due to the central differencing. Both hemisphere are already added together and the coefficients are stored in the index range of the "northern hemisphere" ((nmlat+1)/2 to nmlat). In the "southern hemisphere" index range (1 to (nmlat+1)/2), the same values are stored as in the northern range ((nmlat+1)/2 to nmlat) except of the two mixed terms which change sign.

$$\text{zigmc}(SH) \rightarrow -\frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi} \quad (7.157)$$

$$\text{zigm2}(SH) \rightarrow -\frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi} \quad (7.158)$$

The polar value of  $\frac{\Sigma_{\phi\phi}^T(0)}{\cos\lambda_0\Delta\phi^2}$  is set to zero to avoid floating point exception. The polar value is not used in the electrodynamo equation since the potential at the pole is prescribed.

The subroutine **stencmd** or subroutine **stencil** is called for each conductance term eq. (7.153)–(7.156) and the finite difference stencil is updated for the contributions of the corresponding conductance term. First the conductance is copied into a working array in subroutine **htrpex** and the longitudinal wrap around points, necessary for the longitudinal derivatives, are set. Note that there are 5 different grid levels and therefore there are 16 additional points on either side of the working array. The working array stores the values from the equator (index 1) to the pole (index (nmlat+1)/2).

The contributions to the stencil from the different conductances are determined in subroutine **cnmmod** and/or subroutine **cnm**. Subroutine **cnmmod**

is called if the flag `isolve=2` is set, and then only for the finest grid level. This subroutine sets up the coefficient stencil without upwinding method. At all the other grid levels upwinding may be used if necessary. For `isolve`  $\neq 2$  all the stencils are determined with upwinding methods if necessary, which is done in subroutine `cnm`. Please read section 7.11 for more information about the different solver types (flag `isolve`).

From equation (7.116) and the values in table 7.5 we get the following left hand side of the electrodynamo equation.

$$\begin{aligned} \cos\lambda_0 \text{ lhs} = & \frac{\partial}{\partial\phi_0} \left( \frac{\Sigma_{\phi\phi}^T(0)}{\cos\lambda_0} \frac{\partial\Phi}{\partial\phi_0} + \Sigma_{\phi\lambda}^T(0) \frac{\partial\Phi}{\partial\lambda_0} \right) + \\ & \frac{\partial}{\partial\lambda_0} \left( \Sigma_{\lambda\phi}^T(0) \frac{\partial\Phi}{\partial\phi_0} + \Sigma_{\lambda\lambda}^T(0) \cos\lambda_0 \frac{\partial\Phi}{\partial\lambda_0} \right) \end{aligned} \quad (7.159)$$

Note that the right hand side *rhs* in equation (7.148) is already divided by  $\cos\lambda_0$  therefore we have to include the  $\cos\lambda_0$  on the left hand side of eq. (7.159). Replacing the two terms in the brackets in eq. (7.159) by

$$T_\phi = \frac{\Sigma_{\phi\phi}^T(0)}{\cos\lambda_0} \frac{\partial\Phi}{\partial\phi_0} + \Sigma_{\phi\lambda}^T(0) \frac{\partial\Phi}{\partial\lambda_0} \quad (7.160)$$

$$T_\lambda = \Sigma_{\lambda\phi}^T(0) \frac{\partial\Phi}{\partial\phi_0} + \Sigma_{\lambda\lambda}^T(0) \cos\lambda_0 \frac{\partial\Phi}{\partial\lambda_0} \quad (7.161)$$

leads to

$$\cos\lambda_0 \text{ lhs} = \frac{\partial}{\partial\phi_0} T_\phi + \frac{\partial}{\partial\lambda_0} T_\lambda \quad (7.162)$$

For clarity we will omit the dependence on  $\lambda_0$  shown by  $(\cdot)(0)$  in the following e.g. we write  $\Sigma_{\phi\lambda}^T$  instead of  $\Sigma_{\phi\lambda}^T(0)$ . Using central differencing for the finite differences gives

$$\cos\lambda_0 \text{ lhs} = \frac{T_\phi(i + \frac{1}{2}, j) - T_\phi(i - \frac{1}{2}, j)}{\Delta\phi_0} + \frac{T_\lambda(i, j + \frac{1}{2}) - T_\lambda(i, j - \frac{1}{2})}{\Delta\lambda_0} \quad (7.163)$$

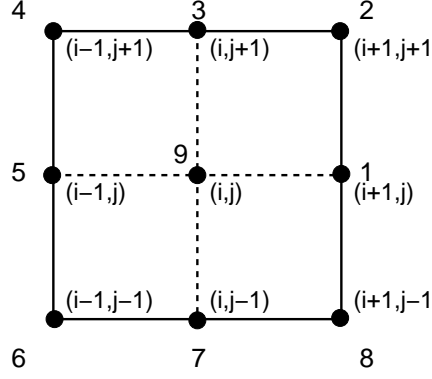


Figure 7.5: Geometry for the 9 point stencil

with

$$\begin{aligned}
 T_\phi(i + \frac{1}{2}, j) &= \frac{\Sigma_{\phi\phi}^T(i + \frac{1}{2}, j)}{\cos\lambda_0(j)} \frac{\Phi(i + 1, j) - \Phi(i, j)}{\Delta\phi_0} + \\
 &\quad \Sigma_{\phi\lambda}^T(i + \frac{1}{2}, j) \frac{\Phi(i + \frac{1}{2}, j + \frac{1}{2}) - \Phi(i + \frac{1}{2}, j - \frac{1}{2})}{\Delta\lambda_0} \\
 T_\phi(i - \frac{1}{2}, j) &= \frac{\Sigma_{\phi\phi}^T(i - \frac{1}{2}, j)}{\cos\lambda_0(j)} \frac{\Phi(i, j) - \Phi(i - 1, j)}{\Delta\phi_0} + \\
 &\quad \Sigma_{\phi\lambda}^T(i - \frac{1}{2}, j) \frac{\Phi(i - \frac{1}{2}, j + \frac{1}{2}) - \Phi(i - \frac{1}{2}, j - \frac{1}{2})}{\Delta\lambda_0} \\
 T_\lambda(i, j + \frac{1}{2}) &= \Sigma_{\lambda\phi}^T(i, j + \frac{1}{2}) \frac{\Phi(i + \frac{1}{2}, j + \frac{1}{2}) - \Phi(i - \frac{1}{2}, j + \frac{1}{2})}{\Delta\phi_0} + \\
 &\quad \Sigma_{\lambda\lambda}^T(i, j + \frac{1}{2}) \cos\lambda_0(j + \frac{1}{2}) \frac{\Phi(i, j + 1) - \Phi(i, j)}{\Delta\lambda_0} \\
 T_\lambda(i, j - \frac{1}{2}) &= \Sigma_{\lambda\phi}^T(i, j - \frac{1}{2}) \frac{\Phi(i + \frac{1}{2}, j - \frac{1}{2}) - \Phi(i - \frac{1}{2}, j - \frac{1}{2})}{\Delta\phi_0} + \\
 &\quad \Sigma_{\lambda\lambda}^T(i, j - \frac{1}{2}) \cos\lambda_0(j - \frac{1}{2}) \frac{\Phi(i, j) - \Phi(i, j - 1)}{\Delta\lambda_0}
 \end{aligned} \tag{7.164}$$

The numbering of the nine point stencil can be seen in figure 7.5 with the index  $i$  denoting the longitude and the index  $j$  for the latitude. The values at half grid points e.g.  $(i + \frac{1}{2}, j)$  are determined by averaging the values of the adjacent grid points, e.g.

$$\Sigma_{\phi\phi}^T(i + \frac{1}{2}, j) = \frac{1}{2} [\Sigma_{\phi\phi}^T(i + 1, j) + \Sigma_{\phi\phi}^T(i, j)] \tag{7.165}$$

