PENTA Documentation

Last updated: 9/28/2011
Note: This is a work in progress!! XX denotes sections to be filled in at a later date.

1. Introduction

This document describes the PENTA code.

2. Fundamental Equations

2.1 Definitions

Note that in the following sections “SN” refers to the Sugama-Nishimura approach, “MBT” to the Maassberg-Beidler-Turkin approach, and “T” to the Taguchi approach. DKE is drift kinetic equation.

2.1.1 Basic definitions

The following symbols are used for the basic plasma parameters of a species denoted by label *a*. T_a, n_a, e_a and m_a are the temperature, density, electric charge and mass, respectively. In all equations T_a is given in electron volts, all other quantities are in mks units. The kinetic pressure is $p_a = n_a T_a$, and the thermal velocity is $v_{Ta} \equiv \sqrt{2T_a / m_a}$.
The radial electric field is $E_r \equiv -\Phi'$, where Φ is the electric potential , and the prime denotes a radial derivative versus the appropriate radial flux coordinate. In PENTA the radial coordinate used is the effective minor radius *r*, defined from the normalized toroidal flux $\rho = r / a$. The parallel electric field is defined as $E_\| \equiv \mathbf{B} \cdot \mathbf{E}$.
The following symbols are regularly used for the magnetic field; $\langle B^2 \rangle$, where $\langle ... \rangle$ denotes a flux surface average, and B_0, which is the "reference" magnetic field strength used when running DKES (see section 2.1.3). The equations used below are all consistent with the SN formulation if $B_0 = \langle B^2 \rangle^{1/2}$. In the MBT formulation, B_0 is defined as the B_{00} component of the Fourier decomposition of the magnetic field strength. The normalized magnetic field strength $b \equiv B / B_0$ is also used in some sections.
The monoenergetic (test particle) velocity is given simply as *v* in the following equations. The normalized monoenergtic velocity and energy are given by

$$x_a \equiv \frac{v}{v_{Ta}} , \tag{2.1.1.1}$$

and

$$K_a \equiv \frac{v^2}{v_{Ta}^2}, \tag{2.1.1.2}$$

respectively.

The energy dependent perpendicular (pitch angle) scattering collision frequency ν_D^a is defined as

$$\nu_D^a \equiv \sum_b \frac{3\sqrt{\pi}}{4}\frac{1}{\tau_{ab}}\frac{v_{Ta}^3}{v^3}H(x_b). \tag{2.1.1.3}$$

where the summation is over *all* species,

$$\frac{3\sqrt{\pi}}{4}\frac{1}{\tau_{ab}} = \frac{n_b e_a^2 e_b^2 \ln\Lambda_{ab}}{4\pi\varepsilon_0^2 m_a^2 v_{Ta}^3}, \tag{2.1.1.4}$$

$$H(x_b) = \left(1 - \frac{1}{2x_b^2}\right) erf(x_b) + \frac{1}{x_b\sqrt{\pi}}\exp(-x_b^2), \tag{2.1.1.5}$$

and erf is the error function. The second term in Eq. 2.1.1.5 comes from the derivative of the error function, and $\ln\Lambda_{ab}$ is the Coulomb logarithm. It is useful to write the collision frequency as

$$\nu_D^a = \frac{e_a^2 \ln\Lambda}{4\pi\varepsilon_0^2 m_a^2 v^3}\sum_b n_b e_b^2 \left[\left(1 - \frac{1}{2x_b^2}\right) erf(x_b) + \frac{1}{x_b\sqrt{\pi}} e^{-x_b^2}\right], \tag{2.1.1.6}$$

where the term in front of the summation is independent of the field species, and the Coulomb logarithm is approximated by

$$\ln\Lambda = 23.4 - 1.15\log(n_e/10^6) + 3.45\log(T_e), \text{ for } T_e < 50 \text{ eV}, \tag{2.1.1.7a}$$

$$\ln\Lambda = 25.3 - 1.15\log(n_e/10^6) + 2.3\log(T_e), \text{ for } T_e > 50 \text{ eV}. \tag{2.1.1.7b}$$

2.1.2 Thermodynamic forces

In the SN approach the thermodynamic forces are labeled as X_{aj} and X_E, where

$$X_{a1} \equiv -\frac{1}{n_a}p_a' + e_a E_r = -T_a\left(\frac{T_a'}{T_a} + \frac{n_a'}{n_a} - \frac{e_a E_r}{T_a}\right), \tag{2.1.2.1a}$$

$$X_{a2} \equiv -T_a', \tag{2.1.2.1b}$$

$$X_E \equiv \frac{\langle BE_\parallel \rangle}{\langle B^2 \rangle^{1/2}}. \tag{2.1.2.1c}$$

In the MBT approach (and in the DKES papers, with slight modifications) the forces are labeled as A_{aj}, where

$$A_{a1} \equiv \frac{n_a'}{n_a} - \frac{3}{2}\frac{T_a'}{T_a} - \frac{e_a E_r}{T_a}, \tag{2.1.2.2a}$$

$$A_{a2} \equiv \frac{T_a'}{T_a}, \tag{2.1.2.2b}$$

$$A_{a3} \equiv \frac{e_a}{T_a} \frac{\left\langle BE_{\parallel} \right\rangle}{\left\langle B^2 \right\rangle} B_0 . \tag{2.1.2.2c}$$

In most of the PENTA equations the A_{aj} forces are preferred, however both methods have their advantages. The X forces allow the DKE to be written simply in terms of the Sonine polynomials, and have a species independent parallel electric field drive. The A_{aj} forces, on the other hand, are better suited to writing the equation for the energy flux (as opposed to the heat flux), and allow for easier comparison to the original DKES papers and later monoenergetic benchmarking work. The X forces are written in terms of the A_{aj} as

$$X_{a1} = -T_a \left(A_{a1} + \frac{5}{2} A_{a2} \right), \tag{2.1.2.3a}$$

$$X_{a2} = -T_a A_{a2} , \tag{2.1.2.3b}$$

$$X_E = \frac{T_a}{e_a} \frac{\left\langle B^2 \right\rangle^{1/2}}{B_0} A_{a3} . \tag{2.1.2.3c}$$

And the inverse relationship is

$$A_{a1} = -\frac{X_{a1}}{T_a} + \frac{5}{2} \frac{X_{a2}}{T_a} , \tag{2.1.2.4a}$$

$$A_{a2} = -\frac{X_{a2}}{T_a} , \tag{2.1.2.4b}$$

$$A_{a3} = X_E \frac{e_a}{T_a} \frac{B_0}{\left\langle B^2 \right\rangle^{1/2}} . \tag{2.1.2.4c}$$

2.1.3 DKES coefficient definitions

The three independent monoenergetic transport coefficients from DKES are D_{11}^a, D_{31}^a, and D_{33}^a $\left(D_{13}^a = -D_{31}^a\right)$. Unfortunately the definition of the coefficients is the cause of much confusion. The definition changes between the different versions of DKES, a bug exists in some versions of DKES which puts the coefficients off by factors of $\left\langle B^2 \right\rangle$ and $\left\langle B^2 \right\rangle^{1/2}$, and the notation is different in the MBT and SN papers. In all PENTA notation the D_{ij}^a refer to the monoenergetic coefficients with units of m^2/s, and are identical to the definitions used by MBT. "Normalized" versions of these cofficients are calculated by DKES (with definitions that change between the versions) and are used directly by the PENTA code. These definitions are also given in this section.

There are three primary sources of confusion with the DKES coefficients. The biggest issue is a bug in some versions of DKES which causes the D_{31}^a and D_{33}^a coefficients to be off by factors of $\left\langle B^2 \right\rangle^{1/2}$ and $\left\langle B^2 \right\rangle$, respectively, where B is in units of Tesla. When using the output directly from DKES2, for example, these coefficients must be multiplied by the above factors. As this is a BUG, all equations in this document assume that this "B correction" has already been applied.

The second issue is specific to the parallel electric conductivity coefficient, D_{33}^{a}. In the earliest version of DKES the output contained the entire coefficient, however in later versions the collisional contribution to the D_{33}^{a} coefficient was excluded and only the remainder given. To get the physical D_{33}^{a} the collisional, or "Spitzer" contribution had to be added to the DKES output. The collisional contribution to D_{33}^{a} is given by

$$D_{33}^{Spitzer-a} = \frac{1}{3}\frac{v^2}{\nu_D^a}\frac{\langle B^2 \rangle}{B_0^2} = \frac{2}{3}\frac{T_a K_a}{m_a \nu_D^a}\frac{\langle B^2 \rangle}{B_0^2} \ . \tag{2.1.3.1}$$

In the SN formulation the D_{33}^{a} used is defined as the total D_{33}^{a} minus the collisional contribution. In the MBT formulation, on the other hand, the total D_{33}^{a} is used. In PENTA an option exists whereby the normalized D_{33}^{a} file (see section XX) can be specified to contain either the total coefficient or the one with the collisional contribution excluded. This option is in the XX file as XX.

In the SN (and the original DKES) formulation the three coefficients have the following units: D_{11}^{a}[m^2/s], D_{31}^{a} [Tm^2/s], and D_{33}^{a} [T^{2}m^2/s] where in the MBT formulation (and in this document) all three coefficients have units of [m^2/s]. To convert between the definitions (recall again that the "B correction" is always assumed), the following relations can be used

$$D_{11}^{a-SN} = D_{11}^{a}, \tag{2.1.3.2a}$$

$$D_{13}^{a-SN} = B_0 D_{13}^{a} = -B_0 D_{31}^{a}, \tag{2.1.3.2b}$$

$$D_{33}^{a-SN} = \frac{1}{3}\langle B^2 \rangle \frac{v^2}{\nu_D^a} - B_0^2 D_{33}^{a} = \frac{2}{3}\langle B^2 \rangle \frac{T_a}{m_a}\frac{K_a}{\nu_D^a} - B_0^2 D_{33}^{a}, \tag{2.1.3.2b}$$

where D_{ij}^{a-SN} are the coefficients used in the SN papers.

