

Calculation of Thermodynamic Parameters for Dense High-Temperaure Plasma

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The present paper is essentially the report submitted by a first-year student, Pavel Chvykov, after his internship (summer, 2008) (sections 1-4). The embedded tables are created by the Fortran code, which is the part of the BATS-RUS code development for the CRASH project.

In the installed version of the SWMF code one can use command 'make PDF' from the SWMF subdirectory SWMF/util/CRASH/doc to make this document. The Fortran code will automatically compile the executable IONIZ.exe and run it, which will calculate the ionization equilibrium in Xe within wide ranges of parameters and put the output data to the tables used in the text

1 Introduction and Background

Understanding the processes that go on in high-density and high-temperature plasmas, as well as the response of such plasmas to various external disturbances has become increasingly important in the modern world. Such plasmas play the key role in many important emerging or possible future applications, such as thermonuclear fusion chain reaction, laser particle acceleration, and the x-ray laser pumped by nuclear reactions. However, experiments with such plasmas are extremely difficult to carry out in a controlled lab environment, since the temperatures and densities reached are comparable to those of the sun, or of a nuclear explosion, the tests with which have been banned around a decade ago. This significantly hinders the progress that can be made in understanding such plasmas and in the development of the related technologies.

Hence, computer modeling of the processes that occur in these extremely dense and hot plasmas becomes irreplaceable. This is true not only due to the complexity of the real world experiments, which are still necessary to conduct, but also due to the measurement limitations of such experiments – not all important parameters of such plasmas can be measured experimentally, and hence some calculations and modeling are still necessary.

This work presents a way of calculating the temperature, as well as several other fundamental plasma parameters (pressure, degree of ionization, heat capacity), assuming that some set of the thermodynamic variables is given. Usually in Computational Fluid Dynamics (CFD) the pressure should be expressed in terms of the internal energy density or via the average internal energy per atomic unit in the plasma, the plasma density being the other input parameter for the Equation Of State (EOS). This calculation, which is very simple for ideal gases, becomes more complex when dealing with plasmas. Furthermore, this calculation is described for multi-element, as well as for single component plasmas.

Although this calculation is described for the general case, this work was done based on a particular experiment, in which Beryllium foil is accelerated via laser radiation along a thin plastic tube ($C_{22}H_{10}N_2$) filled in with Xenon. In the process, all these substances are heated to such temperatures that they form a mixture plasma, which then carries shock waves formed by the acceleration process, the dynamics of which are then examined.

2 Ionization Equilibrium

2.1 Basics

To find the thermodynamic characteristics of the plasma one should first describe the ionization equilibrium in it.

Population of an ion (P_i) in a plasma is the probability of finding that particle in the state possessing a certain charge, i . Similarly, if we let N_a be the heavy particle density – the total number of atoms and ions per unit of volume in a plasma – then, $N_i = P_i * N_a$, where N_i is the concentration of i -level ions (ions that lost i electrons), and P_i , their populations. Furthermore, since the total of probabilities of all the alternative events is always equal to

one, we get

$$\sum_{i=0}^X P_i = 1, \quad (1)$$

where X is the atomic number of the element – hence the maximum charge it can attain. Or, similarly:

$$\sum_{i=0}^X N_i = N_a, \quad (2)$$

which is the same equation multiplied by N_a . Furthermore, since in a single-component plasma, each of the N_i ions loses i electrons, which is further true for each of the X types of ions, we obtain the formula for the total number of free electrons per unit volume, N_e :

$$N_e = \sum_{i=0}^X i N_i, \quad (3)$$

which is the condition of plasma neutrality – the total positive charge on the ions per unit of volume in a plasma must be equal to the total number of free electrons in that volume. If we divide this equation by N_a , we get:

$$Z = \langle i \rangle = \sum_{i=0}^X i P_i, \quad (4)$$

where $Z = N_e/N_a$ – the average positive charge per ion in the plasma (measured in elementary charge units). Here $\langle i \rangle$ illustrates that this is the statistical average of the charge per ion.

From all these formulas we can see that to calculate practically any property of a plasma, we need to know the populations of all the levels of ions.

2.2 Boltzmann Distribution

To calculate the population of an i -level ion at a certain temperature, we need to know for how many atoms/ions, the energy per atomic cell is greater than or equal to the energy level of the i^{th} ion. Thus, we need to know the energy distribution between the atoms and ions for a given temperature T .

Here, recall the Maxwell-Boltzmann distribution, which formulates that the probability of finding a particle with certain energy in some volume of gas

(population of that energy state) is proportional to the Boltzmann factor:

$$g_i e^{-\frac{E_i}{k_B T}}, \quad (5)$$

where the exponent gives the probability of finding a particle in a specific state with energy E_i , while g_i – degeneracy – is the number of such distinct states that have the same desired energy. In the case of a plasma, however, the degeneracy value includes not only the number of states that the i-charged ion might have, but also the number of distinct states possible for all of the i electrons that have separated from the original atom. Since each of these electrons has the same degeneracy value, g_e , the total number of possible states for all of these electrons will be $(g_e)^i$. Therefore, in Eq.(5), g_i will be replaced by $g_i * (g_e)^i$. Furthermore, recalling that the sum of the populations of all alternative states must equal one, we can find the proportionality constant for the Boltzmann factor. Dividing each of these factors by the value of their sum, we will normalize them so that their sum after the transformation will be equal to unity (Eq. 1). Hence, if we also use the ion energy levels for E_i (energy needed to ionize a neutral atom to an i-charged ion), then the ion populations become:

$$P_i = \frac{g_i (g_e)^i e^{-\frac{E_i}{k_B T}}}{\sum_{i=0}^X g_i (g_e)^i e^{-\frac{E_i}{k_B T}}}, \quad (6)$$

Here, the sum in the denominator is called the partition function. The main difficulty with finding the actual populations using this equation comes from the g_e and g_i values. Through statistical and quantum mechanics we can find that the value of g_e is:

$$g_e = \frac{2}{N_e \Lambda^3} \quad \Lambda = \sqrt{\frac{h^2}{2\pi m_e k_B T}}, \quad (7)$$

where Λ is the thermal De Broglie wavelength of an electron.

Note that to calculate the value for g_e , we need to know N_e , which is found from Eq.(3) (or 4), which in turn takes the populations as an input parameter. Hence, we will have to solve a system of coupled equations, instead of a single equation, to find the correct population values. This will be addressed later on in the paper. In regards to the g_i values, on the other

hand, note that in most cases in a realistic plasma, while the value of g_e might be of the order of 10^{15} , the value of g_i is usually not greater than 3. Hence, after normalization, the effect of g_i on the final population values will be negligibly small in comparison.

Furthermore, since in most cases we are not interested in the actual population values, but rather in properties of plasma, such as Z (Eq.4), the slight inaccuracies in the populations will be evened out by the summation often used to calculate such properties, making the approximation even less evident. Hence, from now on, we will ignore the g_i values in our equations, approximating them by $g_i \approx 1$.