Accordingly, the values at  $(i - \frac{1}{2}, j)$ ,  $(i, j + \frac{1}{2})$  and  $(i, j - \frac{1}{2})$  can be calculated. The difference at half points in latitude and longitude e.g.  $(i + \frac{1}{2}, j + \frac{1}{2})$  is also resolved by averaging the values of the adjacent grid points which leads to e.g.

$$\begin{aligned} \Phi(i + \frac{1}{2}, j + \frac{1}{2}) - \Phi(i + \frac{1}{2}, j - \frac{1}{2}) = \\ \frac{1}{4} [\Phi(i + 1, j + 1) - \Phi(i + 1, j - 1) + \Phi(i, j + 1) - \Phi(i, j - 1)] \end{aligned} \quad (7.166)$$

Accordingly,  $\Phi(i - \frac{1}{2}, j + \frac{1}{2}) - \Phi(i - \frac{1}{2}, j - \frac{1}{2})$ ,  $\Phi(i + \frac{1}{2}, j + \frac{1}{2}) - \Phi(i - \frac{1}{2}, j + \frac{1}{2})$  and  $\Phi(i + \frac{1}{2}, j - \frac{1}{2}) - \Phi(i - \frac{1}{2}, j - \frac{1}{2})$  are discretized. The resulting contributions from the conductance terms to the nine point stencil in figure 7.5 are summarized in table 7.6. Therein, we are using the abbreviations  $A, B, C, D$  from equations (7.153)–(7.156) for the conductance quantities.

**Upwinding** In the following the contributions to the stencil are denoted by the variable  $c$ , e.g. at node 9 the coefficient would be  $c(i, j)$ . The stability is not preserved if the stencil coefficient of adjacent points of  $c(i, j)$  are changing sign e.g.  $c(i + 1, j)c(i - 1, j) < 0$  or  $c(i, j + 1)c(i, j - 1) < 0$ . To avoid instabilities the diagonal dominance of the coefficient matrix has to be preserved. This can be done by using upwinding methods depending on the orientation of the flux (i.e. the sign of the stencil coefficients). The derivatives with respect to e.g.  $\lambda_0$  for the central differencing is

$$\frac{d\Phi(i + \frac{1}{2}, j)}{d\lambda_0} = \frac{1}{\Delta\lambda_0} [\Phi(i + \frac{1}{2}, j + \frac{1}{2}) - \Phi(i + \frac{1}{2}, j - \frac{1}{2})] \quad (7.167)$$

and the upwinding leads to

$$\begin{aligned} \frac{d\Phi(i + \frac{1}{2}, j)}{d\lambda_0} &= \frac{1}{2} \left[ \frac{d\Phi(i + 1, j)}{d\lambda_0} + \frac{d\Phi(i, j)}{d\lambda_0} \right] \\ &= \frac{1}{2} \left[ \frac{\Phi(i + 1, j + 1) - \Phi(i + 1, j - 1)}{2\Delta\lambda_0} + \frac{\Phi(i, j + 1) - \Phi(i, j - 1)}{\Delta\lambda_0} \right] \\ \frac{d\Phi(i + \frac{1}{2}, j)}{d\lambda_0} &= \frac{1}{2} \left[ \frac{d\Phi(i + 1, j)}{d\lambda_0} + \frac{d\Phi(i, j)}{d\lambda_0} \right] \\ &= \frac{1}{2} \left[ \frac{\Phi(i + 1, j + 1) - \Phi(i + 1, j - 1)}{2\Delta\lambda_0} + \frac{\Phi(i, j) - \Phi(i, j - 1)}{\Delta\lambda_0} \right] \end{aligned} \quad (7.168)$$

node	$A = \frac{\Sigma_{\phi\phi}^T}{\Delta\phi^2 \cos\lambda_0}$	$B = \frac{\Sigma_{\lambda\lambda}^T(0) \cos\lambda_0}{\Delta\lambda_0^2}$	$C = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$	$D = \frac{\Sigma_{\lambda\phi}^T(0)}{4\Delta\lambda_0\Delta\phi}$
1	$A(i + \frac{1}{2}, j)$	-	-	$D(i, j + \frac{1}{2}) - D(i, j - \frac{1}{2})$
2	-	-	$C(i + \frac{1}{2}, j)$	$D(i, j + \frac{1}{2})$
3	-	$B(i, j + \frac{1}{2})$	$C(i + \frac{1}{2}, j) - C(i - \frac{1}{2}, j)$	-
4	-	-	$-C(i - \frac{1}{2}, j)$	$-D(i, j + \frac{1}{2})$
5	$A(i - \frac{1}{2}, j)$	-	-	$-D(i, j + \frac{1}{2}) + D(i, j - \frac{1}{2})$
6	-	-	$C(i - \frac{1}{2}, j)$	$D(i, j - \frac{1}{2})$
7	-	$B(i, j - \frac{1}{2})$	$-C(i + \frac{1}{2}, j) + C(i - \frac{1}{2}, j)$	-
8	-	-	$-C(i + \frac{1}{2}, j)$	$-D(i, j - \frac{1}{2})$
9	$-A(i + \frac{1}{2}, j) - A(i - \frac{1}{2}, j)$	$-B(i, j + \frac{1}{2}) - B(i, j - \frac{1}{2})$	-	-

Table 7.6: Contributions from conductance terms to nine point stencil using central differencing for all terms (see subroutine `cnm` and subroutine `cnmmmod`)

node	$C = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$	$D = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$
1	-	$2D(i, j + \frac{1}{2}) - 2D(i, j - \frac{1}{2})$
3	$2C(i + \frac{1}{2}, j) - 2C(i - \frac{1}{2}, j)$	-
5	-	-
7	-	-
9	$-2C(i + \frac{1}{2}, j) + 2C(i - \frac{1}{2}, j)$	$-2D(i, j + \frac{1}{2}) + 2D(i, j - \frac{1}{2})$

Table 7.7: Modification to stencil due to upwinding with positive flux  $f_l > 0$  in subroutine `cnm` and subroutine `cnmmod`

and for the derivative with respect to longitude  $\phi$  the upwinding results in

$$\begin{aligned}
\frac{d\Phi(i, j + \frac{1}{2})}{d\phi_0} &= \frac{1}{2} \left[ \frac{d\Phi(i, j + 1)}{d\phi_0} + \frac{d\Phi(i, j)}{d\phi_0} \right] \\
&= \frac{1}{2} \left[ \frac{\Phi(i + 1, j + 1) - \Phi(i - 1, j + 1)}{\Delta\phi_0} + \frac{\Phi(i + 1, j) - \Phi(i, j)}{2\Delta\phi_0} \right] \\
\frac{d\Phi(i, j - \frac{1}{2})}{d\phi_0} &= \frac{1}{2} \left[ \frac{d\Phi(i, j + 1)}{d\phi_0} + \frac{d\Phi(i, j)}{d\phi_0} \right] \\
&= \frac{1}{2} \left[ \frac{\Phi(i + 1, j + 1) - \Phi(i - 1, j + 1)}{2\Delta\phi_0} + \frac{\Phi(i, j) - \Phi(i - 1, j)}{\Delta\phi_0} \right]
\end{aligned} \tag{7.169}$$

The flux at the center of the stencil (i, j) is determined by the flux average of the two adjacent points in the corresponding direction. Thus, the latitudinal flux at the center  $c(i, j)$  is  $f_l = \frac{1}{2}[c(i, j + 1) + c(i, j - 1)]$  and the longitudinal flux is  $f_l = \frac{1}{2}[c(i + 1, j) + c(i - 1, j)]$ . For positive flux  $f_l > 0$  the values in table 7.7 are used and for negative flux  $f_l < 0$  the modifications in table 7.8 are applied. If the flux at the two adjacent points goes into the same direction  $c(i + 1, j)c(i - 1, j) > 0$  or  $c(i, j + 1)c(i, j - 1) > 0$  the central differencing in table 7.6 is used.