Finally, there remains some question about the sign of the D_{13}^{a} and D_{31}^{a} coefficients. It is possible that SN use different definitions, and that in their notation both D_{13}^{a} and D_{31}^{a} have the same sign. Further, in the D_{31}^{a} given for HSX (assuming that VMEC and DKES were run correctly) have the wrong sign given a "physical" inspection of the expected sign of the bootstrap current to a parallel electric field. These issues remain to be resolved satisfactorily XX.

XX talk about relationship between coefficients XX

2.1.4 Classical friction coefficients

The classical friction coefficients are defined as

$$\frac{l_{j+1,k+1}^{ab}}{n_a m_a} \equiv \delta_{ab} \sum_{b'} \frac{M_{jk}^{ab'}}{\tau^{ab'}} + \frac{N_{jk}^{ab}}{\tau^{ab}}, \tag{2.1.4.1}$$

where XX.

It is useful to consider the cases of like species and unlike species collisions

$$\frac{l_{j+1,k+1}^{aa}}{n_a m_a} = \sum_{b'} \frac{M_{jk}^{ab'}}{\tau^{ab'}} + \frac{N_{jk}^{aa}}{\tau^{aa}} = \sum_{b' \neq a} \frac{M_{jk}^{ab'}}{\tau^{ab'}} + \frac{M_{jk}^{aa} + N_{jk}^{aa}}{\tau^{aa}}, \tag{2.1.4.2}$$

$$\left. \frac{l_{j+1,k+1}^{ab}}{n_a m_a} \right|_{b \neq a} = \frac{N_{jk}^{ab}}{\tau^{ab}}, \tag{2.1.4.3}$$

2.1.5 Sonine polynomials

Despite it being somewhat sloppy notation, to conserve space the argument of the Sonine polynomial K_a is dropped in the following equations.

The coefficient c_j is defined as

$$c_j \equiv 3\frac{2^j j!}{(2j+3)!!}, \tag{2.1.5.1}$$

where the double factorial $N!! \equiv N(N-2)(N-4)\ldots$.

It is useful to express c_j in terms of gamma functions using the following identities

$$\Gamma\left(n+\frac{1}{2}\right) = \frac{(2n-1)!!}{2^n}\sqrt{\pi}\,, \tag{2.1.5.2a}$$

$$\Gamma(n) = (n-1)!\,. \tag{2.1.5.2b}$$

Then we have

$$c_j = \frac{3\sqrt{\pi}}{4}\frac{\Gamma(j+1)}{\Gamma\left(j+\frac{5}{2}\right)}. \tag{2.1.5.3}$$

The low order polynomials are used explicitly in deriving the following equations

$$L_0^{(3/2)}(K_a) = 1, \tag{2.1.5.4a}$$

$$L_1^{(3/2)}(K_a) = \frac{5}{2} - K_a. \tag{2.1.5.4b}$$

The orthogonality condition for the Sonine polynomials is

$$\frac{2}{\sqrt{\pi}}\int_0^\infty dK_a K_a^{3/2} e^{-K_a} L_j^{(3/2)} L_k^{(3/2)} = \frac{2}{\sqrt{\pi}}\frac{(j+3/2)!}{j!}\delta_{jk}\,, \tag{2.1.5.5}$$

which is related to the coefficient c as

$$\frac{2}{\sqrt{\pi}}\frac{(j+3/2)!}{j!}\delta_{jk} = \frac{(2j+3)!!}{j!2^{j+1}}\delta_{jk} = \frac{3}{2}\frac{\delta_{jk}}{c_j}\,. \tag{2.1.5.6}$$

2.1.6 Energy integrals

In the SN formulation the Sonine polynomial weighted energy integral is given by

$$A_{j+1,k+1}^a \equiv n_a \frac{2}{\sqrt{\pi}}\int_0^\infty dK_a K_a^{1/2} e^{-K_a} L_j^{(3/2)} L_k^{(3/2)} A_a\,, \tag{2.1.6.1}$$

where A_a is a monoenergetic coefficient (function of K_a) and $A_{j+1,k+1}^a$ is the corresponding thermal coefficient.

In the MBT formulation the following definition is used

$$\left\|A_a\right\|_j^{MBT} \equiv \frac{4}{\sqrt{\pi}}\int_0^\infty dx_a x_a^2 e^{-x_a^2} L_j^{(3/2)} A_a\,, \tag{2.1.6.2}$$

which, using the relation $dK_a = 2x_a dx_a$ is equivalent to

$$\left\| A_a \right\|_j^{MBT} = \frac{2}{\sqrt{\pi}} \int_0^\infty dK_a K_a^{1/2} e^{-K_a} L_j^{(3/2)} A_a . \tag{2.1.6.3}$$

In the PENTA equations the energy integral includes the density and is defined as

$$\left\| A_a \right\|_j = n_a \frac{2}{\sqrt{\pi}} \int_0^\infty dK_a K_a^{1/2} e^{-K_a} L_j^{(3/2)} A_a . \tag{2.1.6.4}$$

2.1.7 Pfirsch-Schlüter Factor

XX – to be written

2.1.8 Coefficients used by SN and T

The thermal transport coefficients used by SN are

$$\left[M_{j+1,k+1}^a, N_{j+1,k+1}^a, L_{j+1,k+1}^a \right] \equiv n_a \frac{2}{\sqrt{\pi}} \int_0^\infty dK_a K_a^{1/2} e^{-K_a} L_j^{(3/2)} L_k^{(3/2)} \left[M_a, N_a, L_a \right], \tag{2.1.8.1}$$

which can be related to the Sonine weighted energy integral (Eq. 2.1.5.4) as

$$\left[M_{j+1,k+1}^a, N_{j+1,k+1}^a, L_{j+1,k+1}^a \right] = \left\| L_k^{(3/2)} \left[M_a, N_a, L_a \right] \right\|_j . \tag{2.1.8.2}$$

The monoenergetic coefficients are defined as

$$M_a \equiv \frac{m_a^2}{T_a} \left[\nu_D^a \right]^2 D_{33}^{a-SN} \left[1 - \frac{3}{2} \frac{m_a}{T_a \left\langle B^2 \right\rangle} \frac{\nu_D^a D_{33}^{a-SN}}{K_a} \right]^{-1}, \tag{2.1.8.3a}$$

$$N_a \equiv \frac{m_a}{T_a} \nu_D^a D_{13}^{a-SN} \left[1 - \frac{3}{2} \frac{m_a}{T_a \left\langle B^2 \right\rangle} \frac{\nu_D^a D_{33}^{a-SN}}{K_a} \right]^{-1}, \tag{2.1.8.3b}$$

$$L_a \equiv \frac{1}{T_a} \left(D_{11}^a - \left\langle \tilde{U}^2 \right\rangle \frac{2}{3} \frac{m_a T_a}{e_a^2} K_a \nu_D^a + \frac{3}{2} \frac{m_a}{T_a \left\langle B^2 \right\rangle} \frac{\nu_D^a \left[D_{13}^{a-SN} \right]^2}{K_a} \left[1 - \frac{3}{2} \frac{m_a}{T_a \left\langle B^2 \right\rangle} \frac{\nu_D^a D_{33}^{a-SN}}{K_a} \right]^{-1} \right). \tag{2.1.8.3c}$$

Next we wish to convert these to use the D_{ij}^a. Defining the common term (this term is added by SN to make the parallel momentum equations agree with the tokamak moment approach, see section XX) as

$$F_a \equiv \frac{m_a}{T_a} \nu_D^a \left[1 - \frac{3}{2} \frac{m_a}{T_a \left\langle B^2 \right\rangle} \frac{\nu_D^a D_{33}^{a-SN}}{K_a} \right]^{-1} = \frac{2}{3} \frac{\left\langle B^2 \right\rangle}{B_0^2} \frac{K_a}{D_{33}^a} . \tag{2.1.8.4}$$

We then have

$$M_a = \left(\frac{2}{3} \left\langle B^2 \right\rangle T_a K_a - m_a B_0^2 \nu_D^a D_{33}^a \right) F_a , \tag{2.1.8.5a}$$

$$N_a = -B_0 D_{31}^a F_a , \tag{2.1.8.5b}$$

$$L_a = \frac{1}{T_a}\left(D_{11}^a - \left\langle \tilde{U}^2 \right\rangle \frac{2}{3}\frac{m_a T_a}{e_a^2} K_a \nu_D^a + \frac{3}{2}\frac{B_0^2}{\left\langle B^2 \right\rangle}\frac{\left[D_{31}^a\right]^2}{K_a} F_a \right), \tag{2.1.8.5a}$$

or

$$M_a = \frac{2}{3}\left\langle B^2 \right\rangle \left(\frac{2}{3}\left\langle B^2 \right\rangle \frac{T_a}{B_0^2}\frac{K_a^2}{D_{33}^a} - m_a \nu_D^a K_a \right), \tag{2.1.8.6a}$$

$$N_a = -\frac{2}{3}\frac{\left\langle B^2 \right\rangle}{B_0}\frac{D_{31}^a}{D_{33}^a} K_a, \tag{2.1.8.6b}$$

$$L_a = \frac{1}{T_a}\left(D_{11}^a - \left\langle \tilde{U}^2 \right\rangle \frac{2}{3}\frac{m_a T_a}{e_a^2} K_a \nu_D^a + \frac{\left[D_{31}^a\right]^2}{D_{33}^a} \right). \tag{2.1.8.6c}$$