2.3 Saha Ionization Equation and Calculation Speed Improvement

Another similar approach to finding the population values (if the value of g_e is known) is using the Saha Ionization Equation. This equation is obtained by taking the ratio of the populations of the two consecutive level ions as given by Eq.(6):

$$\frac{P_{i+1}}{P_i} = g_e \frac{g_{i+1}}{g_i} e^{-\frac{E_{i+1}-E_i}{k_B T_e}} = \frac{2}{N_e \Lambda^3} \frac{g_{i+1}}{g_i} e^{-\frac{I_{i+1}}{k_B T_e}}, \quad (8)$$

or, similarly:

$$\frac{N_{i+1} N_e}{N_i} = \frac{2}{\Lambda^3} \frac{g_{i+1}}{g_i} e^{-\frac{I_{i+1}}{k_B T_e}}, \quad (9)$$

which is a better known form of the Saha Equation. Note that here $I_{i+1} = E_{i+1} - E_i$ denotes the ionization energy – energy required to remove a single electron from an i -charged ion, forming $(i+1)$ -level ion. These equations can provide an advantage in finding the populations if the speed of calculation is important. First, realize that if such is the case, than it is better to avoid the complex exponents of Eq.(6), which would take a long time to calculate. To do this, we could instead start with the natural logarithm of Eq.(8) (now ignoring the ratio $g_{i+1}/g_i \approx 1$):

$$\ln P_{i+1} - \ln P_i = \ln g_e - \frac{I_{i+1}}{k_B T_e}, \quad (10)$$

Then, we will let $P_0 = 1$ ($\ln P_0 = 0$), and using this relationship, build up and array of non-normalized values of $P_1, P_2, P_3, \dots, P_X$. The values of

this array will vary greatly, and some will be very large. To avoid having to find exponents of huge numbers, we can normalize this array so that the population of the most probable ion $P_{max} = 1$ ($\ln P_{max} = 0$). Note that normalizing an array of logarithms is done by subtraction, rather than division, since $\log(P_i/C) = \log P_i - \log C$, and hence we simply need to subtract $\ln P_{max}$ from every term. After this is done, to simplify the calculations even further, we can get rid of all the values of the array $j-7$, for example, because the actual populations corresponding to these values will be negligibly small – $P_i < e^{-7} = 0.00091$, and can be approximated as zeros. Finally, at this point, it should not take long to find the exponents of the remaining part of the array, and normalize them as before so that their sum equals one. This method can then be used instead of Eq.(6) any time the population values are needed.

3 Ionization Equilibrium at a Given Temperature

In CFD of an ideal gas, the temperature of a fluid is not important. As long as a conservative numerical scheme is used, the EOS can be applied to express the plasma pressure (the momentum flux) in terms of the total energy density, a constitutive part of the latter is the internal energy.

On the other hand, the crucial parameter of the ionization equilibrium is the plasma temperature. That is why while implementing the EOS for the plasma, the temperature should be first solved from the input parameters and then the ion populations should be solved at the given temperature. The latter problem is discussed in this section

3.1 The System of Equations

Both of the methods for finding the populations presented above can only be used if the value of g_e is known. However, g_e depends on N_e , which in turn depends on the populations themselves, and hence we find ourselves faced with solving a system of two equations – Eq.(3) (or 4) and Eq.(6) must both be satisfied in order to obtain the correct population values.

To solve this system, we first need to rewrite the term g_e as a function of

Z:

$$g_e = \frac{2}{N_e \Lambda^3} = \frac{2}{Z N_a \Lambda^3} = \frac{C_1}{Z}, \quad (11)$$

C_1 , which is independent of Z, is introduced here only to simplify this ratio. Hence, the Boltzmann factor from Eq.(5) becomes:

$$P_i \propto \left(\frac{C_1}{Z} \right)^i e^{-\frac{E_i}{k_B T_e}} = p_i. \quad (12)$$

Since this term appears frequently in the further discussion, we will denote it as p_i , to simplify the notation. Now, we can combine equations (4) and (6) into a single equation in Z:

$$Z = \sum_{i=0}^X i P_i = \sum_{i=0}^X \left(i \frac{p_i}{\sum_{j=0}^X p_j} \right) = \frac{\sum_{i=0}^X i p_i}{\sum_{i=0}^X p_i}, \quad (13)$$

3.2 Iterative Algorithm

Finally, all the terms in the above equation are known. However, this expression is too complex to solve by simple algebraic methods and requires an iterative approach. Direct iterations will converge to the answer very slowly, if at all. Hence, we will use the Newton-Rapson iteration method:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. \quad (14)$$

This method is used to approximate zeros of the function f. If x_n is an approximation of the solution (or a trial solution), then x_{n+1} will be a much better approximation. This method does have limitation as to whether it will converge to the answer, but if $f'(x_n) \geq 1$, then convergence is guaranteed. Further, since this method works only for finding zeros of the function, considering equation (13), let

$$f(Z) = Z - \frac{\sum i \left(\frac{C_1}{Z} \right)^i e^{-\frac{E_i}{k_B T_e}}}{\sum \left(\frac{C_1}{Z} \right)^i e^{-\frac{E_i}{k_B T_e}}}, \quad (15)$$

then when $f(Z)=0$, Z will have the desired value. Now, to use the method as in Eq.(14), we need to know $f'(Z)$.

Let's first find the derivative as follows:

$$\begin{aligned} \frac{\partial}{\partial Z} \left[\sum \left(\frac{C_1}{Z} \right)^i e^{-\frac{E_i}{k_B T_e}} \right] &= \sum i \left(\frac{C_1}{Z} \right)^{i-1} \frac{-C_1}{Z^2} e^{-\frac{E_i}{k_B T_e}} = \\ &= -\frac{C_1}{Z^2} \frac{Z}{C_1} \sum i \left(\frac{C_1}{Z} \right)^i e^{-\frac{E_i}{k_B T_e}} = -\frac{1}{Z} \sum i p_i, \end{aligned} \quad (16)$$

and similarly:

$$\frac{\partial}{\partial Z} \left[\sum i p_i \right] = -\frac{1}{Z} \sum i^2 p_i. \quad (17)$$

Now, combining these answers to find $f'(Z)$, we get:

$$\begin{aligned} \frac{\partial f}{\partial Z} &= 1 - \frac{-\frac{1}{Z} \sum i^2 p_i}{\sum p_i} - \frac{-\sum i p_i}{(\sum p_i)^2} \left(-\frac{1}{Z} \sum i p_i \right) = \\ &= 1 + \frac{1}{Z} \left(\frac{\sum i^2 p_i}{\sum p_i} - \left(\frac{\sum i p_i}{\sum p_i} \right)^2 \right), \end{aligned} \quad (18)$$

Therefore, looking back on Eq.(14) and combining Eq.(15) and (18), we get the overall resulting equation that can be used to find Z :

$$Z_{n+1} = Z_n - \frac{Z_n - \frac{\sum i p_i}{\sum p_i}}{1 + \frac{1}{Z_n} \left(\frac{\sum i^2 p_i}{\sum p_i} - \left(\frac{\sum i p_i}{\sum p_i} \right)^2 \right)}, \quad (19)$$

where the values for p_i can be found from equation (12), using Z_n for Z and all sums are across the entire span of possible ion charges. Further, notice that this equation is equivalent to:

$$Z_{n+1} = Z_n - \frac{Z_n - \langle i \rangle_n}{1 + \frac{1}{Z_n} (\langle i^2 \rangle_n - \langle i \rangle_n^2)}, \quad (20)$$

where $\langle i \rangle$ is the approximate average charge per ion, and $\langle i^2 \rangle$ is the approximate average of the squares of charges. This equation can also be used to find Z by first, finding the population values through either of the presented methods, using Z_n for Z in the calculation of g_e , and then find the values of $\langle i \rangle_n$ and $\langle i^2 \rangle_n$ using the formulas:

$$\langle i \rangle = \sum_{i=1}^X i P_i \quad \langle i^2 \rangle = \sum_{i=1}^X i^2 P_i, \quad (21)$$

Also, from Eq.(20), it can be seen that since the average of the squares is always greater than the square of the average, $\langle i^2 \rangle - \langle i \rangle^2 \geq 0$, and hence $f'(Z) \geq 1$, which then necessarily means that the iterations will converge. Hence, with these equations, we can fairly quickly find Z , if our initial guess is reasonably close.