**Equatorial boundary** At the equator the coefficient stencil has to be modified to take into account the boundary condition which was described in section 7.8 eq. (7.109)–(7.114). The discrete modification to the right hand side was described in the paragraph on page 197 eq. (7.151) but the derivation will be explained in the following together with the left hand side. Including the equatorial boundary condition eq. (7.109) into the electrodynamic equation eq. (7.32) leads to eq. (7.112). The boundary condition can

node	$C = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$	$D = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$
1	-	-
3	-	-
5	-	$-2D(i, j + \frac{1}{2}) + 2D(i, j - \frac{1}{2})$
7	$-2C(i + \frac{1}{2}, j) + 2C(i - \frac{1}{2}, j)$	-
9	$2C(i + \frac{1}{2}, j) - 2C(i - \frac{1}{2}, j)$	$2D(i, j + \frac{1}{2}) - 2D(i, j - \frac{1}{2})$

Table 7.8: Modification to stencil due to upwinding with negative flux  $f_l < 0$  in subroutine `cnm` and subroutine `cnmmod`

be rewritten as

$$\Sigma_{\lambda\phi} \frac{\partial\Phi}{\partial\phi_m} + \Sigma_{\lambda\lambda} \cos\lambda_m \frac{\partial\Phi}{\partial|\lambda_m|} = R_0 \cos\lambda_m K_{m\lambda}^D \quad (7.170)$$

and from which in discrete form follows that

$$T_\lambda(i, j_{eq} + \frac{1}{2}) + T_\lambda(i, j_{eq} - \frac{1}{2}) = R_0 \cos\lambda_0 (j_{eq} + \frac{1}{2}) K_{m\lambda}^D(i, j_{eq} + \frac{1}{2}) + R_0 \cos\lambda_0 (j_{eq} - \frac{1}{2}) K_{m\lambda}^D(i, j_{eq} - \frac{1}{2}) \quad (7.171)$$

with  $T_\lambda$  defined in eq. (7.161). The electrodynamic equation at the equator (7.112)) is discretized by

$$\begin{aligned} \frac{1}{\cos\lambda_0(j_{eq})} \left[ \frac{T_\phi(i + \frac{1}{2}, j_{eq}) - T_\phi(i - \frac{1}{2}, j_{eq})}{\Delta\phi_0} + \frac{T_\lambda(i, j_{eq} + \frac{1}{2}) - T_\lambda(i, j_{eq} - \frac{1}{2})}{\Delta\lambda_0} \right] = \\ \frac{R_0}{\cos\lambda_0(j_{eq})\Delta\phi_0} \left[ K_{m\phi}^{D,modT}(i + \frac{1}{2}, j_{eq}) - K_{m\phi}^{D,modT}(i - \frac{1}{2}, j_{eq}) \right] + \\ \frac{R_0}{\cos\lambda_0(j_{eq})\Delta\lambda_0} \left[ K_{m\lambda}^{DT}(i, j_{eq} + \frac{1}{2}) \cos\lambda_0(j_{eq} + \frac{1}{2}) - K_{m\lambda}^{DT}(i, j_{eq} - \frac{1}{2}) \cos\lambda_0(j_{eq} - \frac{1}{2}) \right] \end{aligned} \quad (7.172)$$

Inserting equation (7.171) into the electrodynamic equation (7.172) the values  $K_{m\lambda}^{DT}(i, j_{eq} - \frac{1}{2})$  and  $T_\lambda(i, j_{eq} - \frac{1}{2})$  are substituted by  $K_{m\lambda}^{DT}(i, j_{eq} + \frac{1}{2})$  and

node	$A = \frac{\Sigma_{\phi\phi}^T}{\Delta\phi^2 \cos\lambda_0}$	$B = \frac{\Sigma_{\lambda\lambda}^T(0) \cos\lambda_0}{\Delta\lambda_0^2}$	$C = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$	$D = \frac{\Sigma_{\phi\lambda}^T(0)}{4\Delta\lambda_0\Delta\phi}$
1	$A(i + \frac{1}{2}, j)$	-	-	$D(i, j + \frac{1}{2})$
2	-	-	-	$D(i, j + \frac{1}{2})$
3	-	$B(i, j + \frac{1}{2})$	-	-
4	-	-	-	$-D(i, j + \frac{1}{2})$
5	$A(i - \frac{1}{2}, j)$	-	-	$-D(i, j + \frac{1}{2})$
6	-	-	-	-
7	-	-	-	-
8	-	-	-	-
9	$-A(i + \frac{1}{2}, j) - A(i - \frac{1}{2}, j)$	$-B(i, j + \frac{1}{2})$	-	-

Table 7.9: Modification to stencil at the equator (see `subroutine cnm` or `subroutine cnmmod` )

$T_\lambda(i, j_{eq} + \frac{1}{2})$  which lead to

$$\begin{aligned}
& \frac{T_\phi(i + \frac{1}{2}, j_{eq}) - T_\phi(i - \frac{1}{2}, j_{eq})}{\Delta\phi_0} + \frac{2T_\lambda(i, j_{eq} + \frac{1}{2})}{\Delta\lambda_0} = \\
& \frac{R_0}{\Delta\phi_0} \left[ K_{m\phi}^{D, modT}(i + \frac{1}{2}, j_{eq}) - K_{m\phi}^{D, modT}(i - \frac{1}{2}, j_{eq}) \right] + \\
& \frac{R_0}{\Delta\lambda_0} \left[ 2K_{m\lambda}^{DT}(i, j_{eq} + \frac{1}{2}) \cos\lambda_0(j_{eq} + \frac{1}{2}) \right]
\end{aligned} \tag{7.173}$$

with  $\cos\lambda_0(j_{eq}) = 1$  and the value  $T_\phi = \frac{\Sigma_{\phi\phi}^{modT}(0)}{\cos\lambda_0} \frac{\partial\Phi}{\partial\phi_0}$  at the equator. Therefore the stencil has to be modified at the equator according to table 7.9 with  $B(i, j - \frac{1}{2}) = 0$ ,  $D(i, j - \frac{1}{2}) = 0$  and no  $\Sigma_{\phi\lambda}$  contributions. The coefficients for A are not changing (see table 7.6).

**Coefficient stencil** In table 7.10 the longitudinal and latitudinal dimensions of the 5 different grid levels are given. On the finest grid level the right hand side is stored in `c0(:, :, 10)`. Therefore the dimension is 10 instead of 9, which is the size at all other grid levels. At the pole ( $j = nmlat^*$ ) the off diagonal terms are set to zero and the diagonal terms to one  $c^*(i, nmlat^*, 9) = 1$  in `subroutine edges` with  $(\cdot)^*$  denoting the different grid levels. The right hand side is set to one at the pole  $c0(i, nmlat, 10) = 1$ . The left hand side *lhs* is finally divided by  $\cos\lambda_0$  in `subroutine divide`.



grid level	variable $c^*$	long.dimension	lat.dimension $nmlat^*$	"points" of stencil
0	c0	81	49	10
1	c1	41	25	9
2	c2	21	13	9
3	c3	11	7	9
4	c4	6	4	9

Table 7.10: Coefficient matrix name and dimensions at the different grid levels

## 7.11 Solving for the electric potential

In TIEGCM a multigrid solver is used which was developed by J. Adams. The source code and information can be found at <http://www.scd.ucar.edu/css/software/mudpack/>. In the original mudpack solver the finite differencing and the setting of all the boundary conditions are part of solver package. For TIEGCM the stencil and the boundary conditions are already set up in the TIEGCM code, and therefore the multigrid solver was modified accordingly. We have three different solver options in TIEGCM which are all based on the mudpack multigrid package.