In the Taguchi formulation (as printed in S&N 2008) the following coefficients are defined for the flow equation

$$\left[A_{j+1,k+1}^a, B_{j+1,k+1}^a, Z_{j+1,k+1}^a\right] \equiv n_a \frac{2}{\sqrt{\pi}}\int_0^\infty dK_a K_a^{1/2} e^{-K_a} L_j^{(3/2)} L_k^{(3/2)} \left[A_a, B_a, Z_a\right], \tag{2.1.8.7}$$

where

$$A_a \equiv m_a \nu_D^a D_{33}^{a-SN}, \tag{2.1.8.8a}$$

$$B_a \equiv D_{13}^{a-SN}, \tag{2.1.8.8b}$$

$$Z_a \equiv -D_{33}^{a-SN} + \frac{2}{3}\frac{T_a K_a \left\langle B^2 \right\rangle}{m_a \nu_D^a}. \tag{2.1.8.8c}$$

Converting these to D_{ij}^a gives

$$A_a = \frac{2}{3}\left\langle B^2 \right\rangle T_a K_a - m_a B_0^2 \nu_D^a D_{33}^a, \tag{2.1.8.9a}$$

$$B_a = -B_0 D_{31}^a, \tag{2.1.8.9b}$$

$$Z_a = B_0^2 D_{33}^a. \tag{2.1.8.9c}$$

The flux equation uses two additional coefficients,

$$\left[N_{j+1,k+1}^{a-T}, L_{j+1,k+1}^{a-T}\right] \equiv n_a \frac{2}{\sqrt{\pi}}\int_0^\infty dK_a K_a^{1/2} e^{-K_a} L_j^{(3/2)} L_k^{(3/2)} \left[N_a^T, L_a^T\right], \tag{1.2.8.10}$$

where

$$N_a^T \equiv \frac{m_a}{T_a}\nu_D^a D_{13}^{a-SN}, \tag{2.1.8.11a}$$

$$L_a^T \equiv \frac{1}{T_a}\left(D_{11}^{a-SN} - \left\langle \tilde{U}^2 \right\rangle \frac{2}{3}\frac{T_a m_a}{e_a^2}\nu_D^a K_a \right), \tag{2.1.8.11b}$$

Converting these to D_{ij}^a gives

$$N_a^T = -B_0 \frac{m_a}{T_a}\nu_D^a D_{31}^a, \tag{2.1.8.12a}$$

$$L_a^T = \frac{1}{T_a}\left(D_{11}^a - \left\langle \tilde{U}^2 \right\rangle \frac{2}{3} \frac{T_a m_a}{e_a^2} \nu_D^a K_a \right). \tag{2.1.8.12b}$$

2.1.9 Definition of the parallel flow moments

In the MBT approach the parallel flow moments are defined as

$$U_k^a = \frac{1}{n_a} \int d^3 v v_{\|} L_k^{3/2} f_a . \tag{2.1.9.1}$$

In the SN approach the following definition is used.

$$u_{\|aj} = \frac{c_j}{n_a} \int d^3 v v_{\|} L_k^{3/2} f_a . \tag{2.1.9.2}$$

The flow moments are then simply related as

$$U_k^a = \frac{u_{\|aj}}{c_j} . \tag{2.1.9.3}$$

2.2 Flow equations

Nominally there are three different flow equations to be considered.

2.2.1 SN Flow Equation

In the SN formulation, the flow equation is written for j=0,1,...,j_{max}

$$\sum_{k=0}^{j\max} M_{j+1,k+1}^a \frac{\left\langle B u_{\|ak} \right\rangle}{\left\langle B^2 \right\rangle} + N_{j+1,1}^a X_{a1} - N_{j+1,2}^a X_{a1} = \sum_b \sum_{k=0}^{j\max} l_{j+1,k+1}^{ab} \left\langle B u_{\|bk} \right\rangle + \delta_{j0} n_a e_a \left\langle B^2 \right\rangle^{1/2} X_E , \tag{2.2.1.1}$$

where j_{max} is the truncation order for the Sonine polynomials. Using equations 2.1.2.3, 2.1.7.2 and 2.1.7.6 we can write 2.2.1.1 as

$$\begin{aligned} &\sum_{k=0}^{j\max} \left(\left\| L_k^{(3/2)} \left(\frac{2}{3} \frac{\left\langle B^2 \right\rangle}{B_0} \frac{K_a^2}{D_{33}^a} - \frac{m_a B_0}{T_a} \nu_D^a K_a \right) \right\|_j \frac{\left\langle B u_{\|ak} \right\rangle}{\left\langle B^2 \right\rangle} - \frac{3}{2} \frac{B_0}{T_a} \sum_b l_{j+1,k+1}^{ab} \frac{\left\langle B u_{\|bk} \right\rangle}{\left\langle B^2 \right\rangle} \right). \\ &= - \left\| \frac{D_{31}^a}{D_{33}^a} K_a \right\|_j A_{a1} - \left\| K_a^2 \frac{D_{31}^a}{D_{33}^a} \right\|_j A_{a2} + \delta_{j0} \frac{3}{2} n_a A_{a3} \end{aligned} \tag{2.2.1.2}$$

If the reference magnetic field strength is given as $B_0 \equiv \left\langle B^2 \right\rangle^{1/2}$ the flow equation can be written as

$$\begin{aligned} &\sum_{k=0}^{j\max} \left(\left\| L_k^{(3/2)} \left(\frac{2}{3} \frac{K_a^2}{D_{33}^a} - \frac{m_a}{T_a} \nu_D^a K_a \right) \right\|_j \left\langle b u_{\|ak} \right\rangle - \frac{3}{2} \frac{1}{T_a} \sum_b l_{j+1,k+1}^{ab} \left\langle b u_{\|bk} \right\rangle \right). \\ &= - \left\| \frac{D_{31}^a}{D_{33}^a} K_a \right\|_j A_{a1} - \left\| K_a^2 \frac{D_{31}^a}{D_{33}^a} \right\|_j A_{a2} + \delta_{j0} \frac{3}{2} n_a A_{a3} \end{aligned} \tag{2.2.1.3}$$

2.2.2 MBT flow equation

In the MBT formulation the flow equation is given for j=0,1,...,j_{max}

$$\sum_{k=0}^{j\max}\left[\frac{\left\langle Bu_{\|ak}\right\rangle}{B_0 c_k}\left\{n_a\delta_{kj}-c_k\frac{B_0^2}{\left\langle B^2\right\rangle}\frac{m_a}{T_a}\left(\left\|\nu_D^a L_k^{(3/2)}D_{33}^a\right\|_j+\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^a\right\|_j\left\{\frac{M_{lk}^{aa}+N_{lk}^{aa}}{\tau^{aa}}+\sum_{b\neq a}\frac{M_{lk}^{ab}}{\tau^{ab}}\right\}\right)\right\}\right. \quad (2.2.2.1)$$
$$\left.-c_k\frac{B_0^2}{\left\langle B^2\right\rangle}\frac{m_a}{T_a}\sum_{b\neq a}\frac{\left\langle Bu_{\|bk}\right\rangle}{B_0 c_k}\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^a\right\|_j\frac{N_{lk}^{ab}}{\tau^{ab}}\right]=-\left\|D_{31}^a\right\|_j A_{a1}-\left\|K_a D_{31}^a\right\|_j A_{a2}-\left\|D_{33}^a\right\|_j A_{a3}$$

Using equations XX and XX we can write

$$\sum_{k=0}^{j\max}\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}\left[\left(\frac{\left\langle B^2\right\rangle}{B_0 c_k}n_a\delta_{kj}-B_0\frac{m_a}{T_a}\left\|\nu_D^a L_k^{(3/2)}D_{33}^a\right\|_j\right)-\frac{B_0}{n_a T_a}\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^a\right\|_j\sum_b l_{l+1,k+1}^{ab}\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\right]. \quad (2.2.2.2)$$
$$=-\left\|D_{31}^a\right\|_j A_{a1}-\left\|K_a D_{31}^a\right\|_j A_{a2}-\left\|D_{33}^a\right\|_j A_{a3}$$

Or, if reference magnetic field strength is given as $B_0\equiv\left\langle B^2\right\rangle^{1/2}$ then

$$\sum_{k=0}^{j\max}\left\langle bu_{\|ak}\right\rangle\left[\left(\delta_{kj}\frac{n_a}{c_k}-\frac{m_a}{T_a}\left\|\nu_D^a L_k^{(3/2)}D_{33}^a\right\|_j\right)-\frac{1}{n_a T_a}\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^a\right\|_j\sum_b l_{l+1,k+1}^{ab}\left\langle bu_{\|bk}\right\rangle\right]. \quad (2.2.2.3)$$
$$=-\left\|D_{31}^a\right\|_j A_{a1}-\left\|K_a D_{31}^a\right\|_j A_{a2}-\left\|D_{33}^a\right\|_j A_{a3}$$

2.2.3 Taguchi Flow Equation

The T flow equation given for j=0,1,...,j_{max} as

$$\sum_{k=0}^{j\max}A_{j+1,k+1}^a\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}+B_{j+1,1}^a X_{a1}-B_{j+1,2}^a X_{a2}=\frac{1}{n_a}\sum_{m=0}^{j\max}Z_{j+1,m+1}^a c_m\sum_b\sum_{k=0}^{j\max}l_{m+1,k+1}^{ab}\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}+\frac{1}{\left\langle B^2\right\rangle^{1/2}}Z_{j+1,1}^a e_a X_E\cdot \quad (2.2.3.1)$$