3.3 Initial Approximation

In order to make the above iterative approach quick and efficient, it is important to find a decent first approximation for what the value of Z is. Since in most cases in plasma, there is a single ion whose population is much higher than that of all the others, a good first guess would be that Z is approximately the same as the charge of that ion. Hence, we need to find the value of i that maximizes P_i , or $\ln P_i$ (which will occur at the same i , but is easier to find). Recall that at a local extrema of any function, its first derivative is equal to 0. Since the populations are not defined by a continuous function, we can similarly say that $\Delta(\ln P_i)/\Delta i$ is closest to 0 at the maximum value of $\ln P_i$. Eq.(10) essentially gives an expression for $\Delta(\ln P_i)/\Delta i$. Hence, since we decided to initially approximate $Z \approx i_{P_{max}}$, we can build a sequence of values of what $\Delta(\ln P_i)/\Delta i$ would be if the current i was equal to $i_{P_{max}}$, and hence to Z . Hence, we will approximate $g_e = C_1/Z \approx C_1/i$. Further, when this derivative of the $\ln P_i$ sequence is ≈ 0 , P_i will be $\approx P_{i+1}$, and hence $i+1$ can be used for Z here just as well. Hence we get:

$$\frac{\Delta(\ln P_i)}{\Delta i} = \frac{\ln P_i - \ln P_{i-1}}{1} = \ln\left(\frac{C_1}{i}\right) - \frac{I_i}{k_B T_e}, \quad (22)$$

Then, the value of i for which the right side of this equation is closest to 0, will be a reasonable initial approximation for Z . Further, since, as mentioned, i as well as $i-1$ could be used for Z here, a better initial approximation would actually be between the two: $Z \approx i - 0.5$. A separate case arises when the plasma is weak and the vast majority of the atoms are not ionized ($Z \approx 0$). This implies that the populations of higher level ions will be negligible compared to those of P_0 , or even P_1 , and hence, Eq.(13) becomes:

$$Z = \frac{\sum_{i=0}^X i p_i}{\sum_{i=0}^X p_i} \approx \frac{p_1}{p_0} = \left(\frac{C_1}{Z}\right) e^{-\frac{I_1}{k_B T_e}}. \quad (23)$$

This can then be easily solved for Z :

$$Z \approx \sqrt{C_1 e^{-\frac{I_i}{k_B T_e}}}, \quad (24)$$

which is a very good and simple approximation. Hence, when the method in Eq.(22) yields $i_{P_{max}} = 1$, the method in Eq.(24) can be used instead, but only as long as it yields a value for Z less than 1 (if it does not, then $Z \approx 1$ and is too large for this method).

3.4 Section Summary

Finally, we have concluded that in order to find the ion populations in a plasma, we can use the following procedure:

1. Approximate the value of Z (average charge per ion) by first, finding the value of i for which

$$\ln\left(\frac{C_1}{i}\right) - \frac{I_i}{k_B T_e}$$

is closest to 0, and then approximating $Z \approx i - 0.5$. Note that if the i value found is $=1$, than Z might be very close to zero, in which case use:

$$Z \approx \sqrt{C_1 e^{-\frac{I_i}{k_B T_e}}}$$

- I_i is the ionization energy (energy required to remove one electron from $(i-1)$ -level ion, creating i charged ion)
- k_B is Boltzmann constant;
- T_e is the electron temperature;
- $C_1 = 2/(N_a \Lambda^3)$
 - N_a is the total concentration of atoms and ions in the plasma
 - $\Lambda = \sqrt{\frac{h^2}{2\pi m_e k_B T}}$, which is the thermal De Broglie wavelength of an electron.
 - * h is Planck's constant
 - * m_e is the electron mass 2.

2. Then, use

$$Z_{n+1} = Z_n - \frac{Z_n - \langle i \rangle_n}{1 + \frac{1}{Z_n} (\langle i^2 \rangle_n - \langle i \rangle_n^2)}$$

to iteratively get a better approximation of Z.

- To find $\langle i \rangle_n$ and $\langle i^2 \rangle_n$, first find the population values using the equation in the next step, and using Z_n for Z. Then, use the formulas:

$$\langle i \rangle = \sum_{i=1}^X i P_i \quad \langle i^2 \rangle = \sum_{i=1}^X i^2 P_i$$

3. Finally, calculate the populations using:

$$P_i = \frac{\left(\frac{C_1}{Z}\right)^i e^{-\frac{E_i}{k_B T_e}}}{\sum_{i=0}^X \left(\frac{C_1}{Z}\right)^i e^{-\frac{E_i}{k_B T_e}}}$$

4. If speed of calculation is important, use the method in section 3 (Eq. 10) instead on the previous step.

Following is the table that was constructed using the above algorithm. It shows the Z values calculated for Xenon at various electron temperatures (given in electron-volts – the value of $k_B T_e$, where k_B is in eV/K) and heavy particle concentrations (given in number of particles per cm^3).

Te[eV]\Na[1/cm ³]	10 ¹⁸	10 ¹⁹	10 ²⁰	10 ²¹	10 ²²	10 ²³
5.	3.4	2.8	2.2	1.3	0.6	0.2
10.	6.3	5.2	4.1	3.0	1.7	0.7
15.	7.3	6.9	5.9	4.4	2.7	1.1
20.	9.2	7.7	6.9	5.6	3.6	1.6
25.	11.8	9.4	7.6	6.5	4.5	2.1
30.	13.8	11.5	8.9	7.1	5.4	2.6
35.	15.7	13.3	10.4	7.8	6.0	3.1
40.	17.2	14.9	12.1	8.7	6.6	3.6
45.	18.1	16.4	13.4	9.9	7.1	4.1
50.	19.0	17.4	14.7	11.1	7.6	4.6
55.	20.5	18.1	15.9	12.3	8.2	5.0
60.	22.0	19.0	16.9	13.3	8.8	5.5
65.	23.3	20.1	17.6	14.3	9.6	5.9
70.	24.4	21.4	18.2	15.2	10.4	6.2
75.	25.3	22.6	19.0	16.1	11.2	6.6
80.	25.7	23.6	19.8	16.8	12.0	6.9
85.	25.9	24.5	20.8	17.4	12.7	7.3
90.	25.9	25.1	21.9	17.9	13.5	7.7
95.	26.0	25.5	22.8	18.5	14.2	8.0
100.	26.1	25.7	23.6	19.1	14.8	8.4
105.	26.2	25.9	24.3	19.7	15.4	8.9
110.	26.4	25.9	24.8	20.5	16.0	9.3
115.	26.9	26.0	25.2	21.3	16.5	9.8
120.	27.5	26.1	25.5	22.0	17.0	10.2
125.	28.3	26.2	25.7	22.7	17.5	10.7

4 Plasma Thermodynamic Parameters at a Given Temperature

4.1 Pressure

After having set the populations of the ions as above, we can now calculate some important thermodynamic characteristics of the plasma. The most straightforward is a formula for the pressure. In neglecting the plasma non-ideality, the pressure is a simple total of the ion contribution, N_aT , and the

electron one: ZN_aT :

$$P = (1 + Z)N_aT. \quad (25)$$

With the above procedure for finding Z as a function of T , N_a the pressure can be easily found.

4.2 Internal Energy

Another important characteristic is the average internal energy per atomic cell (U) – the energy of the total combination of particles that originally comprised a whole neutral atom. In fact, experimentally, this energy, which fundamentally depends on T , is usually much easier to find than the temperature itself, and hence the value of T actually has to be calculated from this energy. This calculation will be further discussed in section 5. First, our goal is to find U as a function of T for plasma. Recall that for an ideal gas, the average internal kinetic energy per particle is given by:

$$U = \frac{3}{2}k_B T. \quad (26)$$

Hence, to find the internal energy of a whole atomic cell in a plasma, we have to find the sum of the kinetic energies of the ion and all the electrons that have separated from it, as well as the energy that was used to separate these electrons (E_i). Then, averaging this out across the various charge ions that are present in the plasma, we get:

$$U = \frac{3}{2}k_B T + \sum_{i=1}^X P_i \left(\frac{3}{2}ik_B T + E_i \right) = \frac{3}{2}k_B T(1 + Z) + \langle E_i \rangle. \quad (27)$$

Note that this also implies that in plasma, ions have the same average kinetic energy as electrons do, despite the immense difference in mass. Furthermore, notice that because of the statistical averages used in this equation (Z and $\langle E_i \rangle$), which depend on the population values that in turn depend on the temperature, this equation cannot be solved for T by simple algebraic methods, and hence finding the temperature will once again require an iterative approach.

