PENTA Documentation

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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*.  and are the temperature, density, electric charge and mass, respectively. In all equations  is given in electron volts, all other quantities are in mks units. The kinetic pressure is , and the thermal velocity is .

The radial electric field is , where  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 . The parallel electric field is defined as .

The following symbols are regularly used for the magnetic field; , where  denotes a flux surface average, and , 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 . In the MBT formulation,  is defined as the B00 component of the Fourier decomposition of the magnetic field strength. The normalized magnetic field strength  is also used in some sections.

The monoenergetic (test particle) velocity is given simply as  in the following equations. The normalized monoenergtic velocity and energy are given by

 , (2.1.1.1)

and

, (2.1.1.2)

respectively.

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

. (2.1.1.3)

where the summation is over *all* species,

, (2.1.1.4)

, (2.1.1.5)

and  is the error function. The second term in Eq. 2.1.1.5 comes from the derivative of the error function, and  is the Coulomb logarithm. It is useful to write the collision frequency as

, (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

, for  eV, (2.1.1.7a)

, for  eV. (2.1.1.7b)

### 2.1.2 Thermodynamic forces

In the SN approach the thermodynamic forces are labeled as  and , where

, (2.1.2.1a)

, (2.1.2.1b)

 . (2.1.2.1c)

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

, (2.1.2.2a)

, (2.1.2.2b)

. (2.1.2.2c)

In most of the PENTA equations the  forces are preferred, however both methods have their advantages. The  forces allow the DKE to be written simply in terms of the Sonine polynomials, and have a species independent parallel electric field drive. The  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  forces are written in terms of the  as

, (2.1.2.3a)

, (2.1.2.3b)

. (2.1.2.3c)

And the inverse relationship is

, (2.1.2.4a)

, (2.1.2.4b)

. (2.1.2.4c)

### 2.1.3 DKES coefficient definitions

The three independent monoenergetic transport coefficients from DKES are , , and  . 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  and , and the notation is different in the MBT and SN papers. In all PENTA notation the  refer to the monoenergetic coefficients with units of m2/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  and  coefficients to be off by factors of  and, 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, . In the earliest version of DKES the output contained the entire coefficient, however in later versions the collisional contribution to the  coefficient was excluded and only the remainder given. To get the physical  the collisional, or "Spitzer" contribution had to be added to the DKES output. The collisional contribution to  is given by

 . (2.1.3.1)

In the SN formulation the  used is defined as the total  minus the collisional contribution. In the MBT formulation, on the other hand, the total  is used. In PENTA an option exists whereby the normalized  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: [m2/s],  [Tm2/s], and  [T2m2/s] where in the MBT formulation (and in this document) all three coefficients have units of [m2/s]. To convert between the definitions (recall again that the "B correction" is always assumed), the following relations can be used

, (2.1.3.2a)

, (2.1.3.2b)

, (2.1.3.2b)

where  are the coefficients used in the SN papers.

Finally, there remains some question about the sign of the  and  coefficients. It is possible that SN use different definitions, and that in their notation both  and  have the same sign. Further, in the  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

, (2.1.4.1)

where XX.

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

, (2.1.4.2)

, (2.1.4.3)

XX

### 2.1.5 Sonine polynomials

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

The coefficient  is defined as

, (2.1.5.1)

where the double factorial .

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

, (2.1.5.2a)

. (2.1.5.2b)

Then we have

. (2.1.5.3)

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

, (2.1.5.4a)

. (2.1.5.4b)

The orthogonality condition for the Sonine polynomials is

, (2.1.5.5)

which is related to the coefficient c as

. (2.1.5.6)

### 2.1.6 Energy integrals

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

, (2.1.6.1)

where  is a monoenergetic coefficient (function of ) and  is the corresponding thermal coefficient.

In the MBT formulation the following definition is used

, (2.1.6.2)

which, using the relation is equivalent to

. (2.1.6.3)

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

. (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

, (2.1.8.1)

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

. (2.1.8.2)

The monoenergetic coefficients are defined as

, (2.1.8.3a)

, (2.1.8.3b)

. (2.1.8.3c)

Next we wish to convert these to use the . 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

. (2.1.8.4)

We then have

, (2.1.8.5a)

, (2.1.8.5b)

, (2.1.8.5a)

or

, (2.1.8.6a)

, (2.1.8.6b)

. (2.1.8.6c)

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

, (2.1.8.7)

where

, (2.1.8.8a)

, (2.1.8.8b)

. (2.1.8.8c)

Converting these to  gives

, (2.1.8.9a)

, (2.1.8.9b)

. (2.1.8.9c)

The flux equation uses two additional coefficients,

, (1.2.8.10)

where

, (2.1.8.11a)

, (2.1.8.11b)

Converting these to  gives

, (2.1.8.12a)

. (2.1.8.12b)

### 2.1.9 Definition of the parallel flow moments

In the MBT approach the parallel flow moments are defined as

. (2.1.9.1)

In the SN approach the following definition is used.