Using equations XX and XX, and changing the index of the second summation from m to l

$$\sum_{k=0}^{j\max}\left[\left(\frac{2}{3}\frac{\left\langle B^2\right\rangle}{B_0}\left\|L_k^{(3/2)}K_a\right\|_j-B_0\frac{m_a}{T_a}\left\|\nu_D^a L_k^{(3/2)}D_{33}^a\right\|_j\right)\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}-\frac{B_0}{n_a T_a}\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^a\right\|_j\sum_b l_{l+1,k+1}^{ab}\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\right]. \quad (2.2.3.2)$$
$$=-\left\|D_{31}^a\right\|_j A_{a1}-\left\|K_a D_{31}^a\right\|_j A_{a2}+\left\|D_{33}^a\right\|_j A_{a3}$$

This is now very similar to the MBT flow equation except for the first term in brackets and the sign of the last term on the RHS. The first integral can be evaluated directly using the orthogonality condition of the Sonine polynomials (Eq. 2.1.5.6)

$$\left\|L_k^{(3/2)}K_a\right\|_j=n_a\frac{2}{\sqrt{\pi}}\int_0^\infty dK_a K_a^{3/2}e^{-K_a}L_j^{(3/2)}L_k^{(3/2)}=n_a\frac{3}{2}\frac{\delta_{jk}}{c_j}, \quad (2.2.3.3)$$

And we can write

$$\sum_{k=0}^{j\max}\left[\left(\frac{\left\langle B^2\right\rangle}{B_0 c_j}n_a\delta_{jk}-B_0\frac{m_a}{T_a}\left\|\nu_D^a L_k^{(3/2)}D_{33}^a\right\|_j\right)\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}-\frac{B_0}{n_a T_a}\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^a\right\|_j\sum_b l_{l+1,k+1}^{ab}\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\right]. \quad (2.2.3.4)$$
$$=-\left\|D_{31}^a\right\|_j A_{a1}-\left\|K_a D_{31}^a\right\|_j A_{a2}+\left\|D_{33}^a\right\|_j A_{a3}$$

Now the only difference is in the sign of the last term. After talking to Beidler, it appears that the definition of A_{a3} used in their paper is not the same as used to derive the equations as printed. The actual definition uses the loop voltage, which introduces another minus sign on the parallel electric field drive, so I think everything agrees XX.

2.3 Flux Equations

Again we nominally have three separate equations.

2.3.1 SN Flux Equations

The radial fluxes are written in the SN formulation as

$$\Gamma_{aj}^{bn} = \sum_{k=0}^{j\max} N_{j+1,k+1}^{a} \frac{\langle Bu_{a\|k} \rangle}{\langle B^2 \rangle} + L_{j+1,1}^{a} X_{a1} - L_{j+1,2}^{a} X_{a2} . \tag{2.3.1.1}$$

where Γ_{aj}^{bn} is the banana-non-axisymmetric component of the flux, and the total flux is

$$\Gamma_{aj} = \Gamma_{aj}^{bn} + \Gamma_{aj}^{PS} . \tag{2.3.1.2}$$

The physical fluxes are given by j=0,1 as

$$\Gamma_{a0} = \Gamma_a , \tag{2.3.1.3a}$$

$$\Gamma_{a1} = -\frac{q_a}{T_a} . \tag{2.3.1.3b}$$

Substituting the coefficients and forces gives

$$\Gamma_{aj}^{bn} = -\frac{2}{3} \frac{\langle B^2 \rangle}{B_0} \sum_{k=0}^{j\max} \left\| L_k^{(3/2)} K_a \frac{D_{31}^a}{D_{33}^a} \right\|_j \frac{\langle Bu_{a\|k} \rangle}{\langle B^2 \rangle} - \left\| L_a^{SN} \right\|_j A_{a1} - \left\| K_a L_a^{SN} \right\|_j A_{a2} , \tag{2.3.1.4}$$

where I have defined

$$L_a^{SN} \equiv \left(D_{11}^a - \langle \tilde{U}^2 \rangle \frac{2}{3} \frac{m_a T_a}{e_a^2} K_a \nu_D^a + \frac{\left[D_{31}^a \right]^2}{D_{33}^a} \right), \tag{2.3.1.5}$$

as a radial particle diffusion coefficient.
The PS flux is written as

$$\Gamma_{aj}^{PS} = -\sum_b \frac{\langle \tilde{U}^2 \rangle}{e_a e_b} \left(l_{j+1,1}^{ab} X_{b1} - l_{j+1,2}^{ab} X_{b2} \right). \tag{2.3.1.6}$$

Substituting for the forces and writing just the physical fluxes gives

$$\begin{bmatrix} \Gamma_a^{PS} \\ \dfrac{q_a^{PS}}{T_a} \end{bmatrix} = \frac{\langle \tilde{U}^2 \rangle}{e_a} \sum_b \frac{T_b}{e_b} \begin{bmatrix} l_{11}^{ab} & -l_{12}^{ab} \\ -l_{21}^{ab} & l_{22}^{ab} \end{bmatrix} \begin{bmatrix} \left(A_{b1} + \dfrac{5}{2} A_{b2} \right) \\ A_{b2} \end{bmatrix} . \tag{2.3.1.7}$$

Most of the time, however, we want the total energy flux (i.e., conductive heat flux plus convective flux).

$$Q_a = q_a + \frac{5}{2} T_a \Gamma_a , \tag{2.3.1.8}$$

So we can write

$$\begin{bmatrix} \Gamma_a^{PS} \\ \dfrac{Q_a^{PS}}{T_a} \end{bmatrix} = \frac{\langle \tilde{U}^2 \rangle}{e_a} \sum_b \frac{T_b}{e_b} \left\{ \left(A_{b1} + \frac{5}{2} A_{b2} \right) \left(\begin{bmatrix} 1 \\ 5/2 \end{bmatrix} l_{11}^{ab} - \begin{bmatrix} 0 \\ 1 \end{bmatrix} l_{21}^{ab} \right) - A_{b2} \left(\begin{bmatrix} 1 \\ 5/2 \end{bmatrix} l_{12}^{ab} - \begin{bmatrix} 0 \\ 1 \end{bmatrix} l_{22}^{ab} \right) \right\} , \tag{2.3.1.9}$$

but we can "simplify" this (or at least remove the radial electric field dependence) by noting

$$\left(A_{b1}+\frac{5}{2}A_{b2}\right)=\left(\frac{n_b'}{n_b}-\frac{e_bE_r}{T_b}+\frac{T_b'}{T_b}\right), \tag{2.3.1.10}$$

when this is substituted the E_r term ends up proportional to $E_r\sum_b l_{j1}^{ab}$, which sums to zero from momentum conservation.

$$\begin{bmatrix}\Gamma_a^{PS}\\ \dfrac{Q_a}{T_a}\end{bmatrix}=\frac{\langle\tilde{U}^2\rangle}{e_a}\sum_b\frac{T_b}{e_b}\left\{\left(\frac{n_b'}{n_b}+\frac{T_b'}{T_b}\right)\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{11}^{ab}-\begin{bmatrix}0\\1\end{bmatrix}l_{21}^{ab}\right)-\frac{T_b'}{T_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{12}^{ab}-\begin{bmatrix}0\\1\end{bmatrix}l_{22}^{ab}\right)\right\}, \tag{2.3.1.11}$$

finally, using

$$\left(\frac{n_b'}{n_b}+\frac{T_b'}{T_b}\right)=\frac{(n_bT_b)'}{n_bT_b}, \tag{2.3.1.12}$$

we get

$$\begin{bmatrix}\Gamma_a^{PS}\\ \dfrac{Q_a^{PS}}{T_a}\end{bmatrix}=\frac{\langle\tilde{U}^2\rangle}{e_a}\sum_b\frac{1}{e_b}\left\{\frac{(n_bT_b)'}{n_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{11}^{ab}-\begin{bmatrix}0\\1\end{bmatrix}l_{21}^{ab}\right)-T_b'\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{12}^{ab}-\begin{bmatrix}0\\1\end{bmatrix}l_{22}^{ab}\right)\right\}. \tag{2.3.1.13}$$

Now we can look again at the banana-non-axisymmetric flux, and put in the L_a^{SN}

$$\begin{aligned}\Gamma_{aj}^{bn}=&-\left\|D_{11}^a\right\|_j A_{a1}-\left\|K_aD_{11}^a\right\|_j A_{a2}-\left\|\frac{\left[D_{31}^a\right]^2}{D_{33}^a}\right\|_j A_{a1}-\left\|K_a\frac{\left[D_{31}^a\right]^2}{D_{33}^a}\right\|_j A_{a2}\\ &-\frac{2}{3}\frac{\langle B^2\rangle}{B_0}\sum_{k=0}^{j\max}\left\|L_k^{(3/2)}K_a\frac{D_{31}^a}{D_{33}^a}\right\|_j\frac{\langle Bu_{a\|k}\rangle}{\langle B^2\rangle}+\langle\tilde{U}^2\rangle\frac{2}{3}\frac{m_aT_a}{e_a^2}\left(\left\|K_a\nu_D^a\right\|_j A_{a1}+\left\|K_a^2\nu_D^a\right\|_j A_{a2}\right)\end{aligned}, \tag{2.3.1.14}$$