- `isolve=0` multigrid solver `mudcr2` (see section 7.11.1)
- `isolve=1` multigrid solver `muhcr2` as direct solver (see section 7.11.2)
- `isolve=2` modified multigrid solver `mudcr2` (see section 7.11.3)

### 7.11.1 Multigrid solver `mudcr2`

The subroutine `mud2cr` attempts to compute the second-order difference approximation to a two-dimensional linear nonseparable elliptic partial differential equation with cross derivative terms on a rectangle. The approximation is generated on a uniform grid covering the rectangle. The parameters used for the multigrid solver in TIEGCM are the following:

- `intl=0`: this is an input to the subroutine and is zero for the initial call to `mud2cr` to check for errors. After the initial call of `mud2cr` `intl=1` will be set and the PDE is solved.
- boundary conditions: with `x` being the longitudinal direction and `y` the latitudinal one from the equator to the pole.
  - `nxa = 0` : flags boundary conditions on the edge `x=xa`. `nxa = 0` means the boundary condition is periodic in `x` on `[xa,xb]`.
  - `nxb = 0`: flags boundary conditions on the edge `x=xb`. `nxb = 0` means the boundary condition is periodic in `x` on `[xa,xb]`.
  - `nyc = 2`: flags boundary conditions on the edge `y=yc` (equator). `nyc = 2` means that there are mixed derivative boundary conditions at `y=yc`.

- $nyd = 1$ : flags boundary conditions on the edge  $y=yd$  (pole).  $nyd=1$  means that the boundary condition is specified and input thru the variable `phi`.
- defining the number of grid points in  $x$  (longitude) and  $y$  (latitude) direction
  - $ixp = 5$ :  $ixp+1$  is the number of points on the coarsest  $x$  grid visited during multigrid cycling.
  - $jyq = 3$ :  $jyq+1$  is the number of points on the coarsest  $y$  grid visited during multigrid cycling.
  - $iey = 5$ : integer exponent of 2 used in defining the number of grid points in the  $x$  direction
  - $jey = 5$ : integer exponent of 2 used in defining the number of grid points in the  $y$  direction
  - $nx$ : number of equally spaced grid points in the interval  $[xa,xb]$   
 $nx = ixp \cdot 2^{iey-1} + 1$
  - $ny$ : number of equally spaced grid points in the interval  $[yc,yd]$   
 $ny = jyq \cdot 2^{jey-1} + 1$
- $iguess = 0$ : no initial guess is used forcing full multigrid cycling
- $tolmax = 0.01$ :  $tolmax$  is the maximum relative error tolerance used to terminate the relaxation iterations. Assume  $\Phi_1$  and  $\Phi_2$  are the last two computed approximations at the finest grid level. If we define  $\Phi_{diff} = \max(|\Phi_2(i,j) - \Phi_1(i,j)|)$  for all  $i,j$  and  $\Phi_{max} = \max(|\Phi_2(i,j)|)$  for all  $i,j$  then convergence is considered to have occurred if and only if  $\frac{\Phi_{diff}}{\Phi_{max}} < tolmax$
- $maxcy = 150$ : if  $tolmax > 0.0$  is input, which means error control is used, then  $maxcy$  is the limit on the number of cycles between the finest and coarsest grid levels. When the multigrid iteration is working correctly only a few cycles are required for convergence.
- $method = 3$ : method of relaxation. If neither  $fx$  (the longitudinal second order derivative  $\Sigma_{\phi\phi}/\Delta\phi^2$ ) or  $fy$  (the latitudinal second order derivative  $\Sigma_{\lambda\lambda}/\Delta\lambda_0^2$ ) dominates over the solution region and they both vary considerably choose  $method = 3$ , which uses line relaxation in both the  $x$  and  $y$  direction

- `nwork`: length of work array  
 $length = [7(nx + 2)(ny + 2) + 4(11 + isx + jsy)nx * ny]/3$
- `mgopt`: multigrid options the default values (2,2,1,3) in the vector `mgopt` were chosen for robustness.
  - `mgopt(1) = 2`: w cycling
  - `mgopt(2) = 2`: the number of pre-relaxation sweeps executed before the residual is restricted and cycling is invoked at the next coarser grid level
  - `mgopt(3) = 1`: the number of post-relaxation sweeps executed after the cycling has been invoked at the next coarser grid level and the residual correction has been transferred back
  - `mgopt(4) = 3`: multicubic prolongation (interpolation) is used to transfer residual corrections and the PDE approximation from the coarse to the fine grid within full multigrid cycling.
- output  $\Phi$ : solution of PDE which is the electric potential
- output `ierror`: indicates invalid input arguments when returned positive and nonfatal warnings when returned negative.

If no convergence is reached with this version of the multigrid solver the direct solver described in section 7.11.2 is used.

### 7.11.2 Multigrid solver `muhcr2` as direct solver

This solver which is in subroutine `muh2cr` is originally a hybrid multigrid/direct method which approximates the same 2-d nonseparable elliptic PDE as the mudpack solver `mud2cr`. Using a direct method combines the efficiency of multigrid iteration with the certainty of a direct method. The basic algorithm is modified by using banded Gaussian elimination in place of relaxation whenever the coarsest subgrid is encountered within the multigrid cycling. The solver becomes a full direct method if grid size arguments are chosen so that the coarsest and finest grids coincide, i.e. choosing `iex=jey=1` and `ixp=nx-1, jyq=ny-1`. This will set the Gaussian elimination on the finest grid. In this case, subroutine `muh2cr` produces a direct solution to the same nonseparable elliptic PDE. In TIEGCM we are using the solver `muhcr2` only as a direct solver.

### 7.11.3 Modified multigrid solver `mudcr2`

This solver is the same as the solver in section 7.11.1 only with the exception that the residual is calculated with the coefficient stencil without upwinding (see section 7.10). Therefore the solution converges toward the solution of the direct solver using the coefficient stencil without the upwinding method. In general upwinding introduces unwanted numerical dissipation. The unmodified coefficient stencil is stored in the array `cofum`. In comparison with the solver in section 7.11.1 the number of relaxation steps has to be increased to get convergence.

- `mgopt(2) = 3`: the number of pre-relaxation sweeps executed before the residual is restricted and cycling is invoked at the next coarser grid level
- `mgopt(3) = 2`: the number of post-relaxation sweeps executed after cycling has been invoked at the next coarser grid level and the residual correction has been transferred back

All the other parameters remain the same and can be found in section 7.11.1. If no convergence is reached with this multigrid solver the direct solver described in section 7.11.2 is called.

## 7.12 Electric Field

In subroutine `threed` the two and three dimensional electric field and the three dimensional electric potential is calculated from the two dimensional electric potential  $\Phi$ . The components of the electric field  $E_{d1}$  and  $E_{d2}$  which are in more-or-less magnetic eastward and downward/equatorward direction are determined by

$$E_{d1} = -\frac{1}{R_0 \cos \lambda_m} \frac{\partial \Phi}{\partial \phi_m} \quad (7.174)$$

$$E_{d2} = \frac{1}{R_0 \sin I_m} \frac{\partial \Phi}{\partial \lambda_m} \quad (7.175)$$

In the code the equally spaced latitudinal grid point distribution  $\lambda_0$  in  $\lambda_m^*$  is used to calculate the derivatives. Therefore the mapping factors from the irregular latitudinal spaced grid  $\lambda_m^*$  to  $\lambda_0$  have to be taken into account. Including these factors the discrete derivatives are

$$E_{d1}(i, j) = -\frac{1}{R_0} \frac{\cos \lambda_0(j)}{\cos \lambda_m^*(j)} \frac{\Phi(i-1, j) - \Phi(i+1, j)}{2 \cos \lambda_0(j) \Delta \phi_m} \quad (7.176)$$

$$E_{d2}(i, j) = \frac{1}{R_0} \frac{\partial \lambda_0(j)}{|\sin I_m(j)| \partial \lambda_m^*(j)} \frac{\Phi(i, j-1) - \Phi(i, j+1)}{2 \Delta \lambda_0} \quad (7.177)$$

The polar values are averaged over the four surrounding points. At the equator a second order polynomial of the electric potential is fitted through the adjacent points and thus the derivative of the polynomial at the equator is determined.

The three dimensional electric potential and electric field is calculated assuming that the dipolar magnetic field lines are equipotential. At each grid point  $(\phi(i), \lambda_m^*(j), h(k))$  the foot point of the magnetic field line going through this grid point is determined. Having found the foot point of the field line at height  $h_0$  the values, i.e. electric potential and electric field, at this point can be determined by a two dimensional interpolation of the surrounding points. The polar values are determined by longitudinal averaging all the polar values.