4.3 Heat Capacity

Another important thermodynamic parameter of a plasma is its heat capacity at a constant volume. This parameter is needed to study heat transmission

through the plasma and the variation of temperature and internal energy of various parts of the plasma with time. This value will also be needed for the temperature calculation in the next section. First of all, realize that if volume is constant and $dV = 0$, then the change in internal energy of a system is:

$$dU = dQ - dW = dQ - PdV = dQ, \text{ and}$$

$$\frac{dU}{dT} = \frac{dQ}{dT} = C_V, \quad (28)$$

where dQ is the heat added to the system, while dW is the work done by that system.

Hence, our goal now is to find the partial derivative of U , as given by Eq.27, with respect to T . For simplicity, from now on we will use the value of the temperature measured in electron-volts – $T_{eV} = k_B T$, where k_B is in eV/K. First, begin by taking the derivative of Eq.27 only:

$$\begin{aligned} C_V &= \frac{\partial U}{\partial T_{eV}} = \frac{3}{2} + \sum \left[P_i \left(\frac{3}{2}i \right) + \frac{\partial P_i}{\partial T_{eV}} \left(\frac{3}{2}T_{eV}i + E_i \right) \right] = \\ &= \frac{3}{2}(1 + Z) + \sum \left[\frac{\partial P_i}{\partial T_{eV}} \left(\frac{3}{2}T_{eV}i + E_i \right) \right] \end{aligned} \quad (29)$$

Now, we need to find the partial derivative of the populations w.r.t. temperature. For this we can use the expression from Eq. 6, written as:

$$P_i = \frac{p_i}{\sum p_i}, \text{ where} \quad p_i = \left(C_0 \frac{(T_{eV})^{\frac{3}{2}}}{Z} \right)^i e^{-\frac{E_i}{T_{eV}}}, \quad (30)$$

where C_0 is now independent of T_{eV} . Thus:

$$\frac{\partial P_i}{\partial T_{eV}} = \frac{p'_i}{\sum p_i} - \frac{p_i \sum p'_i}{(\sum p_i)^2}, \quad (31)$$

where primes denote the derivatives with respect to T_{eV} . Also, recall that Z is also a function of T , hence for p'_i we have:

$$\begin{aligned} p'_i &= \left(C_0 \frac{(T_{eV})^{\frac{3}{2}}}{Z} \right)^i e^{-\frac{E_i}{T_{eV}}} \left(\frac{E_i}{(T_{eV})^2} \right) + \left(C_0 \right)^i i \left(\frac{(T_{eV})^{\frac{3}{2}}}{Z} \right)^{i-1} \left(\frac{\frac{3}{2}(T_{eV})^{\frac{1}{2}}}{Z} - \frac{(T_{eV})^{\frac{3}{2}}}{Z^2} Z' \right) e^{-\frac{E_i}{T_{eV}}} = \\ &= p_i \left(\frac{E_i}{(T_{eV})^2} + i \frac{Z}{(T_{eV})^{\frac{3}{2}}} \left(\frac{\frac{3}{2}(T_{eV})^{\frac{1}{2}}}{Z} - \frac{(T_{eV})^{\frac{3}{2}}}{Z^2} Z' \right) \right) = p_i \left(\frac{E_i}{(T_{eV})^2} + i \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) \right) \end{aligned} \quad (32)$$

Also, since

$$Z = \frac{\sum ip_i}{\sum p_i}, \text{ it follows that } Z' = \frac{\sum ip'_i}{\sum p_i} - \frac{\sum ip_i \sum p'_i}{(\sum p_i)^2}, \quad (33)$$

where we can then plug in the expression found for p'_i in Eq.32. Let's first simplify $\sum p'_i$:

$$\sum p'_i = \sum \left[\frac{E_i p_i}{(T_{eV})^2} + ip_i \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) \right] = \frac{\sum E_i p_i}{(T_{eV})^2} + \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) \sum ip_i. \quad (34)$$

Further note that for any expression a it is true that its statistical average is $\langle a \rangle = \sum_{i=0}^X a P_i = \frac{\sum a p_i}{\sum p_i}$. Hence, using these formulas in Eq.33 we get:

$$\begin{aligned} Z' &= \frac{1}{(T_{eV})^2} \frac{\sum i E_i p_i}{\sum p_i} + \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) \frac{\sum i^2 p_i}{\sum p_i} - \frac{1}{(T_{eV})^2} \frac{\sum ip_i \sum E_i p_i}{(\sum p_i)^2} - \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) \frac{(\sum ip_i)^2}{(\sum p_i)^2} \\ &= \frac{\langle i E_i \rangle - \langle i \rangle \langle E_i \rangle}{(T_{eV})^2} + \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) (\langle i^2 \rangle - \langle i \rangle^2) \\ \frac{Z'}{Z} &= \frac{\frac{3}{2} T_{eV} (\langle i^2 \rangle - \langle i \rangle^2) + \langle i E_i \rangle - \langle i \rangle \langle E_i \rangle}{(T_{eV})^2 (Z + \langle i^2 \rangle - \langle i \rangle^2)} \end{aligned} \quad (35)$$

Finally, we have reached the bottom of this derivation – everything in the above equation can be found using the methods presented in Part I. Now, we can significantly simplify this whole derivative by working our way up to the beginning. However first, we need to introduce the following transformation, which is true for any two expressions a and b :

$$\langle ab \rangle - \langle a \rangle \langle b \rangle = \langle \delta a \delta b \rangle, \text{ where } \delta a = a - \langle a \rangle \quad (36)$$

$$\begin{aligned} \text{proof: } & \langle (a - \langle a \rangle) (b - \langle b \rangle) \rangle = \langle ab - a \langle b \rangle - b \langle a \rangle + \langle a \rangle \langle b \rangle \rangle = \\ & = \langle ab \rangle - 2 \langle a \rangle \langle b \rangle + \langle a \rangle \langle b \rangle = \langle ab \rangle - \langle a \rangle \langle b \rangle \end{aligned}$$

This transformation makes the computation simpler, as well as, in some cases, gives better accuracy for the value of $\langle \delta a \delta b \rangle$, which can determine the difference between a zero and a non-zero value. Also notice that this transformation can be used in the denominator of Eq. 20. Further, applying

this transformation and combining Eq.35 and Eq.32 we get:

$$\begin{aligned} p'_i &= p_i \left(\frac{E_i}{(T_{eV})^2} + i \frac{\frac{3}{2}T_{eV}(Z + \langle (\delta i)^2 \rangle) - \frac{3}{2}T_{eV}\langle (\delta i)^2 \rangle - \langle \delta i \delta E_i \rangle}{(T_{eV})^2(Z + \langle (\delta i)^2 \rangle)} \right) = \\ &= \frac{p_i}{(T_{eV})^2} \left(E_i + i \frac{\frac{3}{2}T_{eV}Z - \langle \delta i \delta E_i \rangle}{Z + \langle (\delta i)^2 \rangle} \right), \text{ and let this } = \alpha p_i \end{aligned} \quad (37)$$

Here α is introduced only to simplify the notation for the next step, which then transforms Eq.31 as:

$$\begin{aligned} \frac{\partial P_i}{\partial T_{eV}} &= \frac{\alpha p_i}{\sum p_i} - \frac{p_i \sum \alpha p_i}{(\sum p_i)^2} = P_i(\alpha - \langle \alpha \rangle) = P_i(\delta \alpha) = \\ &= \frac{P_i}{(T_{eV})^2} \left(\delta E_i + \delta i \left(\frac{\frac{3}{2}T_{eV}Z - \langle \delta i \delta E_i \rangle}{Z + \langle (\delta i)^2 \rangle} \right) \right), \text{ and let this } = \frac{P_i}{(T_{eV})^2} (\delta E_i + \beta \delta i) \end{aligned} \quad (38)$$