Where the first two terms are just the normal monoenergetic contributions without momentum correction and the last term is from the PS flows. If we write the physical fluxes and add the convective component we get

$$\begin{aligned}\begin{bmatrix}\Gamma_a^{bn}\\ Q_a^{bn}/T_a\end{bmatrix}=&-\begin{bmatrix}\left\|D_{11}^a\right\|_0\\ \left\|K_aD_{11}^a\right\|_0\end{bmatrix}A_{a1}-\begin{bmatrix}\left\|K_aD_{11}^a\right\|_0\\ \left\|K_a^2D_{11}^a\right\|_0\end{bmatrix}A_{a2}-\begin{bmatrix}\left\|\left[D_{31}^a\right]^2/D_{33}^a\right\|_0\\ \left\|K_a\left[D_{31}^a\right]^2/D_{33}^a\right\|_0\end{bmatrix}A_{a1}-\begin{bmatrix}\left\|K_a\left[D_{31}^a\right]^2/D_{33}^a\right\|_0\\ \left\|K_a^2\left[D_{31}^a\right]^2/D_{33}^a\right\|_0\end{bmatrix}A_{a2}\\ &-\frac{2}{3}\frac{\langle B^2\rangle}{B_0}\sum_{k=0}^{j\max}\begin{bmatrix}\left\|K_a\dfrac{D_{31}^a}{D_{33}^a}\right\|_k\\ \left\|K_a^2\dfrac{D_{31}^a}{D_{33}^a}\right\|_k\end{bmatrix}\frac{\langle Bu_{a\|k}\rangle}{\langle B^2\rangle}+\langle\tilde{U}^2\rangle\frac{2}{3}\frac{m_aT_a}{e_a^2}\left(\begin{bmatrix}\left\|K_a\nu_D^a\right\|_0\\ \left\|K_a^2\nu_D^a\right\|_0\end{bmatrix}A_{a1}+\begin{bmatrix}\left\|K_a^2\nu_D^a\right\|_0\\ \left\|K_a^3\nu_D^a\right\|_0\end{bmatrix}A_{a2}\right)\end{aligned}, \tag{2.3.1.15}$$

Now we can add on the PS flux and group all of the terms proportional to the PS factor as

$$\begin{bmatrix}\Gamma_a \\ Q_a/T_a\end{bmatrix} = -\begin{bmatrix}\left\|D_{11}^a\right\|_0 \\ \left\|K_a D_{11}^a\right\|_0\end{bmatrix}A_{a1} - \begin{bmatrix}\left\|K_a D_{11}^a\right\|_0 \\ \left\|K_a^2 D_{11}^a\right\|_0\end{bmatrix}A_{a2} - \begin{bmatrix}\left\|\left[D_{31}^a\right]^2/D_{33}^a\right\|_0 \\ \left\|K_a\left[D_{31}^a\right]^2/D_{33}^a\right\|_0\end{bmatrix}A_{a1} - \begin{bmatrix}\left\|K_a\left[D_{31}^a\right]^2/D_{33}^a\right\|_0 \\ \left\|K_a^2\left[D_{31}^a\right]^2/D_{33}^a\right\|_0\end{bmatrix}A_{a2}$$

$$-\frac{2}{3}\frac{\left\langle B^2\right\rangle}{B_0}\sum_{k=0}^{j\max}\begin{bmatrix}\left\|K_a\frac{D_{31}^a}{D_{33}^a}\right\|_k \\ \left\|K_a^2\frac{D_{31}^a}{D_{33}^a}\right\|_k\end{bmatrix}\frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle} + \left\langle\tilde{U}^2\right\rangle\frac{n_a m_a}{e_a}X_{PS} \quad , (2.3.1.16)$$

where

$$X_{PS}^a \equiv \frac{1}{n_a m_a}\left[\sum_b\left\{\frac{(n_bT_b)'}{e_bn_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{11}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{21}^{ab}\right) - \frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{12}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{22}^{ab}\right)\right\} + \frac{2}{3}\frac{m_aT_a}{e_a}\left(\begin{bmatrix}\left\|K_a\nu_D^a\right\|_0 \\ \left\|K_a^2\nu_D^a\right\|_0\end{bmatrix}A_{a1} + \begin{bmatrix}\left\|K_a^2\nu_D^a\right\|_0 \\ \left\|K_a^3\nu_D^a\right\|_0\end{bmatrix}A_{a2}\right)\right], \quad (2.3.1.17)$$

and it will be shown in section Appendix A that this is equivalent to the X_{PS}^a used in the MBT force equation.

Or, again in terms of the L_a^{SN} coefficient,

$$\begin{bmatrix}\Gamma_a \\ Q_a/T_a\end{bmatrix} = -\begin{bmatrix}\left\|L_a^{SN}\right\|_0 \\ \left\|K_aL_a^{SN}\right\|_0\end{bmatrix}A_{a1} - \begin{bmatrix}\left\|K_aL_a^{SN}\right\|_0 \\ \left\|K_a^2L_a^{SN}\right\|_0\end{bmatrix}A_{a2} - \frac{2}{3}\frac{\left\langle B^2\right\rangle}{B_0}\sum_{k=0}^{j\max}\begin{bmatrix}\left\|K_a\frac{D_{31}^a}{D_{33}^a}\right\|_k \\ \left\|K_a^2\frac{D_{31}^a}{D_{33}^a}\right\|_k\end{bmatrix}\frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle} . \quad (2.3.1.18)$$

$$+\frac{\left\langle\tilde{U}^2\right\rangle}{e_a}\sum_b\left\{\frac{(n_bT_b)'}{e_bn_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{11}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{21}^{ab}\right) - \frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{12}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{22}^{ab}\right)\right\}$$

2.3.2 MBT Flux Equations

The MBT fluxes are written directly as the radial energy and particle fluxes as

$$\begin{bmatrix}\Gamma_a \\ Q_a/T_a\end{bmatrix} = -\begin{bmatrix}\left\|D_{11}^a\right\|_0 \\ \left\|K_aD_{11}^a\right\|_0\end{bmatrix}A_{a1} - \begin{bmatrix}\left\|K_aD_{11}^a\right\|_0 \\ \left\|K_a^2D_{11}^a\right\|_0\end{bmatrix}A_{a2} - \begin{bmatrix}\left\|D_{13}^a\right\|_0 \\ \left\|K_aD_{13}^a\right\|_0\end{bmatrix}A_{a3}$$

$$-\frac{B_0^2}{\left\langle B^2\right\rangle}\frac{m_a}{T_a}\sum_{k=0}^{j\max}\left\{\frac{\left\langle Bu_{\|ak}\right\rangle}{B_0}\left(\begin{bmatrix}\left\|\nu_D^aD_{31}^a\right\|_k \\ \left\|K_a\nu_D^aD_{31}^a\right\|_k\end{bmatrix} + \sum_{l=0}^{j\max}c_l\begin{bmatrix}\left\|D_{31}^a\right\|_l \\ \left\|K_aD_{31}^a\right\|_l\end{bmatrix}\left\{\frac{M_{lk}^{aa}+N_{lk}^{aa}}{\tau^{aa}} + \sum_{b\neq a}\frac{M_{lk}^{ab}}{\tau^{ab}}\right\}\right) + \sum_{b\neq a}\frac{\left\langle Bu_{\|bk}\right\rangle}{B_0}\sum_{l=0}^{j\max}c_l\begin{bmatrix}\left\|D_{31}^a\right\|_l \\ \left\|K_aD_{31}^a\right\|_l\end{bmatrix}\frac{N_{lk}^{ab}}{\tau^{ab}}\right\} \quad , (2.3.2.1)$$

$$+\frac{n_am_a}{e_a}\frac{\left\langle\tilde{G}^2\right\rangle}{B_0^2}X_{PS}^a$$

where

$$X_{PS}^a \equiv \sum_{b\neq a}\left(\frac{(n_aT_a)'}{n_ae_a} - \frac{(n_bT_b)'}{n_be_b}\right)\left(\begin{bmatrix}1\\5/2\end{bmatrix}\frac{M_{00}^{ab}}{\tau^{ab}} - \begin{bmatrix}0\\1\end{bmatrix}\frac{M_{10}^{ab}}{\tau^{ab}}\right) - \frac{T_a'}{e_a}\left(\begin{bmatrix}1\\5/2\end{bmatrix}\sum_{b\neq a}\frac{M_{01}^{ab}}{\tau^{ab}} - \begin{bmatrix}0\\1\end{bmatrix}\left\{\frac{M_{11}^{aa}+N_{11}^{aa}}{\tau^{aa}} + \sum_{b\neq a}\frac{M_{11}^{ab}}{\tau^{ab}}\right\}\right), \quad (2.3.2.2)$$

$$-\sum_{b\neq a}\frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}\frac{N_{01}^{ab}}{\tau^{ab}} - \begin{bmatrix}0\\1\end{bmatrix}\frac{N_{11}^{ab}}{\tau^{ab}}\right) + \frac{2}{3}\frac{T_a}{e_a}\left(\begin{bmatrix}I_0^a\\I_1^a\end{bmatrix}A_{a1} + \begin{bmatrix}I_1^a\\I_2^a\end{bmatrix}A_{a2}\right)$$

and

$$I_n^a \equiv \frac{2}{\sqrt{\pi}}\int_0^\infty dK_aK_a^{n+3/2}e^{-K_a}\nu_D^a = \frac{1}{n_a}\left\|\nu_D^aK_a^{n+1}\right\|_0 . \quad (2.3.2.3)$$

It is shown in appendix A that the X_{PS}^a is equivalent to that defined in section 2.3.1.