### 7.13 Additional features

### 7.13.1 Magnetic perturbations

The magnetic perturbation from a TIEGCM model run can be determined by using the postprocessor program **MagIon**. The program is available upon request together a **MagIon** user guide, a model description is in preparation. The global magnetic perturbations at the ground and above the ionosphere at low orbiting satellite heights can be determined, or what a magnetometer would measure at the ground. For details about the calculation and the necessary assumption we refer to [?], [13] and the **MagIon** user guide.

To calculate the magnetic perturbation the radial component of the field-aligned current  $J_{qr}$  and the height-integrated current densities  $K_{m\phi}$  and  $K_{m\lambda}$  have to be known. In addition, if the influence of gravity and plasma pressure gradient driven current should be included the height dependent  $K_{m\phi}^{int}$  have to be determined with and without the current driven by gravity and plasma pressure gradient. The calculation of these currents is not the default in the TIEGCM source code, thus the flag `icalkqlam == 1` in the `module dynamo` has to be set. In the following the calculation of the different currents  $J_{qr}$ ,  $K_{q\phi}$  and  $K_{q\lambda}$ , which can be found in the file `current.F`, is described.

#### Field-aligned current $J_{qr}$

The field-aligned current can be determined from the electrodynamic equation (7.32) without the assumption of symmetrical hemispheres which leads to

$$\begin{aligned} & \frac{\partial}{\partial \phi_m} \left( \frac{\Sigma_{\phi\phi}}{\cos \lambda_m} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\phi\lambda} \frac{\partial \Phi}{\partial |\lambda_m|} \right) + \frac{\partial}{\partial |\lambda_m|} \left( \Sigma_{\lambda\phi} \frac{\partial \Phi}{\partial \phi_m} + \Sigma_{\lambda\lambda} \cos \lambda_m \frac{\partial \Phi}{\partial |\lambda_m|} \right) \\ &= R \frac{\partial K_{m\phi}^D}{\partial \phi_m} + R \frac{\partial K_{m\lambda \cos \lambda_m}^D}{\partial |\lambda_m|} + R^2 \cos \lambda_m J_{mr} \end{aligned} \quad (7.178)$$

Note that compared to the electrodynamic equation (7.32) the conductances and the wind driven current are different in the northern and southern hemisphere denoted by e.g.  $\Sigma_{\phi\phi}$  instead of  $\Sigma_{\phi\phi}^T$ . Therefore we determine the finite difference coefficient stencil for both hemispheres instead of only one as described in section 7.10 on page 199. The set up of the finite difference stencil is analog to the one for only one hemisphere. The `subroutine nosocoeff` sets up the coefficient stencil for both hemisphere and also saves the wind



driven current. The **subroutine** **nosocoe** is called shortly after the field line integrations i.e. before the conductances and wind driven currents are added together from the two hemispheres (see table 7.5). The conductances are prepared for the finite differencing and represent

$$A = \frac{\Sigma_{\phi\phi}(0)}{\cos\lambda_0\Delta\phi^2} \rightarrow nszigm11 \quad (7.179)$$

$$B = \frac{\Sigma_{\lambda\lambda}^{(0)}\cos\lambda_0}{\Delta\lambda_0^2} \rightarrow nszigm22 \quad (7.180)$$

$$C = \frac{\Sigma_{\phi\lambda}(0)}{4\Delta\lambda_0\Delta\phi} \rightarrow nszigmc \quad (7.181)$$

$$D = \frac{\Sigma_{\phi\lambda}(0)}{4\Delta\lambda_0\Delta\phi} \rightarrow nszigm2 \quad (7.182)$$

The set up of the stencil is analog to section 7.10 see table 7.6 and 7.9 with A, B, C and D from the definitions above eq. (7.179)–(7.182).

The calling tree is

```
...
call nsstencil
    call nscnm
...
```

Note that the stencil is only calculated on the finest grid. In addition no up-winding method to preserve the diagonal dominance is used since the finite difference stencil is not used for solving. The numbering of the nine node stencil for the southern hemisphere is the same as for the northern hemisphere, which is illustrated in figure 7.6 for both hemispheres. This means that e.g. points 6", 7" and 8" in the southern hemisphere are toward the poles and not toward the equator as for the northern hemisphere points 6, 7 and 8. This switch of the nodes 6, 7, 8 with 4, 3, 2 is reflected in the set up of the stencil in the southern hemisphere done in **subroutine** **nscnm**. The result is stored in the array **nscoef**. The wind driven currents of the right hand side are treated in the same way as in the dynamo equation in section 7.10 on page 197. The right hand side is saved in the array **nsrhs**.

Having set up the finite difference coefficient matrix  $\bar{\mathbf{C}}$  of the left hand side, as described in the previous paragraph, and determined the wind driven

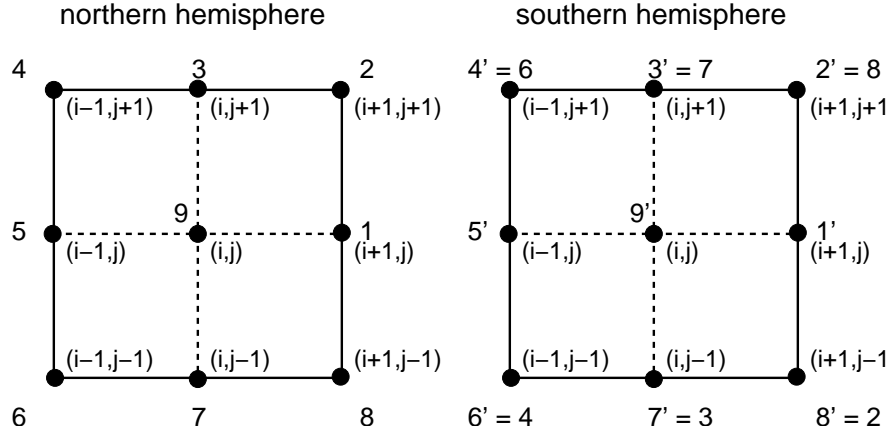


Figure 7.6: Geometry for the 9 point stencil in the northern and southern hemisphere

current of the right hand side vector **rhs** we can insert the calculated electric potential vector  $\Phi$  into equation (7.178) to solve for the field aligned current vector  $J_{mr}$ .

$$R_0^2 \frac{\cos \lambda_m}{\cos \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_m^*} J_{mr} = \bar{C} \Phi - \text{rhs} \quad (7.183)$$

Note that the whole electrodynamo equation was multiplied by  $\frac{1}{\cos \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_m^*}$  as mentioned on page 167. The current calculation is done in **subroutine nosocrtrt**. For the polar values the average values at adjacent latitudinal point are extrapolated by

$$J_{mr}(j_{pole}) = \frac{1}{8nmlon} \left[ 9 \sum_{i=1}^{nmlon} J_{mr}(i, j_{pole} \mp 1) - \sum_{i=1}^{nmlon} J_{mr}(i, j_{pole} \mp 2) \right] \quad (7.184)$$

with  $nmlon$  the number of longitudes and  $j_{pole}$  the latitudinal index at the north / south pole and the  $\mp$  sign referring to the poles respectively. Close to the magnetic equator there is no distinct allocation of the current to either the height integrated current density  $K_{m\lambda}$  or the field-aligned current  $J_{mr}$  since the magnetic field lines are almost horizontal in this region. Therefore the allocation to either one of the two currents  $K_{m\lambda}$  and  $J_{mr}$  depends strongly on the reference height  $h_0$ . Raising the reference height will shift the current from the field line to the ionospheric current sheet  $K_{m\lambda}$ . The exact distribution of the current at the equator can be neglected for the calculation of the

magnetic perturbations. Therefore we linearly interpolate the field-aligned current between  $\pm 12^\circ$  latitude.

$$J_{mr}(j) = \frac{J_{mr}(\lambda_m^{max})J_{mr}(\lambda_m^{min})}{\lambda_m^{max} - \lambda_m^{min}}(\lambda_m - \lambda_m^{min}) + J_{mr}(\lambda_m^{min}) \quad (7.185)$$

$$\text{for } \lambda_m^{min} \leq \lambda_m \leq \lambda_m^{max} \quad (7.186)$$

with  $\lambda_m^{min} = -12^\circ$  and  $\lambda_m^{max} = 12^\circ$ . Due to the linear interpolation at each latitude higher frequency modes are introduced which are smoothed by a weighted average in longitude.

$$J_{mr}(j) = \frac{1}{5}[J_{mr}(i+1, j) + 3J_{mr}(i, j) + J_{mr}(i-1, j)] \quad (7.187)$$

Since the field-aligned current  $J_{mr}$  is used to calculate the ionospheric equator-/ downward current sheet contribution  $K_{m\lambda}$  the total current system is adjusted automatically to satisfy that it is divergence free.