Here, again, we introduce β only for simplicity of notation. At this point, we can finally come back to our original Eq.29. First, however, note that the transformation given in Eq.36 can also be written as:

$$\langle \delta a \ b \rangle = \langle ab - a \rangle b = \langle ab \rangle - \langle a \rangle \langle b \rangle = \langle \delta a \ \delta b \rangle, \quad (39)$$

Using this and Eq.38 we can now transform Eq.29 as follows:

$$\begin{aligned} C_V &= \frac{\partial U}{\partial T_{eV}} = \frac{3}{2}(1+Z) + \sum \left[\frac{P_i}{(T_{eV})^2} (\delta E_i + \beta \delta i) \left(\frac{3}{2}T_{eV}i + E_i \right) \right] = \\ &= \frac{3}{2}(1+Z) + \frac{1}{(T_{eV})^2} \langle (\delta E_i + \beta \delta i) \left(\frac{3}{2}T_{eV}\delta i + \delta E_i \right) \rangle = \\ &= \frac{3}{2}(1+Z) + \frac{1}{(T_{eV})^2} \langle (\delta E_i)^2 + \left(\frac{3}{2}T_{eV} + \beta \right) \delta i \delta E_i + \frac{3}{2}T_{eV}\beta(\delta i)^2 \rangle = \\ &= \frac{3}{2}(1+Z) + \frac{1}{(T_{eV})^2} \left(\langle (\delta E_i)^2 \rangle + \left(\frac{\frac{3}{2}T_{eV}(Z + \langle (\delta i)^2 \rangle) + \frac{3}{2}T_{eV}Z - \langle \delta i \delta E_i \rangle}{Z + \langle (\delta i)^2 \rangle} \right) \langle \delta i \delta E_i \rangle \right) = \\ &+ \frac{3}{2}T_{eV} \frac{\frac{3}{2}T_{eV}Z - \langle \delta i \delta E_i \rangle}{Z + \langle (\delta i)^2 \rangle} \langle (\delta i)^2 \rangle = \\ &= \frac{3}{2}(1+Z) + \frac{1}{(T_{eV})^2} \left(\langle (\delta E_i)^2 \rangle + \frac{3T_{eV}Z \langle \delta i \delta E_i \rangle - \langle \delta i \delta E_i \rangle^2 + \frac{9}{4}(T_{eV})^2Z \langle (\delta i)^2 \rangle}{Z + \langle (\delta i)^2 \rangle} \right) = \\ &= \frac{3}{2}(1+Z) + \langle \left(\frac{\delta E_i}{T_{eV}} \right)^2 \rangle + \frac{3Z \left(\frac{3}{4} \langle (\delta i)^2 \rangle + \langle \delta i \frac{\delta E_i}{T_{eV}} \rangle \right) - \langle \delta i \frac{\delta E_i}{T_{eV}} \rangle^2}{Z + \langle (\delta i)^2 \rangle} = C_V. \end{aligned}$$

This equation can then be used to find the heat capacity at constant volume when the temperature is known. Following is a table built using this equation, as well as Eq. 27, that shows the values of average internal energy [eV] and heat capacity per atomic cell, calculated at various values of T_{eV} and N_a .

Na[1/cm ³]	10 ¹⁸	10 ¹⁹	10 ²⁰	10 ²¹	U
Te[eV]	$U_{av} C_v$	$U_{av} C_v$	$U_{av} C_v$	$U_{av} C_v$	U
5.	117.5 — 45.3	90.3 — 23.7	63.7 — 22.7	37.5 — 14.5	20.1
10.	416.7 — 66.6	298.9 — 52.5	207.4 — 37.8	128.4 — 22.0	71.0
15.	612.8 — 56.0	540.3 — 29.5	423.3 — 47.4	267.6 — 32.1	146.9
20.	1112.9 — 132.1	762.1 — 70.4	607.9 — 31.1	446.0 — 37.4	247.8
25.	1931.1 — 171.2	1248.7 — 119.5	814.4 — 56.3	617.6 — 31.2	373.7
30.	2735.6 — 164.4	1954.7 — 149.0	1183.9 — 90.2	779.0 — 35.8	516.4
35.	3629.0 — 190.3	2662.4 — 139.9	1711.9 — 119.5	996.5 — 52.2	662.0
40.	4500.1 — 140.6	3402.6 — 157.4	2329.3 — 121.8	1306.2 — 71.6	808.3
45.	5091.1 — 115.7	4207.2 — 155.2	2932.9 — 121.6	1711.8 — 89.8	964.7
50.	5846.8 — 197.5	4880.7 — 114.0	3568.9 — 132.5	2193.0 — 100.3	1148.3
55.	7040.3 — 265.5	5426.5 — 113.5	4247.5 — 134.4	2699.4 — 101.5	1371.1
60.	8381.5 — 263.1	6113.8 — 165.7	4880.2 — 115.7	3210.4 — 103.4	1640.0
65.	9634.2 — 239.0	7090.4 — 218.8	5416.2 — 101.1	3740.0 — 108.6	1956.0
70.	10803.8 — 224.5	8236.9 — 232.8	5937.1 — 110.4	4293.6 — 111.8	2314.0
75.	11776.1 — 155.5	9376.3 — 220.8	6561.8 — 141.1	4848.2 — 108.3	2702.0
80.	12376.8 — 90.4	10445.0 — 207.1	7358.3 — 175.1	5370.3 — 99.9	3107.0
85.	12749.5 — 62.0	11434.6 — 184.4	8292.5 — 194.5	5853.3 — 93.7	3524.0
90.	13033.9 — 53.6	12248.2 — 138.4	9274.4 — 195.8	6327.0 — 96.2	3952.0
95.	13303.8 — 55.3	12827.5 — 95.8	10236.4 — 188.0	6834.6 — 107.2	4392.0
100.	13604.6 — 66.3	13238.7 — 71.0	11150.9 — 176.3	7413.3 — 124.3	4841.0
105.	13999.8 — 94.6	13561.9 — 60.0	11992.4 — 158.4	8081.0 — 142.0	5292.0
110.	14599.0 — 150.0	13855.4 — 57.5	12720.7 — 131.9	8828.1 — 155.5	5740.0
115.	15542.8 — 229.0	14149.8 — 61.3	13312.0 — 104.9	9625.1 — 162.0	6177.0
120.	16876.5 — 295.3	14478.6 — 71.4	13782.6 — 84.0	10438.4 — 162.0	6606.0
125.	18426.4 — 315.7	14893.9 — 93.2	14167.1 — 70.9	11239.2 — 157.6	7033.0

5 Temperature Calculation from a Given Internal Energy

For all of the above calculations, it was assumed that the temperature of the plasma was a given input parameter for the problem. However, in realistic experiments, it is usually not possible, or not easy, to measure the temperature directly. It is, however, possible to measure the total internal energy of a volume of plasma, which can then, using a known heavy particle density value, be converted to the average internal energy per atomic cell (U). This energy can then be used to find the value of the temperature, however, as can be seen from Eq. 27, this cannot be done algebraically and hence, we will once again use the Newton-Rapson iterations method. As before, since this approach can only be used to iteratively find the zeros of a function, this function needs to be

$$f(T) = \frac{3}{2}k_B T(1 + Z) + \langle E_i \rangle - U, \quad (41)$$

where U is a given constant. Then when $f(T) = 0$, we will have the desired value for T . Furthermore, to use this method, we also need to have an expression for $f'(T)$, which now becomes simply $\partial U / \partial T = C_V$. Hence, we have everything needed to proceed with the Newton's method:

$$T_{n+1} = T_n - \frac{U(T_n) - U_{given}}{C_V(T_n)}, \text{ where } U = \frac{3}{2}k_B T(1 + Z) + \langle E_i \rangle \text{ and } (42)$$

$$C_V = \frac{3}{2}(1+Z) + \left\langle \left(\frac{\delta E_i}{T_{eV}} \right)^2 \right\rangle + \frac{3Z \left(\frac{3}{4} \langle (\delta i)^2 \rangle + \langle \delta i \frac{\delta E_i}{T_{eV}} \rangle \right) - \langle \delta i \frac{\delta E_i}{T_{eV}} \rangle^2}{Z + \langle (\delta i)^2 \rangle},$$

while for any expression a , $\langle a \rangle = \sum_{i=0}^X a P_i$ and $\delta a = a - \langle a \rangle$, where the populations are found using the trial value of T and the method presented in section 3.

