Creating a global plasma model using Disturbed Bilateral Relations

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Abstract. Disturbed Bilateral Relations offer a way of categorizing plasma processes by their deviation from equilibrium. This method can be used to create a simple plasma model that solves key plasma parameters, namely the electron temperature, electron density and heavy particle temperature. An implementation of this method is presented, and the results validated against a detailed plasma simulation, for a wide range of parameters.

1. Introduction

Plasma modeling is an indispensable part of plasma physics research. It is a very broad field that has a very wide variety of different models, each appropriate for different plasmas and with their own drawbacks and strengths. This wide variety is of course related to the breadth of plasma physics research itself. A useful distinction in modeling is the distinction between global models and grand models.

Global models are models that rely on a high number of assumptions to simplify a problem as much as is feasible, and then solve the simplified problem. They are usually zero or one-dimensional, can be analytical or numerical, and if they are numerical, the numerical cost is small. Because the basic physics is not clouded by numerical details, the successful use of global models for plasma simulation can give a good understanding of the fundamental physics involved in a problem.

With the advent of cheap and powerful computers, grand models have become a popular method of describing plasmas. Using this method, it is possible to create a computer model that, given only elemental input such as reaction and collision cross sections, and external plasma parameters such as geometry, power incoupling and gas feeds, gives an accurate description of the plasma.

In this contribution, we will discuss the creation of a global model that is based on the principle of Disturbed Bilateral Relations (dBR). Briefly, this approach categorized various processes in the plasma based on whether they are in equilibrium or not. This powerful and flexible approach will be used to construct a model that is applicable over a wide parameter range. This allows one to use a simple, single model to browse a large part of the parameter space over which plasmas can exist. We will compare the results of a parameter study with this model with the results obtained with a validated grand model.
2. Disturbed Bilateral Relations
In an equilibrium situation between one state $\alpha$ and a second state $\beta$, in which there is a forward and backwards process which are inverse processes and are in equilibrium, one can write

$$n_\alpha \nu_f = n_\beta \nu_b,$$

with $n$ the densities, $\nu_f$ the forward rate and $\nu_b$ the backward rate [1].

Such an equilibrium can be disturbed by a transport term $n_\beta \nu_t$, which without loss of generality can be considered as a loss term for state $\beta$. This modifies Equation (1) to

$$n_\alpha \nu_f - n_\beta \nu_b = n_\beta \nu_t$$

(2)

In Equation (2), we will refer to the second term as the proper term, while the third term is an improper term. Because industrial and laboratory plasmas are designed to get something out of them, this improper term might be quite large for many processes in the plasma. We will use this fact during the construction of the algorithm we use to solve the model.

3. The model
In this section, we will describe a global model based on the principle of disturbed bilateral relations. We will, for the moment, restrict our discussion to a quasineutral atomic plasma, with a modest (<1%) degree of ionization. These assumptions are not fundamental, but will allow us to make the discussion more concrete.

In order to obtain the key plasma properties, three global balance equations are solved, namely the electron particle balance, the electron energy balance and the heavy particle energy balance. These give three key plasma properties, namely the electron temperature $T_e$, the electron density $n_e$, and the heavy particle temperature $T_h$, respectively.

The model is most accurate for plasmas with a low degree of ionization. For plasmas with a high degree of ionization, much simpler models that are based on a Local Thermal Equilibrium can be made.

3.1. The electron particle balance
In the plasmas under consideration, electron impact ionization is the most important source of ionization. In this process, a high-energy electron impacts on an atom, ionizing it and releasing a second electron. The proper inverse process for this is two-electron recombination, in which two electrons and an ion recombine to form an ion and an electron. An equilibrium between these processes is called Saha equilibrium. We will, however, include a second, improper loss term for the electrons, namely ambipolar diffusion to the walls. This yields the following equation for the electron particle balance:

$$n_e n_1 K_{\text{ion}} - n_e^2 n_+ K_{\text{rec}} = \frac{D_{\text{amb}} n_e}{\Lambda^2}.$$  

Here, $n_1$ is the ground state density, $K_{\text{ion}}$ is the ionization rate, $K_{\text{rec}}$ is the recombination rate, $D_{\text{amb}}$ is the ambipolar diffusion coefficient and $\Lambda$ is the typical length scale of the smallest dimension.