**Eastward current  $J_{e1}$  and height integrated current densities  $K_{q\phi}$ ,  $K_{q\lambda}$**

To calculate the eastward height integrated current density  $K_{q\phi}$ , see also eq. (7.4) in [14],

$$K_{q\phi} = \int_{h_l}^{h_u} \left( \frac{R_E + h}{R_0} \right)^{5/2} \frac{J_{e1}}{F} dh \quad (7.188)$$

the eastward current  $J_{e1}$  has to be known. The eastward current  $J_{e1}$  is determined by, see also eq. (5.7) in [14],

$$\frac{J_{e1}}{D} = \sigma_P \frac{d_1^2}{D} (E_{d1} + u_{e2} B_{e3}) + \left( \sigma_P \frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D} - \sigma_H \right) (E_{d2} - u_{e1} B_{e3}) + \text{fac} \frac{J_{e1}^{p,g}}{D} \quad (7.189)$$

The downward-/ equatorward current component  $J_{e2}$  is only calculated for postprocessing reasons.

$$\frac{J_{e2}}{D} = \sigma_P \frac{d_2^2}{D} (E_{d2} - u_{e1} B_{e3}) + \left( \sigma_P \frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D} + \sigma_H \right) (E_{d1} + u_{e2} B_{e3}) + \text{fac} \frac{J_{e2}^{p,g}}{D} \quad (7.190)$$

with  $\text{fac} = 10^4$  being the conversion factor from  $\frac{1}{\text{cm}^2}$  to  $\frac{1}{\text{m}^2}$ . The current components are computed on the half pressure levels. The input quantities  $\sigma_H$ ,  $\sigma_P$ ,  $\frac{d_1^2}{D}$ ,  $\frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{D}$ ,  $u_{e1}$ ,  $u_{e2}$  and  $B_{e3}$  are all stored at half pressure levels. Only the electric field  $E_{d1}$  and  $E_{d2}$  are at full pressure levels and have to be converted to half levels by

$$E_{d1}(k') = \frac{1}{2}(E_{d1}(k) + E_{d1}(k+1)) \quad (7.191)$$

with  $k'$  denoting the half pressure level index  $k' = k + \frac{1}{2}$ . We assume that  $\frac{d_2^2}{D} = 1$  everywhere which is approximately true. In addition to this simplification the height variation of the magnetic field component  $B_{e3}$  is neglected. The current contribution due to plasma pressure gradient and gravity  $J_{e1}^{p,g}$  is

$$\frac{J_{e1}^{p,g}}{D} = \frac{\mathbf{J}_p \cdot \mathbf{d}_1 + \mathbf{J}_g \cdot \mathbf{d}_1}{D} \quad (7.192)$$

with  $\mathbf{J}_p$  determined in section 7.9.2 by eq. (7.123) and the gravity term  $\mathbf{J}_g$  in section 7.9.1 by eq. (7.118). The gravity and plasma pressure gradient current is calculated in **subroutine magpres\_grav** on the geographic grid and is mapped afterward to the geomagnetic grid. Both terms  $\mathbf{J}_p$  and  $\mathbf{J}_g$  are stored at half pressure levels.

Once the eastward current  $J_{e1}$  is determined the height integrated eastward current density  $K_{m\phi}$  can be calculated by using eq. (7.188) with the dipole field quantity  $F$  quantity, see also eq. (6.9) in [14],

$$F = \frac{\sin \lambda_m}{\sin \lambda_q} \frac{\sin I}{\sin I_m} \left( \frac{R_E + h}{R_0} \right)^3 D \quad (7.193)$$

Inserting eq. (7.193) into eq. (7.188) leads to

$$K_{q\phi} = \int_{h_l}^{h_u} \frac{J_{e1}}{D} \frac{\sin \lambda_q}{\sin \lambda_m} \frac{\sin I_m}{\sin I} \left( \frac{R_0}{R_E + h} \right)^{1/2} dh \quad (7.194)$$

which is calculated at full pressure levels. The height integrated current densities are calculated assuming a dipole field which is indicated by the index  $(\cdot)_q$  of  $K_{q\phi}$ . Therefore the height integration is done in height rather than along the field line. The difference between height and field line integration at mid- and high latitude is small since the field lines are almost vertical

through the ionospheric current sheet. The dipole latitude  $\lambda_q$  in eq. (7.194) is

$$\sin\lambda_q(h) = \sin\lambda_m(h_0) \quad (7.195)$$

We assume dipolar field lines such that  $\lambda_m(h)$  can be computed by

$$\cos^2\lambda_m(h) = \frac{R_0}{R} \cos^2\lambda_q \quad (7.196)$$

The sinus of the inclination angle  $I_m$  is determined by

$$\sin I_m = \frac{2\sin\lambda_m(h_0)}{\sqrt{1 + 3\sin^2\lambda_m(h_0)}} \quad (7.197)$$

and the sinus of the angle  $I$  by

$$\sin I = \frac{B_z}{|B_0|} \quad (7.198)$$

with  $|B_0|$  the magnitude of the geomagnetic field and  $B_z$  the downward component. Note that we assume that both quantities vary in the same way in height and therefore no height variation is taken into account. The equatorial values of  $\sin I$  and  $\sin\lambda_q$  are taken from the adjacent grid point in latitude. The height integral is the sum over all height levels with

$$K_{q\phi} = \sum_{k=-2}^{\text{mlev}} S(k') J_{e1}(k') dh(k) \quad (7.199)$$

with  $J_{e1}(k')$  the eastward current at the half pressure level between  $k$  and  $k+1$ . The term  $S$  denotes  $\frac{\sin\lambda_q}{\sin\lambda_m} \frac{\sin I}{\sin I_m} (\frac{R_0}{R_E+h})^{1/2}$  which is known at the full level e.g.  $k$  and  $k+1$  and therefore has to be interpolated to the half pressure level. The discrete height  $dh$  is determined by  $dh = \frac{1}{100}[z(k+1) - z(k)]$  in [m].