However, unlike with iterations on Z , here convergence is not guaranteed when starting at any value of T . Although in most cases the iterations will eventually converge, they will do so slowly and before approaching the correct value, they might make huge jumps from one side of the correct T to another, which can lead to T becoming negative at one of the iterations. Since to calculate the populations and Z , which is necessary to do for every iteration,

we need to at some point find the value of $\sqrt{T^3}$, when T becomes negative, this has no real answer and will make further iterations impossible. To make matters worse, because the relationship between U and T is so complex, there is no nice way to initially approximate the value of T so as to speed up the iterations and avoid huge jumps.

Therefore, the only way left to avoid this problem is to hard-code some limits on the iteration jumps, such as not letting the iterations jump lower than half or higher than twice the trial value of T . This way, the Newton-Rapson equation will initially only point out the general direction of the correct value of T relative to the trial value, while the iterations will only half or double the trial value until it gets close enough to the actual T . Following is a table of the temperature values [eV] calculated at the given internal energies [eV] and heavy particle densities [$1/cm^3$]. The number of iterations it took to find each temperature value is also given.

Na[1/cm ³]	10 ¹⁸	10 ¹⁹	10 ²⁰	10 ²¹	10 ²²
U[eV]	Te (Iterations)				
100.	4.6 (9)	5.4 (3)	6.6 (3)	8.6 (3)	12.1 (4)
200.	6.5 (5)	7.9 (3)	9.8 (3)	12.8 (3)	17.8 (4)
300.	8.4 (4)	10.0 (3)	12.4 (3)	16.0 (3)	22.2 (4)
400.	9.8 (6)	11.7 (4)	14.5 (3)	18.8 (3)	26.0 (3)
500.	11.8 (6)	13.8 (4)	16.8 (3)	21.5 (3)	29.4 (3)
600.	14.8 (6)	16.9 (3)	19.8 (3)	24.4 (3)	32.8 (3)
700.	16.3 (5)	19.0 (4)	22.6 (3)	27.7 (3)	36.3 (3)
800.	17.4 (5)	20.5 (4)	24.7 (4)	30.6 (3)	39.7 (3)
900.	18.3 (5)	21.7 (4)	26.4 (4)	33.0 (4)	43.0 (3)
1000.	19.1 (5)	22.7 (4)	27.8 (4)	35.1 (4)	46.0 (3)
1100.	19.9 (5)	23.7 (4)	29.0 (4)	36.9 (4)	48.8 (4)
1200.	20.6 (5)	24.6 (4)	30.2 (4)	38.5 (4)	51.3 (4)
1300.	21.3 (5)	25.4 (4)	31.2 (4)	39.9 (4)	53.5 (4)
1400.	22.0 (5)	26.2 (4)	32.2 (4)	41.3 (4)	55.6 (4)
1500.	22.6 (5)	26.9 (4)	33.2 (4)	42.5 (4)	57.5 (4)
1600.	23.1 (5)	27.6 (3)	34.0 (4)	43.7 (4)	59.3 (4)
1700.	23.7 (5)	28.3 (3)	34.9 (4)	44.9 (4)	61.0 (4)
1800.	24.3 (5)	29.0 (3)	35.7 (3)	46.0 (4)	62.6 (4)
1900.	24.8 (5)	29.6 (3)	36.5 (3)	47.0 (4)	64.2 (4)
2000.	25.4 (5)	30.3 (3)	37.3 (3)	48.1 (4)	65.6 (4)
2100.	26.0 (5)	31.0 (3)	38.1 (4)	49.1 (3)	67.1 (4)
2200.	26.6 (5)	31.7 (3)	38.9 (3)	50.1 (3)	68.4 (4)
2300.	27.3 (5)	32.4 (3)	39.8 (3)	51.1 (3)	69.8 (4)
2400.	27.9 (5)	33.1 (3)	40.6 (3)	52.1 (3)	71.1 (4)
2500.	28.5 (5)	33.8 (3)	41.4 (3)	53.0 (3)	72.4 (4)
2600.	29.2 (5)	34.6 (3)	42.2 (3)	54.0 (3)	73.7 (4)
2700.	29.8 (6)	35.3 (3)	43.1 (3)	55.0 (3)	75.0 (4)
2800.	30.4 (6)	36.0 (3)	43.9 (3)	56.0 (3)	76.2 (4)
2900.	31.0 (6)	36.7 (3)	44.7 (3)	57.0 (3)	77.5 (4)
3000.	31.6 (5)	37.4 (3)	45.5 (3)	58.0 (3)	78.7 (4)
3100.	32.1 (5)	38.0 (3)	46.4 (3)	58.9 (3)	79.9 (4)
3200.	32.7 (5)	38.7 (3)	47.1 (3)	59.9 (3)	81.1 (4)
3300.	33.2 (5)	39.3 (3)	47.9 (3)	60.9 (3)	82.3 (4)
3400.	33.8 (5)	40.0 (3)	48.7 (3)	61.8 (3)	83.5 (4)
3500.	34.3 (5)	40.6 (3)	49.5 (3)	62.8 (3)	84.7 (4)
3600.	34.8 (5)	41.2 (3)	50.2 (3)	63.7 (3)	85.9 (4)
3700.	35.4 (5)	41.20(3)	51.0 (3)	64.6 (3)	87.1 (3)
3800.	35.9 (5)	42.5 (3)	51.7 (3)	65.6 (3)	88.2 (3)
3900.	36.4 (5)	43.1 (3)	52.4 (3)	66.5 (3)	89.4 (3)
4000.	37.0 (5)	43.7 (3)	53.2 (3)	67.4 (3)	90.5 (3)

The use of non-conservative scheme may also require to find the internal energy density as a function of the given pressure:

Na[1/cm ³]	10 ¹⁸	10 ¹⁹	10 ²⁰	10 ²¹	10 ²²
P/Na[eV]	Te (Iterations)				
50.	8.1 (6)	8.8 (2)	9.8 (3)	11.5 (3)	14.1 (3)
100.	12.6 (4)	13.3 (3)	14.7 (3)	17.0 (3)	20.7 (3)
150.	16.9 (4)	18.1 (3)	19.3 (2)	21.5 (3)	26.0 (3)
200.	19.8 (4)	21.7 (3)	23.8 (3)	26.1 (2)	30.7 (3)
250.	22.2 (3)	24.5 (3)	27.4 (3)	30.5 (3)	35.1 (3)
300.	24.2 (3)	26.9 (3)	30.2 (3)	34.4 (3)	39.5 (3)
350.	26.2 (4)	29.0 (3)	32.7 (3)	37.7 (3)	43.7 (3)
400.	28.3 (4)	31.0 (3)	35.0 (3)	40.6 (3)	47.7 (3)
450.	30.2 (4)	33.0 (2)	37.1 (3)	43.1 (3)	51.3 (3)
500.	32.1 (4)	35.0 (3)	39.1 (3)	45.5 (3)	54.6 (3)
550.	33.9 (4)	36.9 (3)	41.1 (3)	47.7 (3)	57.6 (3)
600.	35.6 (4)	38.8 (3)	43.1 (3)	49.8 (3)	60.4 (3)
650.	37.2 (3)	40.5 (3)	45.0 (3)	51.8 (3)	62.9 (4)
700.	38.9 (3)	42.3 (3)	46.9 (3)	53.8 (3)	65.4 (4)
750.	40.8 (3)	44.0 (3)	48.8 (3)	55.8 (3)	67.7 (3)
800.	42.7 (3)	45.6 (2)	50.5 (3)	57.8 (3)	69.9 (3)
850.	44.7 (3)	47.4 (3)	52.3 (3)	59.7 (3)	72.1 (3)
900.	46.6 (2)	49.2 (3)	54.0 (3)	61.6 (3)	74.2 (3)
950.	48.4 (3)	51.1 (3)	55.7 (3)	63.4 (3)	76.2 (3)
1000.	50.0 (3)	53.0 (3)	57.4 (2)	65.3 (3)	78.3 (3)
1050.	51.5 (3)	54.9 (2)	59.2 (3)	67.0 (3)	80.2 (3)
1100.	52.8 (3)	56.7 (3)	60.9 (3)	68.8 (3)	82.2 (3)
1150.	54.2 (3)	58.5 (3)	62.8 (3)	70.5 (3)	84.1 (3)
1200.	55.4 (3)	60.1 (3)	64.6 (3)	72.3 (3)	86.0 (3)
1250.	56.7 (4)	61.6 (3)	66.5 (3)	74.0 (3)	87.9 (3)
1300.	57.9 (4)	63.0 (3)	68.3 (2)	75.7 (3)	89.7 (3)
1350.	59.2 (4)	64.4 (3)	70.1 (3)	77.4 (2)	91.6 (3)
1400.	60.4 (4)	65.7 (3)	71.8 (3)	79.2 (2)	93.4 (3)
1450.	61.7 (4)	67.0 (3)	73.5 (3)	80.9 (3)	95.1 (3)
1500.	62.9 (4)	68.3 (3)	75.1 (3)	82.7 (3)	96.9 (3)
1550.	64.2 (4)	69.5 (3)	76.6 (3)	84.5 (3)	98.7 (3)
1600.	65.4 (4)	70.8 (3)	78.1 (3)	86.3 (3)	100.4 (3)
1650.	66.7 (4)	72.0 (3)	79.5 (3)	88.1 (3)	102.2 (3)
1700.	68.0 (4)	73.2 (3)	80.9 (3)	89.9 (3)	103.9 (3)
1750.	69.2 (4)	74.5 (2)	82.2 (3)	91.6 (2)	105.6 (3)
1800.	70.5 (4)	75.7 (2)	83.5 (3)	93.3 (3)	107.3 (3)
1850.	71.8 (4)	77.22(2)	84.8 (3)	95.0 (3)	109.0 (3)
1900.	73.1 (4)	78.2 (2)	86.1 (3)	96.6 (3)	110.7 (3)
1950.	74.4 (4)	79.5 (2)	87.3 (3)	98.2 (3)	112.5 (3)
2000.	75.8 (4)	80.7 (2)	88.6 (3)	99.8 (3)	114.2 (3)

6 Plasma Parameters for Mixtures

6.1 The Basics

In many cases in practice, the plasma does not consist of just a single element, as was assumed for all of the above calculations, but rather of a mixture of several different elements. If such is the case, then all the main formulas that the above methods were based on now take on a slightly different form. Hence, the entire procedure for finding the ionization equilibrium and then thermodynamic plasma parameters will have to be reevaluated for this case. On the other hand, the changes will not be too drastic as the basic principles of plasma formation are still in effect.

First, let's introduce the element concentration factors C_j that give the part of the entire mixture, by number of heavy particles, that the element with index j comprises:

$$C_j = \frac{N_j}{N_a} = \frac{\sum_{i=0}^X N_{ij}}{N_a}, \text{ and hence also } \sum_{j=1}^n C_j = 1. \quad (43)$$

Here, the index i , as before, refers the i -charged ion. Furthermore, these concentration factors will be taken here as a given input parameter to the problem.

With regards to the populations, note that a population of a certain ion, by definition, still remains as the part that the ion comprises out of all the ions of only that same element, and not out of the entire N_a . Hence, we get the following formulas for the populations:

$$P_{ij} = \frac{N_{ij}}{N_j} \quad \sum_{i=0}^X P_{ij} = 1. \quad (44)$$

Combining Eq. 43 and 44 we can then obtain the expression for the part that a certain charge ion of a certain element comprises out of the entire mixture:

$$\frac{N_{ij}}{N_a} = C_j P_{ij} \quad (45)$$

Further, we can also obtain a formula for the total number of free electrons per unit of volume of plasma, which will be just the sum of the electrons coming from each element, which in turn is still calculated as in Eq. 3:

$$N_e = \sum_{j=1}^n \left[\sum_{i=1}^X i N_{ij} \right] \quad (46)$$

Then dividing both sides by N_a , we obtain the average charge per ion:

$$Z = \langle i_j \rangle = \sum_{j=1}^n \left[C_j \sum_{i=1}^X i P_{ij} \right] = \sum_{j=1}^n (C_j \langle i \rangle_j) \quad (47)$$

Notice that here, $\langle i_j \rangle$ denotes the average along two dimensions, instead of just one as was done before and as in $\langle i \rangle_j$. Hence, we can see that basically the only thing that is different about calculating the properties of a mixture plasma is that each calculation has to be performed separately for each of the elements in the mixture, and then the statistical average of the obtained values has to be taken across all of the elements present.

6.2 Ionization Equilibrium

When finding the population values for a mixture plasma, we see, from Eq. 6, or the Saha Equation (Eq. 8), that the various elements in the mixture do not interact with each other in any way other than through the free electrons, or similarly, through the value of Z. Hence, the only difference in the calculation will be in the expression that we use for Z. Hence, transforming Eq. 13 to fit the form in Eq. 47, we get:

$$Z = \sum_{j=1}^n \left[C_j \frac{\sum i p_{ij}}{\sum p_{ij}} \right], \text{ where as before } p_{ij} = \left(\frac{C_1}{Z} \right)^i e^{-\frac{E_{ij}}{k_B T_e}} \quad (48)$$

Since Z has to be found iteratively anyway, we do not need to worry about the additional complexity introduced by the double summation here. Furthermore, since C_j values are given constants, they will not affect the value of the derivative of this expression with respect to Z, which is also needed to use the Newton's method. Hence, this derivative of the above expression becomes, using Eq. 18:

$$-\frac{1}{Z} \sum_{j=1}^n C_j \left(\langle i^2 \rangle_j - \langle i \rangle_j^2 \right) = -\frac{1}{Z} \sum_{j=1}^n C_j \langle (\delta i)^2 \rangle_j. \quad (49)$$

Hence, the equation that defines the Newton's iterative method here becomes:

$$Z_{n+1} = Z_n - \frac{Z_n - \sum_j [C_j < i >_j]}{1 + \frac{1}{Z_n} \sum_j [C_j < (\delta i)^2 >_j]}. \quad (50)$$

Here, once again, for any expression a , $< a >_j = \sum_{i=0}^X a P_{ij}$, and $\delta a = a - < a >$.

This equation can then be used to find the population values and Z for a mixture plasma, while finding the populations exactly as for a single component plasma.

6.3 Thermodynamic Parameters

As with most other characteristics of a mixture plasma, to find the average internal energy per atomic cell, we need to use Eq. 27 to find this energy for each individual element, and then find the statistical average of these values across all elements. Also, note that from here on, for any expression a , $\ll a \gg = \sum_j [C_j \sum_i (P_{ij} a_{ij})]$, which is the statistical average first, across the populations and then, across the elements.

$$U = \sum_j C_j \left(\frac{3}{2} k_B T (1 + < i >_j) + < E_i >_j \right) = \frac{3}{2} k_B T (1 + Z) + \ll E_{ij} \gg. \quad (51)$$

Hence, the equation remains essentially the same, except here all averages are taken along 2 dimensions – first across the populations and then across the elements.