Equation (3) can be rewritten to:

$$K_{\text{ion}} = \frac{D_{\text{amb}}}{n_1 \Lambda^2} + \frac{n_e n_+}{n_1} K_{\text{rec}}.$$  

(4)

Because $K_{\text{ion}}$ is strongly dependent on $T_e$, the particle balance in fact gives us an equation for $T_e$. 

3.2. The electron energy balance
The electrons in a plasma undergo elastic collisions with the neutrals in the plasma. Due to the high mass ratio between electrons and ions, the energy transfer between them is quite inefficient, causing two different temperatures to exist, one for the electrons and one for all the heavy particles.

The electron energy balance has the following form:

\[ n_e n_a K_{\text{heat}} (k_B T_e - k_B T_h) = \epsilon - (n_e n_a K_{\text{ion}} - n_e^2 n_a K_{\text{rec}}) E_{\text{ion}}, \quad (5) \]

where \( n_a \) is the heavy particle density, \( K_{\text{heat}} \) is the heat transfer coefficient, \( \epsilon \) the dissipated power and \( E_{\text{ion}} \) the ionization energy.

All terms in Equation (5), except \( \epsilon \), are proportional to \( n_e \). This means, that Equation (5) can be used to find the density of \( n_e \), when the coefficients and \( \epsilon \) are known.

3.3. The heavy particle energy balance
The heavy particles are heated by elastic collisions with the electrons, and lose their heat via heat conduction to the wall:

\[ n_e n_a K_{\text{heat}} (k_B T_e - k_B T_h) = \lambda \frac{T_h - T_{\text{wall}}}{\Lambda^2}, \quad (6) \]

with \( K_{\text{cond}} \) the coefficient of heat conduction and \( T_{\text{wall}} \) the wall temperature. Equation (6) can be used to obtain a value for \( T_h \).

3.4. The coefficients
The three balance Equations (4), (5) and (6) give a values for \( T_e, n_e \) and \( T_h \), provided that the coefficients \( K_{\text{ion}}, K_{\text{rec}}, D_{\text{amb}}, K_{\text{heat}} \) and \( K_{\text{cond}} \) are known. These coefficients depend on \( T_e \) and \( T_h \), and on the physical properties gas in which the plasma exists.

The ionization rate coefficient \( K_{\text{ion}} \) can be approximated by an Arrhenius rate. This rate has the following general form:

\[ K_{\text{ion}} = k_{\text{rate}} T_e^q \exp \left( -\frac{I}{k_B T_e} \right), \quad (7) \]

The factor \( q, I \) is the energy threshold for the reaction, and the constant \( k_{\text{rate}} \) depend on the gas [2].

The most efficient ionization process in a plasma is not necessarily direct ionization, as stepwise ionization may be a more important mechanism. The rate that is implemented should reflect this, i.e. if direct ionization is dominant, the \( q, I \) and \( k_{\text{rate}} \) of the direct process should be used, and if stepwise ionization is dominant, the \( q, I \) and \( k_{\text{rate}} \) of excitation to the first excited state should be used. [3] gives a more thorough explanation of this.

From Equation (4), it follows that a value of \( K_{\text{ion}} \) is necessary to compensate for the losses. Because \( K_{\text{ion}} \) depends on \( T_e \), this gives the value for \( T_e \). The recombination rate coefficient \( K_{\text{rec}} \) can be obtained using the principle of detailed balancing [2] from \( K_{\text{ion}} \):

\[ K_{\text{rec}} = \left( \frac{h}{2\pi m_e k T_e} \right)^\frac{3}{2} \frac{k_{\text{rate}} T_e^q}{G} \exp \left( \frac{E_{\text{ion}} - I}{k_B T_e} \right), \quad (8) \]

where \( G \) is the ratio of the degeneracy of the ion state and the ground state. The factor 2 in the denominator factors in the degeneracy of the electron.