For the calculation of the magnetic perturbations due to plasma pressure gradient and gravity driven current, the height distribution of the eastward current density denoted by  $K_{m\phi}^{int}$  has to be known. The previous assumption that most of the current is flowing in a thin current shell is not valid anymore since the current due to gravity and plasma pressure gradient is flowing in

the E- and F-region. Therefore the height dependent current density at pressure level  $k^*$  is calculated by

$$K_{m\phi}^{\text{int}}(k^*) = \sum_{k=-2}^{k^*} S(k') J_{e1}(k') dh(k) \quad (7.200)$$

Once the height integrated eastward current density  $K_{q\phi}$  and the radial component of the field aligned current  $J_{mr}$  are determined by equations (7.183) and (7.199) the height integrated northward current density  $K_{q\lambda}$  can be calculated such that the current system is divergence free

$$J_{mr} = \frac{-1}{R \cos \lambda_q} \left[ \frac{\partial K_{q\phi}}{\partial \phi_q} + \frac{\partial (K_{q\lambda} \cos \lambda_q)}{\partial \lambda_q} \right] \quad (7.201)$$

Solving eq. (7.201) for the the height integrated northward current density  $K_{q\lambda}$  leads to

$$K_{q\lambda}(\phi_q, \lambda_q^*) = -\frac{1}{\cos \lambda_q^*} \int_{-\frac{\pi}{2}}^{\lambda_q^*} \left[ J_{mr} R \cos \lambda_q + \frac{\partial K_{q\phi}}{\partial \phi_q} \right] d\lambda_q \quad (7.202)$$

The derivative  $\frac{\partial K_{q\phi}}{\partial \phi_q}$  is approximated by central differencing

$$\frac{dK_{q\phi}(i, j)}{d\phi_q} = \frac{K_{q\phi}(i + \frac{1}{2}, j) - K_{q\phi}(i - \frac{1}{2}, j)}{2\Delta\phi_q} \quad (7.203)$$

with  $i$  being the longitudinal index and  $i + \frac{1}{2}$  denoting the average between the grid points  $i$  and  $i+1$ . We substitute the following term for simplicity

$$T(i, j) = J_{mr}(i, j) R \cos \lambda_q(j) + \frac{dK_{q\phi}(i, j)}{d\phi_q} \quad (7.204)$$

into equation (7.202). The integration is done over the southern and northern hemisphere separately since the total current in both hemispheres has to cancel.

$$S^{SH}(i, j^*) = - \sum_{j=2}^{j^*} T(i, j - \frac{1}{2}) [\lambda_j - \lambda_{j-1}] \quad \frac{nmlat + 1}{2} \geq j^* > 2 \quad (7.205)$$

$$S^{NH}(i, j^*) = \sum_{j=nmlat-1}^{j^*} T(i, j + \frac{1}{2}) [\lambda_j - \lambda_{j-1}] \quad \frac{nmlat + 1}{2} < j^* \leq nmlat-1 \quad (7.206)$$

In addition the integral of the absolute northward current is computed by

$$|S^{SH}(i, j^*)| = - \sum_{j=2}^{j^*} |T(i, j - \frac{1}{2})[\lambda_j - \lambda_{j-1}]| \quad \frac{nmlat+1}{2} \geq j > 2 \quad (7.207)$$

$$|S^{NH}(i, j^*)| = \sum_{j=nmlat-1}^{j^*} |T(i, j + \frac{1}{2})[\lambda_j - \lambda_{j-1}]| \quad \frac{nmlat+1}{2} < j \leq nmlat-1 \quad (7.208)$$

The northward current  $K_{q\lambda}$  has to be corrected to assure that the sum over both hemispheres vanishes. The magnitude of the correction  $\epsilon^{SH}$  and  $\epsilon^{NH}$  for the two hemispheres is calculated at each longitude  $\phi_q(i)$ .

$$\epsilon^{SH}(i) = \frac{1}{2} \frac{S^{SH}(i, j^*) - S^{NH}(i, j^*)}{|S^{SH}(i, j^*)|} \quad \text{with } j^* = nmlat \quad (7.209)$$

$$\epsilon^{NH}(i) = \frac{1}{2} \frac{S^{SH}(i, j^*) - S^{NH}(i, j^*)}{|S^{NH}(i, j^*)|} \quad \text{with } j^* = nmlat \quad (7.210)$$

The corrected northward height integrated current densities in the southern and northern hemisphere are

$$K_{q\lambda}^{cor}(i, j) = \frac{1}{\cos \lambda_q} [S^{SH}(i, j) - \epsilon^{SH}(i)|S^{SH}(i, j)|] \quad \frac{nmlat+1}{2} \geq j > 2 \quad (7.211)$$

$$K_{q\lambda}^{cor}(i, j) = \frac{1}{\cos \lambda_q} [S^{NH}(i, j) + \epsilon^{NH}(i)|S^{NH}(i, j)|] \quad \frac{nmlat+1}{2} < j \leq nmlat-1 \quad (7.212)$$

with the error  $\epsilon$  distributed according to the weight of  $|S(i, j)| = |K_{q\lambda}(i, j)|$ . The eastward current  $J_{e1}$ , the height integrated current densities  $K_{q\phi}$  and  $K_{q\lambda}^{cor}$ , as well as the height dependent current density  $K_{q\phi}^{int}$  are all calculated in subroutine `nosocrdens`.

**7.13.2 No electrodynamo calculation**



physical field	variable	unit	pressure level	timestep
electric field: east-, north-, upward	$R * E_{m\phi}, R * E_{m\lambda}, 2\Delta z * E_z$  $B_x, B_y, B_z$  B  $\mathbf{J}_{mag} = \frac{\partial s_{mag}}{\partial s_{geo}}$	V	interface	$t_n$
geomagnetic direction on geographic grid				
geomagnetic field (north-, east-, downward)		Gauss	-	-
geomagnetic field strength		Gauss	-	-
Jacobian		-	-	-

Table 7.11: Input fields to subroutine `ionvel`

physical field	variable	unit	pressure level	timestep
electric field: geographic east-, north-, upward	$E_x, E_y, E_z$ $v_{ExB,x}, v_{ExB,y}, v_{ExB,z}$	V/cm cm/s	interface interface	$t_n$ $t_n$
on geographic grid				
electromagnetic drift velocity (geographic east-, north-, upward)				

Table 7.12: Output fields of subroutine `ionvel`

## 7.14 Electrodynamic drift velocity calculation

/

The input to subroutine `ionvel` is summarized in table 7.11. The output of subroutine `ionvel` is summarized in table 7.12. Firstly, the electric field input to this subroutine  $R * E_{m\phi}, R * E_{m\lambda}, \Delta z * E_z$  which is the electric field on the geographic grid but in geomagnetic direction is rotated into the

geographic direction by using the Jacobian matrix  $\mathbf{J}_{mag}$ .

$$\mathbf{J}_{mag} = \frac{\partial s_{mag}}{\partial s_{geo}} = \begin{pmatrix} \frac{\cos \lambda_m}{\cos \lambda_g} \frac{d\phi_m}{d\phi_g} & \cos \lambda_m \frac{d\phi_m}{d\lambda_g} \\ \frac{1}{\cos \lambda_g} \frac{d\lambda_m}{d\phi_g} & \frac{\lambda_m}{\lambda_g} \end{pmatrix} \quad (7.213)$$

with the geographic coordinate system denoted by  $s_{geo}$  and the geomagnetic coordinate system denoted by  $s_{mag}$ . The Jacobian matrix is calculated in the subroutine `apex` by using the eastward  $\mathbf{f}_1$  and northward  $\mathbf{f}_2$  base vector for quasi-dipole coordinates as defined in [15].

$$\mathbf{J}_{mag} = \begin{pmatrix} \mathbf{f}_2(2) & \mathbf{f}_2(1) \\ -\mathbf{f}_1(2) & \mathbf{f}_1(1) \end{pmatrix} \quad (7.214)$$

*check the Jacobian stuff, how does this fit together the two matrices????????.*

The electric field [V/cm] in geographic direction is  $\mathbf{E}_{geo} = \mathbf{J}_{mag} \mathbf{E}_{mag}$  with  $\mathbf{E}_{geo} = (E_x, E_y, E_z)^T$ .

$$E_x = \frac{1}{R} [j_{11} R * E_{m\phi} + j_{21} R * E_{m\lambda}] \quad (7.215)$$

$$E_y = \frac{1}{R} [j_{12} R * E_{m\phi} + j_{22} R * E_{m\lambda}] \quad (7.216)$$

$$E_z = \frac{2\Delta z * E_z}{2\Delta z} \quad (7.217)$$

with the radius  $R = R_E + z$ , and  $2\Delta z = z_{k+1} - z_{k-1}$ . The electric field is extrapolated at the lower and upper boundary with the height index  $k_{bot}$  and  $k_{top}$ .