. (2.1.9.2)

The flow moments are then simply related as

. (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,...,jmax

, (2.2.1.1)

where jmax 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

. (2.2.1.2)

If the reference magnetic field strength is given as  the flow equation can be written as

. (2.2.1.3)

### 2.2.2 MBT flow equation

In the MBT formulation the flow equation is given for j=0,1,...,jmax

. (2.2.2.1)

Using equations XX and XX we can write

. (2.2.2.2)

Or, if reference magnetic field strength is given as  then

. (2.2.2.3)

### 2.2.3 Taguchi Flow Equation

The T flow equation given for j=0,1,...,jmax as

. (2.2.3.1)

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

. (2.2.3.2)

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)

, (2.2.3.3)

And we can write

. (2.2.3.4)

Now the only difference is in the sign of the last term. After talking to Beidler, it appears that the definition of  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

. (2.3.1.1)

where  is the banana-non-axisymmetric component of the flux, and the total flux is

. (2.3.1.2)

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

, (2.3.1.3a)

. (2.3.1.3b)

Substituting the coefficients and forces gives

, (2.3.1.4)

where I have defined

, (2.3.1.5)

as a radial particle diffusion coefficient.

The PS flux is written as

. (2.3.1.6)

Substituting for the forces and writing just the physical fluxes gives

. (2.3.1.7)

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

, (2.3.1.8)

So we can write

, (2.3.1.9)

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

, (2.3.1.10)

when this is substituted the  term ends up proportional to , which sums to zero from momentum conservation.

, (2.3.1.11)

finally, using

, (2.3.1.12)

we get

. (2.3.1.13)

Now we can look again at the banana-non-axisymmetric flux, and put in the 

, (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

, (2.3.1.15)

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

, (2.3.1.16)

where

 , (2.3.1.17)

and it will be shown in section Appendix A that this is equivalent to the  used in the MBT force equation.

Or, again in terms of the  coefficient,

. (2.3.1.18)

### 2.3.2 MBT Flux Equations

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

, (2.3.2.1)

where

, (2.3.2.2)

and

. (2.3.2.3)

It is shown in appendix A that the  is equivalent to that defined in section 2.3.1.

We can use Eqs XX and XX to convert the  and  coefficients to the  and then combine these terms to get

, (2.3.2.4)

we can also see that

, (2.3.2.5)

so we finally have

. (2.3.2.6)

### 2.3.3 T Flux Equations

The Taguchi flux equation is

 , (2.3.3.1)

and substituting for the forces and coefficients gives

. (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

. (2.3.3.3)

Now we can add the PS fluxes to get

. (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

, (3.1.1a)

, (3.1.1b)

. (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

, (3.1.2a)

, (3.1.2b)

. (3.1.2c)

The Spitzer contribution is written in normalized form as

. (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

, (3.2.1.1)

### 3.2.2 Taguchi Flow Equation (or MBT Flow Equation)

. (3.2.2.1)

### 3.2.3 SN Flux Equation

(3.2.3.1)

or

 (3.2.3.2)

 (3.2.3.3)

### 3.2.4 MBT Flux equation (or T Flux Equation)

(3.2.4.1)

### 3.2.5 DKES flux equation

 (3.2.5.1)

### 3.2.6 DKES flow equation

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# Appendix A. Equality of the XPS forces

In the MBT formulation we have

Using Eqs XX and XX we can write















where I also used the relations

,,,





Then

Now each pair of the first six terms can be combined into sums over all species noting that, from momentum conservation,  so . (The following expression can also be obtained by writing the expression for  using Eq 2.1.4.2 and substituting this in for the sum over ).

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, , was implemented as

, (B.1.1)

which is missing a factor of , as compared to equation 3.1.3.

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

, (B.1.2)

which has an extra factor of  on the last term, as compared to equation XX.

The SN flux equations were implemented as

, (B.1.3)

where there is an extra factor of  on last term.

The SN flow equation was implemented as

, (B.1.4)

which is missing a factor of  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.