We can use Eqs XX and XX to convert the M_{lk}^{ab} and N_{lk}^{ab} coefficients to the l_{lk}^{ab} and then combine these terms to get

$$\begin{gathered}\begin{bmatrix}\Gamma_a \\ Q_a/T_a\end{bmatrix} = -\begin{bmatrix}\left\|D_{11}^a\right\|_0 \\ \left\|K_a D_{11}^a\right\|_0\end{bmatrix} A_{a1} - \begin{bmatrix}\left\|K_a D_{11}^a\right\|_0 \\ \left\|K_a^2 D_{11}^a\right\|_0\end{bmatrix} A_{a2} - \begin{bmatrix}\left\|D_{13}^a\right\|_0 \\ \left\|K_a D_{13}^a\right\|_0\end{bmatrix} A_{a3} + \frac{n_a m_a}{e_a}\frac{\left\langle \tilde{G}^2\right\rangle}{B_0^2} X_{PS}^a \\ -\frac{B_0}{n_a T_a}\sum_{k=0}^{j\max}\left\{ n_a m_a \frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}\begin{bmatrix}\left\|\nu_D^a D_{31}^a\right\|_k \\ \left\|K_a \nu_D^a D_{31}^a\right\|_k\end{bmatrix} + \sum_b \frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\sum_{l=0}^{j\max} c_l \begin{bmatrix}\left\|D_{31}^a\right\|_l \\ \left\|K_a D_{31}^a\right\|_l\end{bmatrix} l_{l+1,k+1}^{ab}\right\}\end{gathered}, \qquad (2.3.2.4)$$

we can also see that

$$\left\langle \tilde{U}^2\right\rangle = \frac{\left\langle \tilde{G}^2\right\rangle}{B_0^2}, \qquad (2.3.2.5)$$

so we finally have

$$\begin{gathered}\begin{bmatrix}\Gamma_a \\ Q_a/T_a\end{bmatrix} = -\begin{bmatrix}\left\|D_{11}^a\right\|_0 \\ \left\|K_a D_{11}^a\right\|_0\end{bmatrix} A_{a1} - \begin{bmatrix}\left\|K_a D_{11}^a\right\|_0 \\ \left\|K_a^2 D_{11}^a\right\|_0\end{bmatrix} A_{a2} - \begin{bmatrix}\left\|D_{13}^a\right\|_0 \\ \left\|K_a D_{13}^a\right\|_0\end{bmatrix} A_{a3} + \left\langle \tilde{U}^2\right\rangle \frac{n_a m_a}{e_a} X_{PS}^a \\ -\frac{B_0}{n_a T_a}\sum_{k=0}^{j\max}\left\{ n_a m_a \frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}\begin{bmatrix}\left\|\nu_D^a D_{31}^a\right\|_k \\ \left\|K_a \nu_D^a D_{31}^a\right\|_k\end{bmatrix} + \sum_b \frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\sum_{l=0}^{j\max} c_l \begin{bmatrix}\left\|D_{31}^a\right\|_l \\ \left\|K_a D_{31}^a\right\|_l\end{bmatrix} l_{l+1,k+1}^{ab}\right\}\end{gathered}. \qquad (2.3.2.6)$$

2.3.3 T Flux Equations

The Taguchi flux equation is

$$\begin{gathered}\Gamma_{aj}^{bn} = \sum_{k=0}^{j\max} N_{j+1,k+1}^{a-T}\frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle} + \frac{1}{n_a T_a}\sum_{m=0}^{j\max} B_{j+1,m+1}^a c_m \sum_b \sum_{k=0}^{j\max} l_{m+1,k+1}^{ab}\frac{\left\langle Bu_{b\|k}\right\rangle}{\left\langle B^2\right\rangle} \\ + L_{j+1,1}^{a-T} X_{a1} - L_{j+1,2}^{a-T} X_{a2}\end{gathered}, \qquad (2.3.3.1)$$

and substituting for the forces and coefficients gives

$$\begin{gathered}\Gamma_{aj}^{bn} = -B_0\frac{m_a}{T_a}\sum_{k=0}^{j\max}\left\|L_k^{(3/2)}\nu_D^a D_{31}^a\right\|_j \frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle} - \frac{B_0}{n_a T_a}\sum_{m=0}^{j\max}\left\|L_m^{(3/2)} D_{31}^a\right\|_j c_m \sum_b \sum_{k=0}^{j\max} l_{m+1,k+1}^{ab}\frac{\left\langle Bu_{b\|k}\right\rangle}{\left\langle B^2\right\rangle} \\ -\left\|D_{11}^a\right\|_j A_{a1} - \left\|K_a D_{11}^a\right\|_j A_{a2} + \left\langle \tilde{U}^2\right\rangle \frac{2}{3}\frac{T_a m_a}{e_a^2}\left(\left\|\nu_D^a K_a\right\|_j A_{a1} + \left\|\nu_D^a K_a^2\right\|_j A_{a2}\right)\end{gathered}. \qquad (2.3.3.2)$$

Now we can write the physical fluxes (where I included the convective term and changed the index of the second summation to l) as

$$
\begin{bmatrix} \Gamma_a^{bn} \\ Q_a^{bn}/T_a \end{bmatrix} = -\begin{bmatrix} \left\|D_{11}^a\right\|_0 \\ \left\|K_a D_{11}^a\right\|_0 \end{bmatrix} A_{a1} - \begin{bmatrix} \left\|K_a D_{11}^a\right\|_0 \\ \left\|K_a^2 D_{11}^a\right\|_0 \end{bmatrix} A_{a2}
$$
$$
-\frac{B_0}{n_a T_a} \sum_{k=0}^{j\max} \left\{ n_a m_a \frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle} \begin{bmatrix} \left\|\nu_D^a D_{31}^a\right\|_k \\ \left\|K_a \nu_D^a D_{31}^a\right\|_k \end{bmatrix} + \sum_b \frac{\left\langle Bu_{b\|k}\right\rangle}{\left\langle B^2\right\rangle} \sum_{l=0}^{j\max} c_l \begin{bmatrix} \left\|D_{31}^a\right\|_l \\ \left\|K_a D_{31}^a\right\|_l \end{bmatrix} l_{l+1,k+1}^{ab} \right\} . \qquad (2.3.3.3)
$$
$$
+\left\langle \tilde{U}^2 \right\rangle \frac{2}{3} \frac{T_a m_a}{e_a^2} \left(\begin{bmatrix} \left\|\nu_D^a K_a\right\|_0 \\ \left\|\nu_D^a K_a^2\right\|_0 \end{bmatrix} A_{a1} + \begin{bmatrix} \left\|\nu_D^a K_a^2\right\|_0 \\ \left\|\nu_D^a K_a^3\right\|_0 \end{bmatrix} A_{a2} \right)
$$

Now we can add the PS fluxes to get

$$
\begin{bmatrix} \Gamma_a \\ Q_a/T_a \end{bmatrix} = -\begin{bmatrix} \left\|D_{11}^a\right\|_0 \\ \left\|K_a D_{11}^a\right\|_0 \end{bmatrix} A_{a1} - \begin{bmatrix} \left\|K_a D_{11}^a\right\|_0 \\ \left\|K_a^2 D_{11}^a\right\|_0 \end{bmatrix} A_{a2} + \left\langle \tilde{U}^2 \right\rangle \frac{n_a m_a}{e_a} X_{PS}^a
$$
$$
-\frac{B_0}{n_a T_a} \sum_{k=0}^{j\max} \left\{ n_a m_a \frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle} \begin{bmatrix} \left\|\nu_D^a D_{31}^a\right\|_k \\ \left\|K_a \nu_D^a D_{31}^a\right\|_k \end{bmatrix} + \sum_b \frac{\left\langle Bu_{b\|k}\right\rangle}{\left\langle B^2\right\rangle} \sum_{l=0}^{j\max} c_l \begin{bmatrix} \left\|D_{31}^a\right\|_l \\ \left\|K_a D_{31}^a\right\|_l \end{bmatrix} l_{l+1,k+1}^{ab} \right\} . \qquad (2.3.3.4)
$$

So this is identical to the MBT formulae, except for the Ware pinch term.

3. Computational Form of Equations

This section contains equations in a form as used by the PENTA code.

3.1 Normalized DKES coefficients

The thermal transport coefficients used in the equations above are related to so-called “normalized” coefficients as

$$
D_{11}^* \equiv D_{11}^a \left(\frac{m_a^2 v^3}{2e_a^2} \right)^{-1} = D_{11}^a \left(\frac{m_a^2 v_{Ta}^3}{2e_a^2} K_a^{3/2} \right)^{-1} , \qquad (3.1.1a)
$$

$$
D_{31}^* \equiv D_{31}^a \left(\frac{m_a v^2}{2e_a B_0} \right)^{-1} = D_{31}^a \left(\frac{m_a v_{Ta}^2}{2e_a B_0} K_a \right)^{-1} , \qquad (3.1.1b)
$$

$$
D_{33}^* \equiv D_{33}^a \left(\frac{v}{2B_0^2} \right)^{-1} = D_{33}^a \left(\frac{v_{Ta}}{2B_0^2} K_a^{1/2} \right)^{-1} . \qquad (3.1.1c)
$$

These coefficients are then independent of species and are stored in data files used by PENTA. To convert the equations from section XX it is useful to write the following equations

$$
\frac{1}{D_{33}^a} = \frac{1}{D_{33}^*} \frac{2B_0^2}{v_{Ta}} K_a^{-1/2} , \qquad (3.1.2a)
$$

$$
\frac{D_{31}^a}{D_{33}^a} = B_0 \frac{m_a v_{Ta}}{e_a} \frac{D_{31}^*}{D_{33}^*} K_a^{1/2} , \qquad (3.1.2b)
$$

$$\frac{\left[D_{31}^{a}\right]^{2}}{D_{33}^{a}}=\frac{m_a^2 v_{Ta}^3}{2e_a^2}\frac{\left[D_{31}^{*}\right]^{2}}{D_{33}^{*}}K_a^{3/2}. \tag{3.1.2c}$$

The Spitzer contribution is written in normalized form as

$$D_{33}^{Spitzer-*}\equiv D_{33}^{Spitzer-a}\left(\frac{\nu}{2B_0^2}\right)^{-1}=\frac{2}{3}\frac{\nu}{\nu_D^a}\left\langle B^2\right\rangle. \tag{3.1.3}$$