$$E_z(z_{bot}) = 2E_z(z_{bot} + \Delta z) - E_z(z_{bot} + 2\Delta z) \quad (7.218)$$

$$E_z(z_{top}) = 2E_z(z_{top} - \Delta z) - E_z(z_{top} - 2\Delta z) \quad (7.219)$$

The height  $z_{bot}$  corresponds to  $k_{bot}$ , and  $z_{top}$  to  $k_{top}$  with  $z_{bot} + \Delta z$  is  $k_{bot} + 1$ , and  $z_{top} - \Delta z$  is  $k_{top} - 1$  etc. The electrodynamic drift velocity is determined by

$$\mathbf{v}_{ExB} = -\frac{\mathbf{E} \times \mathbf{B}}{B^2} \quad (7.220)$$

The components of  $\mathbf{B}$  are  $B_x, B_y$ , and  $B_z$  in northward, eastward and downward direction. To be consistent with the geographic direction the magnetic

field vector reads  $(B_y, B_x, -B_z)^T$ .

$$v_{ExB,x} = - \frac{E_y B_z + E_z B_x}{B^2} \quad (7.221)$$

$$v_{ExB,y} = \frac{E_z B_y + E_x B_z}{B^2} \quad (7.222)$$

$$v_{ExB,z} = \frac{E_x B_x - E_y B_y}{B^2} \quad (7.223)$$

$$(7.224)$$

In the code a factor of  $10^6$  is used to convert from  $[\frac{V}{cmGauss}]$  to  $[\frac{V}{mT}] = [m/s]$ . However, after the periodic points are set the electrodynamic drift velocity is converted back from m/s to  $[cm/s]$

# Chapter 8

## Numerical Algorithms

## 8.1

A Shapiro Filter/smoother is used for time-dependent dynamical variables  $T_n, U_n, V_n, O^+, \Psi_O, \Psi_{O_2}, \Psi_{NO}$  and  $\Psi_{N(4S)}$  in the TIEGCM to limit the development of numerical nonlinear instability and short wavelength waves (less than four grid size) that are poorly represented in the model. Shapiro smoothing is used in modules/subroutines that solve equations for these variables.

**\*Note: the following material is from [22], and copyright to the University of Michigan. Some of the material has been modified based on the updated TIEGCM.**

In real world, wave interactions occur that generate larger and smaller wavelength waves. The smaller waves cascade in sizes to reach the characteristic scale of molecular dissipation which is the process that finally eliminates motion. However, in a numerical model that has discrete grid, motion energy cascade from larger wavelength waves to smaller and smaller scales is interrupted. In fact, waves with wavelength smaller than  $2\Delta x$  ( $\Delta x$  is the grid size of a numerical model) are erroneously represented as larger wavelength waves. This phenomenon is called aliasing [12]. The net result of this aliasing is a fictitious energy buildup since energy is added continuously to the model through forcing terms, while energy dissipation processes are cut off. Therefore, even though a numerical scheme is linearly stable, the results can degrade into physically meaningless computational noise. The solutions of model dynamical variables can grow to infinity. This numerical error is commonly referred to as nonlinear instability.

To remove aliasing in the wave presentation, and thus to prevent the nonlinear instability from occurring, short waves with wavelength smaller than  $4\Delta x$  must be eliminated from a numerical model. In addition to the above mentioned nonlinear instability problem, such short waves are also poorly represented in terms of phase and amplitude. And they are expected to dissipate to even smaller scale motions anyway. Therefore, it is desirable to remove these waves completely.

In the TIEGCM the smoothing technique discussed by [19] is used to control computational noise. The Shapiro smoother is a low-pass filter that eliminates waves with wavelength smaller than  $4\Delta x$  each time step, but leaves the large-scale disturbances unaffected. Another way to control nonlinear instability is to enhance the horizontal eddy diffusion by proper parameterization of the subgrid correlation terms. This method is not desirable since it

allows modelers to adjust the eddy diffusion coefficient arbitrarily to change the magnitude of numerical solutions [20],

A one-dimensional, five-point Shapiro smoothing scheme is used in both the TIEGCM to eliminate or constrain any spurious, nonlinear growth of high-frequency waves that may be introduced by roundoff and truncations errors or by the interruption of the energy cascade process that transport energy from large-scale disturbances to small-scale motions. Any time-dependent dynamical variable  $Z(T_n, U_n, V_n, O^+, \Psi_O, \Psi_{O_2}, \Psi_{NO}$  and  $\Psi_{N(^4S)}$ ) is averaged each time step by

$$\bar{Z} = Z_l - \alpha(Z_{l+2} + Z_{l-2} - 4Z_{l+1} + 6Z_l) \quad (8.1)$$

where  $l$  is the index of grid point in either latitude or longitude direction.  $\alpha$  is a smoothing factor and  $0 < \alpha < 0.5$ .  $Z(x)$  can be expressed in terms of a summation of Fourier components of the form

$$Z_l = C + A \cos k(x_l + \varphi) \quad (8.2)$$

where  $C$  is a constant,  $A$  is the amplitude of the wave component with wave number  $k$  ( $k = 2\pi/\lambda$ , where  $\lambda$  is the wavelength of the component). Substituting 8.2 into 8.1 yields

$$\begin{aligned} \bar{Z} &= C + A \cos k(x_l + \varphi) [1 - 2\alpha(\cos 2k\Delta x - 4\cos k\Delta x + 3)] \\ &= C + A[1 - 4\alpha(1 - \cos k\Delta x)^2] \cos k(x_l + \varphi) \end{aligned} \quad (8.3)$$

$\alpha$  is set to be equal to 0.03.  $\alpha$  values are determined by numerical experiments. It is desirable to have  $\alpha$  as small as possible so that longer waves are less affected by the smoothing. The minimum value of  $\alpha$  is obtained by gradually decreasing  $\alpha$  while preserving integrity and stability of the numerical solutions. It is clear from 8.3 that all wavelengths are damped. However, short waves ( $\lambda, 8\Delta x$ ) are heavily damped while long waves are almost unaffected. Successive application of this smoother on a dynamical variable prevents short waves from growing to such a degree that they degrade the numerical solutions.

## 8.2

**\*Note:** the following material is from [22], and copyright to the University of Michigan. Some of the material has been modified

**based on the updated TIEGCM.**

Since the TIEGCM uses a uniform horizontal grid system and finite-difference numerical scheme, computational errors can grow significantly as the grids approach to the poles. The zonal grid sizes decrease in direct proportion to  $\cos\phi$ , where  $\phi$  is the latitude. The truncation error of the finite-difference scheme and other numerical errors may be amplified by the zonal finite difference calculations at the grid points near poles. Non-physical waves are then generated and grow non-linearly to cause computational instability. This pole problem occurs in any simulation that uses finite difference techniques with uniform latitude and longitude grids. One way to avoid this problem is to use much smaller time steps, which is undesirable because it increases the computational cost dramatically by slowing down the entire simulation process.

Another way to solve this pole problem is to apply a Fourier filter at high latitudes to remove non-physical high-frequency zonal waves generated by finite differences in the region with smaller zonal grid sizes. At each time step a Fourier expansion is applied to the prognostic variables of the model. A cutoff frequency was found at each latitude (at high latitudes) as a result of numerical experiments. Waves with frequencies that are higher than the cutoff frequencies are eliminated from the Fourier spectra of prognostic variables. The values of prognostic variables are then recovered through a reverse Fourier transform using modified Fourier spectra. Each latitude grid may have its own cutoff frequency. The cutoff frequency at a particular latitude is determined by the expected time step used by a model. A large time step requires low cutoff frequencies and more zonal waves are filtered out.

In the TIEGCM, Fourier filters are applied to the individual prognostic variables. These variables include  $T_n, U_n, V_n, O^+, \Psi_O, \Psi_{O_2}, \Psi_{NO}, \Psi_{N(^4S)}$  and  $W$ . It should be noted here that to apply a Fourier filter directly and successively on prognostic variables may cause overfiltering which may remove fine structures that are expected to occur at high latitudes.

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