The ambipolar diffusion coefficient \( D_{\text{amb}} \) consists of the ion diffusion coefficient multiplied with a factor to take into account the ambipolar field, and is given by [4]:

\[ D_{\text{amb}} = \left( 1 + \frac{T_e}{T_h} \right) \frac{2}{\beta n_a \sigma_{ia}} \sqrt{\frac{k_B T_h}{\pi M}} \quad (9) \]
where \( \sigma_{ia} \) is the \( T_h \)-dependent ion-atom collision cross section and \( M \) is the ion mass. The heat transfer coefficient \( K_{\text{heat}} \) is the product of the reduced collision frequency (i.e. the collision frequency divided by \( n_a \) and \( n_e \)) and the heat transferred in one such collision, divided by the temperature difference \( T_e - T_h \), which is explicitly accounted for in Equations (5) and (6). This gives the following expression for \( K_{\text{heat}} \) [4]:

\[
n_e n_p \sigma_{ea} \sqrt{\frac{8 k_B T_e}{\pi m_e} \frac{3 m_e}{M} (k_B T_e - k_B T_h)} = n_e n_p (k_B T_e - k_B T_h) K_{\text{heat}}, \tag{10}
\]

where \( m_e \) is the electron mass. We can solve \( K_{\text{heat}} \) from Equation (10) to obtain [2]

\[
K_{\text{heat}} = \frac{3 \sigma_{ea}}{M} \sqrt{\frac{8 k_B T_e m_e}{\pi}}. \tag{11}
\]

The thermal conductivity coefficient \( \lambda \) for the heavy particles is given by [4]

\[
\lambda = \frac{\sqrt{2 k_B}}{\sigma_{aa}} \sqrt{\frac{8 k_B T_h}{\pi M}}, \tag{12}
\]

with \( \sigma_{aa} \) the neutral-neutral collision cross section, which generally depends on \( T_h \).

4. The algorithm

The three balance equations and the five equations for the coefficients in those equations are in principle sufficient to solve for the eight variables in the system. This is not trivial, especially because of the highly nonlinear nature of many of the equation. In this subsection, an iterative algorithm that can reliably solve the equations will be presented. In this algorithm, we use the fact that the ionization degree is low to approximate \( n_1 \) with \( n_a \). The algorithm is schematically represented in Figure 1.

The first part of the algorithm consists of obtaining a good guess for \( T_e \). For this, Equation (4) and the coefficients therein are solved iteratively.

The iteration is started by choosing starting values, denoted with the superscript \( i \), which should be reasonably close to an actual plasma condition, i.e. \( T_e^i = 10000 \text{ K} \), \( T_h^i = 1000 \text{ K} \),
\[ n_e = 10^{24} \text{ m}^{-3}. \]

Next, the right-hand terms of Equation (4) are calculated using Equation (9) and (8) and substituted. This gives a value for \( K_{\text{ion}}. \) \( T_e \) cannot be solved directly from Equation (7), as Equation (7) is a transcendental equation. It is solved by substituting \( T'_e \) in the \( T_e^q \)-term, and solving for the \( T_e \) in the exponential term.

This new value of \( T_e \), which we will call \( T'_e \), can now be used to compute new values for the right-hand terms in Equation (4), and hence, a new value for \( K_{\text{ion}} \). By substituting \( T'_e \) in the exponential term, Equation (7) can be solved for a new value of \( T_e \). This procedure is repeated until convergence is achieved.

With a good estimate for \( T_e \), we now turn our attention to \( T_h \) and \( n_e \). First, \( K_{\text{heat}} \) is computed using Equation (11) and the new value of \( T_e \) and \( \lambda \) is computed using Equation (12) and \( T'_h \).

At this point, all coefficients are known. To solve \( n_e \), we substitute Equation (3) in Equation (5):

\[ n_e n_\alpha k_{\text{heat}}(T_e) - n_e n_\alpha k_{\text{heat}}(T_h) = \epsilon - \left( \frac{D_{\text{amb}} n_e}{A^2} \right) E_{\text{ion}}. \tag{13} \]

We can now solve \( n_e \) from Eq. Equation (13):

\[ n_e = \frac{\epsilon}{n_\alpha K_{\text{heat}}(T_e - T_h) + \left( \frac{D_{\text{amb}}}{A^2} \right) E_{\text{ion}}}, \tag{14} \]

and by substituting the coefficients and \( T_e \) and \( T'_h \), obtain a value for \( n_e \).