3.2 Flow equations

Using these equations we can write the two flow equations (SN and T) as

3.2.1 SN Flow Equation

$$\begin{aligned}&\sum_{k=0}^{j\max}\left(\frac{e_a}{T_a}\left\|L_k^{(3/2)}K_a^{3/2}\left(\frac{2}{3}\left\langle B^2\right\rangle\frac{1}{D_{33}^*}-\frac{\nu_D^a}{\nu}\right)\right\|_j\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}-\frac{3}{2}\frac{e_a}{m_a v_{Ta}T_a}\sum_b l_{j+1,k+1}^{ab}\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\right)\\&=-\left\|K_a^{3/2}\frac{D_{31}^*}{D_{33}^*}\right\|_j A_{a1}-\left\|K_a^{5/2}\frac{D_{31}^*}{D_{33}^*}\right\|_j A_{a2}+\frac{3}{2}\frac{e_a n_a}{m_a v_{Ta}}\frac{\delta_{j0}}{B_0}A_{a3}\end{aligned}, \tag{3.2.1.1}$$

3.2.2 Taguchi Flow Equation (or MBT Flow Equation)

$$\begin{aligned}&\sum_{k=0}^{j\max}\left[\left(\frac{n_a e_a}{T_a}\frac{\left\langle B^2\right\rangle}{c_j}\delta_{jk}-\frac{e_a}{v_{Ta}T_a}\left\|\nu_D^a L_k^{(3/2)}D_{33}^*K_a^{1/2}\right\|_j\right)\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}-\frac{e_a}{n_a T_a m_a v_{Ta}}\sum_{l=0}^{j\max}c_l\left\|L_l^{(3/2)}D_{33}^*K_a^{1/2}\right\|_j\sum_b l_{l+1,k+1}^{ab}\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\right]\\&=-\left\|D_{31}^*K_a\right\|_j A_{a1}-\left\|D_{31}^*K_a^2\right\|_j A_{a2}+\frac{e_a}{B_0 m_a v_{Ta}}\left\|D_{33}^*K_a^{1/2}\right\|_j A_{a3}\end{aligned}. \tag{3.2.2.1}$$

3.2.3 SN Flux Equation

$$\begin{aligned}\begin{bmatrix}\Gamma_a\\ Q_a/T_a\end{bmatrix}=&-\frac{m_a^2 v_{Ta}^3}{2e_a^2}\begin{bmatrix}\left\|K_a^{3/2}\left(D_{11}^*+\left[D_{31}^*\right]^2/D_{33}^*\right)\right\|_0\\ \left\|K_a^{5/2}\left(D_{11}^*+\left[D_{31}^*\right]^2/D_{33}^*\right)\right\|_0\end{bmatrix}A_{a1}-\frac{m_a^2 v_{Ta}^3}{2e_a^2}\begin{bmatrix}\left\|K_a^{5/2}\left(D_{11}^*+\left[D_{31}^*\right]^2/D_{33}^*\right)\right\|_0\\ \left\|K_a^{7/2}\left(D_{11}^*+\left[D_{31}^*\right]^2/D_{33}^*\right)\right\|_0\end{bmatrix}A_{a2}\\&-\frac{2}{3}\left\langle B^2\right\rangle\frac{m_a v_{Ta}}{e_a}\sum_{k=0}^{j\max}\begin{bmatrix}\left\|K_a^{3/2}D_{31}^*/D_{33}^*\right\|_k\\ \left\|K_a^{5/2}D_{31}^*/D_{33}^*\right\|_k\end{bmatrix}\frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle}+\left\langle\tilde{U}^2\right\rangle\frac{n_a m_a}{e_a}X_{PS}\end{aligned} \tag{3.2.3.1}$$

or

$$\begin{bmatrix}\Gamma_a\\ Q_a/T_a\end{bmatrix} = -\begin{bmatrix}\left\|L_a^{SN}\right\|_0\\ \left\|K_a L_a^{SN}\right\|_0\end{bmatrix}A_{a1} - \begin{bmatrix}\left\|K_a L_a^{SN}\right\|_0\\ \left\|K_a^2 L_a^{SN}\right\|_0\end{bmatrix}A_{a2} - \frac{2}{3}\left\langle B^2\right\rangle \frac{m_a v_{Ta}}{e_a}\sum_{k=0}^{j\max}\begin{bmatrix}\left\|K_a^{3/2}\dfrac{D_{31}^*}{D_{33}^*}\right\|_k\\ \left\|K_a^{5/2}\dfrac{D_{31}^*}{D_{33}^*}\right\|_k\end{bmatrix}\frac{\left\langle Bu_{a\|k}\right\rangle}{\left\langle B^2\right\rangle}$$

$$+\frac{\left\langle \tilde{U}^2\right\rangle}{e_a}\sum_b\left\{\frac{(n_bT_b)'}{e_bn_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{11}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{21}^{ab}\right) - \frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{12}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{22}^{ab}\right)\right\} \tag{3.2.3.2}$$

$$L_a^{SN} \equiv \frac{m_a^2 v_{Ta}^3}{2e_a^2}K_a^{3/2}\left(D_{11}^* - \frac{2}{3}\left\langle \tilde{U}^2\right\rangle\frac{\nu_D^a}{\nu} + \frac{\left[D_{31}^*\right]^2}{D_{33}^*}\right) \tag{3.2.3.3}$$

3.2.4 MBT Flux equation (or T Flux Equation)

$$\begin{aligned}\begin{bmatrix}\Gamma_a\\ Q_a/T_a\end{bmatrix} =& -\frac{m_a^2 v_{Ta}^3}{2e_a^2}\begin{bmatrix}\left\|K_a^{3/2}D_{11}^*\right\|_0\\ \left\|K_a^{5/2}D_{11}^*\right\|_0\end{bmatrix}A_{a1} - \frac{m_a^2 v_{Ta}^3}{2e_a^2}\begin{bmatrix}\left\|K_a^{5/2}D_{11}^*\right\|_0\\ \left\|K_a^{7/2}D_{11}^*\right\|_0\end{bmatrix}A_{a2} + \frac{m_a v_{Ta}^2}{2e_aB_0}\begin{bmatrix}\left\|K_aD_{31}^*\right\|_0\\ \left\|K_a^2D_{31}^*\right\|_0\end{bmatrix}A_{a3}\\ &-\sum_{k=0}^{j\max}\left\{\frac{m_a}{e_a}\frac{\left\langle Bu_{\|ak}\right\rangle}{\left\langle B^2\right\rangle}\begin{bmatrix}\left\|\nu_D^aK_aD_{31}^*\right\|_k\\ \left\|K_a^2\nu_D^aD_{31}^*\right\|_k\end{bmatrix} + \frac{1}{n_ae_a}\sum_b\frac{\left\langle Bu_{\|bk}\right\rangle}{\left\langle B^2\right\rangle}\sum_{l=0}^{j\max}c_l\begin{bmatrix}\left\|K_aD_{31}^*\right\|_l\\ \left\|K_a^2D_{31}^*\right\|_l\end{bmatrix}l_{l+1,k+1}^{ab}\right\}\\ &+\frac{\left\langle \tilde{U}^2\right\rangle}{e_a}\left[\sum_b\left\{\frac{(n_bT_b)'}{e_bn_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{11}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{21}^{ab}\right) - \frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}l_{12}^{ab} - \begin{bmatrix}0\\1\end{bmatrix}l_{22}^{ab}\right)\right\} + \frac{2}{3}\frac{m_aT_a}{e_a}\left(\begin{bmatrix}\left\|K_a\nu_D^a\right\|_0\\ \left\|K_a^2\nu_D^a\right\|_0\end{bmatrix}A_{a1} + \begin{bmatrix}\left\|K_a^2\nu_D^a\right\|_0\\ \left\|K_a^3\nu_D^a\right\|_0\end{bmatrix}A_{a2}\right)\right]\end{aligned} \tag{3.2.4.1}$$

3.2.5 DKES flux equation

$$\begin{bmatrix}\Gamma_a\\ Q_a/T_a\end{bmatrix} = -\frac{m_a^2 v_{Ta}^3}{2e_a^2}\begin{bmatrix}\left\|K_a^{3/2}D_{11}^*\right\|_0\\ \left\|K_a^{5/2}D_{11}^*\right\|_0\end{bmatrix}A_{a1} - \frac{m_a^2 v_{Ta}^3}{2e_a^2}\begin{bmatrix}\left\|K_a^{5/2}D_{11}^*\right\|_0\\ \left\|K_a^{7/2}D_{11}^*\right\|_0\end{bmatrix}A_{a2} + \frac{m_a v_{Ta}^2}{2e_aB_0}\begin{bmatrix}\left\|K_aD_{31}^*\right\|_0\\ \left\|K_a^2D_{31}^*\right\|_0\end{bmatrix}A_{a3} \tag{3.2.5.1}$$

3.2.6 DKES flow equation

XX

Appendix A. Equality of the X_{PS} forces

In the MBT formulation we have

$$X_{PS}^{a} \equiv \sum_{b\neq a}\left(\frac{(n_aT_a)'}{n_ae_a}-\frac{(n_bT_b)'}{n_be_b}\right)\left(\begin{bmatrix}1\\5/2\end{bmatrix}\frac{M_{00}^{ab}}{\tau^{ab}}-\begin{bmatrix}0\\1\end{bmatrix}\frac{M_{10}^{ab}}{\tau^{ab}}\right)-\frac{T_a'}{e_a}\left(\begin{bmatrix}1\\5/2\end{bmatrix}\sum_{b\neq a}\frac{M_{01}^{ab}}{\tau^{ab}}-\begin{bmatrix}0\\1\end{bmatrix}\left\{\frac{M_{11}^{aa}+N_{11}^{aa}}{\tau^{aa}}+\sum_{b\neq a}\frac{M_{11}^{ab}}{\tau^{ab}}\right\}\right)$$
$$-\sum_{b\neq a}\frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}\frac{N_{01}^{ab}}{\tau^{ab}}-\begin{bmatrix}0\\1\end{bmatrix}\frac{N_{11}^{ab}}{\tau^{ab}}\right)+\frac{2}{3}\frac{T_a}{e_a}\left(\begin{bmatrix}I_0^a\\I_1^a\end{bmatrix}A_{a1}+\begin{bmatrix}I_1^a\\I_2^a\end{bmatrix}A_{a2}\right)$$