Now, to find the derivative $\partial U / \partial T$, which is again the heat capacity at constant volume, we will use the sum given for U in Eq. 51. Here, the summation across the elements remains outside of the expression unaffected by the differentiation. Further, the derivative of the inside expression is found in the same way as for single component plasma, except for the stage of finding Z' , since Z is now given by Eq. 48. Hence, using Eq. 35, we can obtain the expression for Z' :

$$Z' = \sum_j C_j \left[\frac{< \delta i \delta E_i >}{(T_{eV})^2} + \left(\frac{3}{2T_{eV}} - \frac{Z'}{Z} \right) (< (\delta i)^2 >) \right]$$

$$Z' + \frac{Z'}{Z} \ll (\delta i)^2 \gg = \frac{\frac{3}{2} T_{eV} \ll (\delta i)^2 \gg + \ll \delta i \delta E_i \gg}{(T_{eV})^2}$$

$$\frac{Z'}{Z} = \frac{\frac{3}{2}T_{eV} \ll (\delta i)^2 \gg + \ll \delta i \ \delta E_i \gg}{(T_{eV})^2 (Z + \ll (\delta i)^2 \gg)}. \quad (52)$$

This expression is the same as the one obtained for single component plasma, except now all the averages are separately taken along both dimensions. Now, if we follow this expression through the subsequent steps of the derivation of the heat capacity expression for a single component plasma, presented earlier, then we notice that it translates into the expression for β introduced later on in the derivation. Hence, since the above expression is independent of the element (j), β also becomes independent of j . Therefore, using the derivation for C_V from Eq. 40 and recalling the outside summation from Eq. 51, we obtain:

$$\begin{aligned} C_V &= \sum_j C_j \left[\frac{3}{2}(1 + \langle i \rangle_j) + \frac{1}{(T_{eV})^2} \left(\langle (\delta E_i)^2 \rangle_j + \left(\frac{3}{2}T_{eV} + \beta \right) \langle \delta i \ \delta E_i \rangle_j + \frac{3}{2}T_{eV}\beta \langle (\delta i)^2 \rangle_j \right) \right. \\ &= \frac{3}{2}(1 + Z) + \frac{1}{(T_{eV})^2} \left(\ll (\delta E_i)^2 \gg + \left(\frac{3}{2}T_{eV} + \beta \right) \ll \delta i \ \delta E_i \gg + \frac{3}{2}T_{eV}\beta \ll (\delta i)^2 \gg \right). \end{aligned}$$

This equation is again exactly the same as the one obtained in the derivation for single component plasma, except that all the averages are now separately taken across the elements as well. Therefore, we can conclude that the final expression for the heat capacity here will also be the same as for single element plasma except for the averaging domain. Hence, for a mixture plasma, the heat capacity is given by:

$$C_V = \frac{3}{2}(1 + Z) + \ll \left(\frac{\delta E_i}{T_{eV}} \right)^2 \gg + \frac{3Z \left(\frac{3}{4} \ll (\delta i)^2 \gg + \ll \delta i \ \frac{\delta E_i}{T_{eV}} \gg \right) - \ll \delta i \ \frac{\delta E_i}{T_{eV}} \gg^2}{Z + \ll (\delta i)^2 \gg}, \quad (54)$$

where for any expressions a and b , $\ll \delta a \ \delta b \gg = \sum_j [C_j \sum_i (P_{ij}(a_{ij} - \langle a_i \rangle_j)(b_{ij} - \langle b_i \rangle_j))]$.

Finally, same way as before, we can use these two equations for U and C_V to iteratively find the temperature from a given average internal energy using the Newton-Rapson iterations (first part of Eq. 42).

The results of the thermodynamic calculations for polyimide $C_{22}H_{10}N_2O_5$ is provided in the following table:

Na[1/cm ³]	10 ¹⁸	10 ¹⁹	10 ²⁰	10 ²¹	10 ²²
Te[eV]	$U_{av} C_v$				
5.	80.7 — 55.8	58.1 — 28.2	44.3 — 15.2	30.5 — 10.2	18.7 — 6.1
10.	192.9 — 70.2	175.5 — 52.4	140.8 — 39.7	92.1 — 21.1	56.2 — 9.6
15.	256.3 — 74.0	244.9 — 61.0	219.4 — 39.5	178.1 — 27.6	110.7 — 15.0
20.	292.2 — 51.4	290.8 — 50.5	280.3 — 43.9	245.5 — 28.5	178.0 — 18.2
25.	334.1 — 43.1	326.9 — 39.5	323.3 — 37.9	303.2 — 30.8	242.4 — 19.3
30.	452.3 — 59.5	374.0 — 36.9	360.8 — 32.3	350.2 — 29.5	300.8 — 20.3
35.	658.0 — 83.8	477.5 — 47.2	405.4 — 30.6	390.6 — 27.0	354.3 — 21.2
40.	876.4 — 104.8	646.0 — 62.5	478.2 — 34.5	431.5 — 25.4	402.6 — 21.3
45.	1025.2 — 98.4	836.9 — 77.9	594.4 — 42.5	480.7 — 25.5	446.2 — 20.8
50.	1126.7 — 89.1	1000.9 — 80.3	743.7 — 52.0	547.9 — 27.8	489.1 — 20.5
55.	1226.8 — 82.0	1118.4 — 75.3	903.1 — 59.2	637.4 — 31.7	534.3 — 20.4
60.	1331.7 — 78.8	1215.9 — 70.3	1046.0 — 60.9	748.5 — 36.5	585.4 — 21.0
65.	1433.5 — 79.4	1310.3 — 66.4	1162.5 — 59.2	874.2 — 41.0	644.4 — 22.0
70.	1518.3 — 78.5	1406.7 — 64.6	1261.5 — 56.7	1002.7 — 44.0	713.1 — 23.6
75.	1584.0 — 74.8	1501.0 — 64.5	1352.5 — 54.4	1123.8 — 45.1	792.5 — 25.6
80.	1638.2 — 70.3	1585.5 — 64.2	1441.9 — 52.8	1232.9 — 44.9	881.6 — 27.7
85.	1687.2 — 65.8	1656.4 — 62.5	1530.3 — 52.0	1330.9 — 44.1	978.1 — 29.6
90.	1734.2 — 61.8	1716.4 — 60.1	1616.3 — 51.8	1421.3 — 43.2	1078.5 — 31.2
95.	1780.3 — 58.2	1769.7 — 57.3	1696.2 — 51.5	1507.2 — 42.3	1179.3 — 32.2
100.	1826.0 — 55.1	1819.7 — 54.6	1767.8 — 50.7	1590.5 — 41.7	1277.9 — 32.8
105.	1871.4 — 52.3	1867.7 — 52.0	1831.6 — 49.5	1672.2 — 41.3	1372.7 — 33.1
110.	1916.8 — 49.9	1914.3 — 49.7	1889.3 — 48.1	1751.9 — 41.1	1463.1 — 33.1
115.	1962.0 — 47.7	1960.4 — 47.6	1942.8 — 46.5	1828.6 — 40.9	1550.0 — 32.9
120.	2007.4 — 45.7	2006.1 — 45.7	1993.6 — 45.0	1901.3 — 40.6	1632.9 — 32.8
125.	2052.6 — 44.0	2051.7 — 43.9	2042.5 — 43.5	1968.8 — 40.1	1713.2 — 32.6

7 Conclusion

In this work, a method was presented for calculating such parameters of the plasma as its temperature (T), pressure (P), average ionization state (Z), and populations of various level ions (P_i) from a given average internal energy per atomic unit in that plasma. This method was also somewhat optimized for faster performance in a computer program, since such calculation may need to be performed millions of times within a cell-based plasma modeling

program, which this calculation was meant for.

This file is closed in June, 2009, because the approach of the Boltzmann electron gas does not meet the practical requirements. The CRASH code moved towards an account of the Fermi statistics for electrons, the Coulomb interactions as well as the detailed analysis of the excited level populations. The further progress is described in HEDP.pdf document.