The last property to be determined is \( T_h \). It can be determined by solving Equation (6) for \( T_h \):

\[ T_h = \left( T_e + T_{\text{wall}} \frac{\lambda}{K_{\text{heat}} A^2} \right) \left( 1 + \frac{\lambda}{K_{\text{heat}} A^2} \right)^{-1} \tag{15} \]

We now have obtained values for all coefficients and \( T_e, T_h \) and \( n_e \). This makes it possible to start the main iterative loop. In this loop, we first solve Equations (4), (13) and (15) to obtain \( T_e, n_e \) and \( T_h \), respectively. These plasma properties can now be used to obtain new values for the coefficients \( K_{\text{rec}}, D_{\text{amb}}, K_{\text{heat}}, \) and \( \lambda \) using Eqs. Equation (8), Equation (9), Equation (11) and Equation (12), respectively. By iterating, the equations can be solved to a degree of precision that is in principle only limited by machine accuracy.

The equations for the transport coefficients presented in this section are only the simplest realistic approximation of the true transport coefficients of a plasma. It is, of course, possible, and in fact quite easy to use other, more accurate and complicated expressions for the transport coefficients.

5. Comparison with a grand model

In order to demonstrate the viability of the dBR global model, we will compare the result this approach gives with the results of a grand model. For this, we will use a very simple case, namely an Ar plasma in a cylindrical vessel with radius \( \Lambda \), that is assumed to be infinitely long. By varying \( n_\alpha, \Lambda \) and \( P \), the latter denoting the power per unit length, we can easily browse a large part of the parameters space.

The grand model used is the PLASIMO code. This is a well-validated code, that has been used successfully in the modeling of a wide variety of plasmas [5, 6].

The necessary input data for the model has been obtained from literature. For \( \sigma_{a=\alpha} \), the hard-sphere cross section is used. For \( \sigma_{e=\alpha} \), [7] is used, while for \( \sigma_{i=\alpha} \) [8] is used. The ionization rate is obtained from [3].

We have carried out a parameter study by varying \( n_\alpha, \Lambda \) and \( P \), in both the dBR simulation and the PLASIMO simulation. The default values are \( n_\alpha = 10^{24} \text{ m}^{-3}, 1 \text{ mm} \) and 100 W/m, respectively. The wall of the plasma is cooled to a temperature of 300 K.
Figure 2. A study of the impact of a variation of $P$ on $n_e$, $T_e$ and $T_h$, obtained with dBR and PLASIMO.

Figure 3. A study of the impact of a variation of $\Lambda$ on $n_e$, $T_e$ and $T_h$, obtained with dBR and PLASIMO.

Figure 4. A study of the impact of variation of $n_a$ on $n_e$, $T_e$ and $T_h$, obtained with dBR and PLASIMO.

Figure 2 shows that for increasing $P$, the electron density increases. Furthermore, the increased electron density leads to an increase in electron/heavy particle collision frequency and hence to background gas heating. The match between the dBR and PLASIMO is generally excellent. However, dBR does not take into account the fact that gas heating and ionization redistributes the background gas, and this leads to a discrepancy between the dBR and PLASIMO results.

Figure 3 shows that for decreasing $\Lambda$, $n_e$ increases. This is due to the increase in power density. Furthermore, decreasing $\Lambda$ leads to more diffusive losses and hence a higher $T_e$. The match between dBR and PLASIMO is again very good.

Figure 4 shows two competing trends for $n_e$ as a function of $n_a$. For low $n_a$, the increased diffusive losses lead to a reduction in $n_e$. This also manifests itself in a higher $T_e$ for lower $n_a$. On the other hand, for high values of $n_a$, the increased background gas heating carries away the bulk of the power, leading to a lower $n_e$. The match between dBR and PLASIMO is again very good.

6. Conclusions
A zero-dimensional plasma model that uses Disturbed Bilateral Relations to obtain $n_e$, $T_e$ and $T_h$ for a given set of plasma parameters is presented. In its present form, the model can simulate a wide range of atomic, quasineutral plasmas, and because of the conceptual simplicity and easy implementation of such a method, it is easily expanded to handle other plasmas.
The model has been compared with a well-validated grand plasma model, in this case the PLASIMO code, in a parameter study, to see if the dBR model correctly reproduces the trends. The agreement between both models is excellent, and the results can easily be explained with elementary understanding of plasma physics, which leads to the conclusion that the dBR model produces physically relevant results over a wide parameter range, making it suitable for the global modeling of plasmas.

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