Using Eqs XX and XX we can write

$$\left.\frac{l_{11}^{ab}}{n_am_a}\right|_{b\neq a}=\frac{N_{00}^{ab}}{\tau^{ab}}=-\frac{M_{00}^{ab}}{\tau^{ab}}$$
$$\left.\frac{l_{12}^{ab}}{n_am_a}\right|_{b\neq a}=\frac{N_{01}^{ab}}{\tau^{ab}}$$
$$\left.\frac{l_{21}^{ab}}{n_am_a}\right|_{b\neq a}=\frac{N_{10}^{ab}}{\tau^{ab}}=-\frac{M_{10}^{ab}}{\tau^{ab}}$$
$$\left.\frac{l_{22}^{ab}}{n_am_a}\right|_{b\neq a}=\frac{N_{11}^{ab}}{\tau^{ab}}$$
$$\frac{l_{12}^{aa}}{n_am_a}=\sum_{b'\neq a}\frac{M_{01}^{ab'}}{\tau^{ab'}}+\frac{M_{01}^{aa}+N_{01}^{aa}}{\tau^{aa}}=\sum_{b'\neq a}\frac{M_{01}^{ab'}}{\tau^{ab'}}$$
$$\frac{l_{21}^{aa}}{n_am_a}=\sum_{b'\neq a}\frac{M_{10}^{ab'}}{\tau^{ab'}}+\frac{M_{10}^{aa}+N_{10}^{aa}}{\tau^{aa}}=\sum_{b'\neq a}\frac{M_{10}^{ab'}}{\tau^{ab'}}$$
$$\frac{l_{22}^{aa}}{n_am_a}=\sum_{b'\neq a}\frac{M_{11}^{ab'}}{\tau^{ab'}}+\frac{M_{11}^{aa}+N_{11}^{aa}}{\tau^{aa}}$$

where I also used the relations

$$N_{00}^{ab}=-M_{00}^{ab},\, N_{10}^{ab}=-M_{10}^{ab},\, N_{ij}^{aa}=N_{ji}^{aa},\, M_{ij}^{ab}=M_{ji}^{ab}$$

$$\frac{l_{j+1,k+1}^{aa}}{n_am_a}=\sum_{b'}\frac{M_{jk}^{ab'}}{\tau^{ab'}}+\frac{N_{jk}^{aa}}{\tau^{aa}}=\sum_{b'\neq a}\frac{M_{jk}^{ab'}}{\tau^{ab'}}+\frac{M_{jk}^{aa}+N_{jk}^{aa}}{\tau^{aa}}$$
$$\left.\frac{l_{j+1,k+1}^{ab}}{n_am_a}\right|_{b\neq a}=\frac{N_{jk}^{ab}}{\tau^{ab}}$$

Then

$$X_{PS}^{a} \equiv -\begin{bmatrix}1\\5/2\end{bmatrix}\frac{(n_aT_a)'}{n_ae_a}\sum_{b\neq a}\frac{l_{11}^{ab}}{n_am_a}+\begin{bmatrix}1\\5/2\end{bmatrix}\sum_{b\neq a}\frac{(n_bT_b)'}{n_be_b}\frac{l_{11}^{ab}}{n_am_a}-\begin{bmatrix}0\\1\end{bmatrix}\frac{(n_aT_a)'}{n_ae_a}\frac{l_{21}^{aa}}{n_am_a}-\begin{bmatrix}0\\1\end{bmatrix}\sum_{b\neq a}\frac{(n_bT_b)'}{n_be_b}\frac{l_{21}^{ab}}{n_am_a}$$
$$-\frac{T_a'}{e_a}\left(\begin{bmatrix}1\\5/2\end{bmatrix}\frac{l_{12}^{aa}}{n_am_a}-\begin{bmatrix}0\\1\end{bmatrix}\frac{l_{22}^{aa}}{n_am_a}\right)-\sum_{b\neq a}\frac{T_b'}{e_b}\left(\begin{bmatrix}1\\5/2\end{bmatrix}\frac{l_{12}^{ab}}{n_am_a}-\begin{bmatrix}0\\1\end{bmatrix}\frac{l_{22}^{ab}}{n_am_a}\right)+\frac{2}{3}\frac{T_a}{n_ae_a}\left(\begin{bmatrix}\left\|\nu_D^aK_a^1\right\|_0\\\left\|\nu_D^aK_a^2\right\|_0\end{bmatrix}A_{a1}+\begin{bmatrix}\left\|\nu_D^aK_a^2\right\|_1\\\left\|\nu_D^aK_a^3\right\|_1\end{bmatrix}A_{a2}\right)$$

Now each pair of the first six terms can be combined into sums over all species noting that, from momentum conservation, $\sum_a l_{11}^{ab} = 0$ so $\sum_{a \neq b} l_{11}^{ab} = -l_{11}^{aa}$. (The following expression can also be obtained by writing the expression for l_{11}^{aa} using Eq 2.1.4.2 and substituting this in for the sum over M_{00}^{ab}).

$$n_a m_a X_{PS}^a = \sum_b \left\{ \frac{(n_b T_b)'}{e_b n_b} \left(\begin{bmatrix} 1 \\ 5/2 \end{bmatrix} l_{11}^{ab} - \begin{bmatrix} 0 \\ 1 \end{bmatrix} l_{21}^{ab} \right) - \frac{T_b'}{e_b} \left(\begin{bmatrix} 1 \\ 5/2 \end{bmatrix} l_{12}^{ab} - \begin{bmatrix} 0 \\ 1 \end{bmatrix} l_{22}^{ab} \right) \right\} + \frac{2}{3} \frac{m_a T_a}{e_a} \left(\begin{bmatrix} \left\| K_a \nu_D^a \right\|_0 \\ \left\| K_a^2 \nu_D^a \right\|_0 \end{bmatrix} A_{a1} + \begin{bmatrix} \left\| K_a^2 \nu_D^a \right\|_0 \\ \left\| K_a^3 \nu_D^a \right\|_0 \end{bmatrix} A_{a2} \right)$$

which is equivalent to Eq XX.

Appendix B. Tracking changes to equations

B.1. Fortran version 1.2 to 1.3

In version 1.3 the following bugs in equations were fixed, as compared to version 1.2.

In version 1.2 the normalized Spitzer portion of the parallel electric conductivity coefficient, $D_{33}^{Spitzer-*}$, was implemented as

$$D_{33}^{Spitzer-*} = \frac{2}{3} \frac{\nu}{\nu_D^a}, \tag{B.1.1}$$

which is missing a factor of $\langle B^2 \rangle$, as compared to equation 3.1.3.

The radial particle diffusion coefficient used in the SN flux equations was implemented as

$$L_a^{SN} \equiv \frac{m_a^2 v_{Ta}^3}{2e_a^2} K_a^{3/2} \left(D_{11}^* - \frac{2}{3} \langle \tilde{U}^2 \rangle \frac{\nu_D^a}{\nu} + \frac{\left[D_{31}^* \right]^2}{B_0^2 D_{33}^*} \right), \tag{B.1.2}$$

which has an extra factor of $1/B_0^2$ on the last term, as compared to equation XX.

The SN flux equations were implemented as

$$\begin{bmatrix} \Gamma_a^{bn} \\ Q_a^{bn}/T_a \end{bmatrix} = -\begin{bmatrix} \left\| L_a^{SN} \right\|_0 \\ \left\| K_a L_a^{SN} \right\|_0 \end{bmatrix} A_{a1} - \begin{bmatrix} \left\| K_a L_a^{SN} \right\|_0 \\ \left\| K_a^2 L_a^{SN} \right\|_0 \end{bmatrix} A_{a2} - \frac{2}{3} \frac{\langle B^2 \rangle}{B_0} \frac{m_a v_{Ta}}{q_a} \sum_{k=0}^{j\max} \begin{bmatrix} \left\| K_a^{3/2} \frac{D_{31}^*}{D_{33}^*} \right\|_k \\ \left\| K_a^{5/2} \frac{D_{31}^*}{D_{33}^*} \right\|_k \end{bmatrix} \frac{\langle B u_{a\|k} \rangle}{\langle B^2 \rangle}, \tag{B.1.3}$$

where there is an extra factor of $1/B_0$ on last term.

The SN flow equation was implemented as

$$\begin{aligned} &\sum_{k=0}^{j\max} \left(m_a v_{Ta} B_0 \left\| L_k^{(3/2)} K_a^{3/2} \left(\frac{2}{3} \langle B^2 \rangle \frac{1}{D_{33}^*} - \frac{\nu_D^a}{\nu} \right) \right\|_j \frac{\langle B u_{\|ak} \rangle}{\langle B^2 \rangle} - \frac{3}{2} B_0 \sum_b l_{j+1,k+1}^{ab} \frac{\langle B u_{\|bk} \rangle}{\langle B^2 \rangle} \right) \\ &= -T_a \frac{v_{Ta} m_a B_0}{e_a} \left\| K_a^{3/2} \frac{D_{31}^*}{D_{33}^*} \right\|_j A_{a1} - T_a \frac{v_{Ta} m_a B_0}{e_a} \left\| K_a^{5/2} \frac{D_{31}^*}{D_{33}^*} \right\|_j A_{a2} + T_a \delta_{j0} \frac{3}{2} A_{a3} \end{aligned}, \tag{B.1.4}$$

which is missing a factor of n_a on the last term, as compared to equation 3.2.3.3.

The MBT fluxes had some errors in calculation of the P-S flux, which were insignificant as evaluation of the flow equation convolutions resulted in a much larger error. There is also the issue of the sign on the parallel electric field term, see section 2.1.3.