

# Numerical study of radiatively cooling partially ionized plasma expansion in neutral environment

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**Abstract.** Plasma physics is a vast area of physics, which includes both fundamental aspects, such as, for example, astrophysics, and more applied ones: new compact plasma accelerators, compact powerful sources of X-ray and gamma radiation, new promising, practically inexhaustible sources of clean energy due to controlled thermonuclear fusion, compact ion sources for cancer therapy and isotope sources for nuclear medicine. Currently, studies of non-stationary and non-equilibrium processes in pulsed plasma created under the influence of high-intensity energy flows on matter are topical. Energy flows of multiterawatt and petawatt power levels are created, for example, in laboratory conditions, by electric pulse generators, as well as by short-pulse laser installations. This paper presents a hydrodynamic model that considers ions and neutrals as separate fluids that interact with each other through collisional processes. In this case, the evolution of ions is determined by the system of magnetic hydrodynamics, and of neutrals – by ordinary, non-magnetic hydrodynamics. Such an approximation makes it possible to carry out simulations and study effects in a partially ionized plasma [1, 2]. The code MARPLE3D (Keldysh Institute of Applied Mathematics, Russian Academy of Sciences), developed for solving problems of magnetic radiation gas dynamics on high-performance cluster-type computing systems, was used for simulation [3].

**Keywords:** partially ionized plasma, instabilities, neutral, radiatively cooling, supernova remnant.

## 1. Partially ionized plasma model

Let us describe the model of partially ionized plasma, on the basis of which the calculations are carried out below. Since the physical effects for ions and neutrals are different, the system of equations is divided into 2 parts. For the ionic component (denoted by index  $\alpha$ ):

$$\rho_\alpha = m_\alpha n_\alpha, \quad (1)$$

$$\partial_t \rho_\alpha + \partial_i (\rho_\alpha v_{\alpha,i}) = 0, \quad (2)$$

$$\partial_t (\rho_\alpha v_{\alpha,i}) + \partial_j \left( \rho_\alpha v_{\alpha,i} v_{\alpha,j} + \delta_{ij} \left( p_\alpha + \frac{B^2}{2} \right) - B_i B_j \right) = R_{\alpha\beta,i}, \quad (3)$$

$$\partial_t E_\alpha + \partial_i \left( v_{\alpha,i} \left[ E_\alpha + p + \frac{B^2}{2} \right] - (\mathbf{v}\mathbf{B}) B_i \right) = Q_{\alpha\beta} - Q_{cool} + Q_{heat}, \quad (4)$$

$$\partial_t B + \partial_i (\mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v}) = 0 \quad (5)$$

$$E_\alpha = \rho_\alpha e_\alpha + \frac{\rho_\alpha \mathbf{v}_\alpha^2}{2} + \frac{B^2}{2}.$$

where  $E_\alpha$  is the total energy,  $\rho_\alpha$  is the density,  $\mathbf{v}$  is the velocity,  $p$  is the pressure,  $e$  is the internal energy,  $\mathbf{B}$  is the magnetic field normalized to  $(4\pi)^{1/2}$ ,  $Q_{\alpha\beta}$  is the collisional energy exchange between ions and neutrals,  $Q_{cool}$  is the rate of energy loss by cooling,  $Q_{heat}$  is the heating of the medium,  $R_{\alpha\beta}$  is the force of friction between the fluids (collisional).

For the neutral component (denoted by index  $\beta$ ):

$$\rho_\beta = m_\beta n_\beta, \quad (6)$$

$$\partial_t \rho_\beta + \partial_i (\rho_\beta v_{\beta,i}) = 0, \quad (7)$$

$$\partial_t (\rho_\beta v_{\beta,i}) + \partial_j (\rho_\beta v_{\beta,i} v_{\beta,j} + \delta_{ij} p_\beta) = R_{\alpha\beta,i}, \quad (8)$$

$$\partial_t E_\beta + \partial_i (v_{\beta,i} [E_\beta + p]) = Q_{\alpha\beta} \quad (9)$$

$$E_\beta = \rho_\beta e_\beta + \frac{\rho_\beta \mathbf{v}_\beta^2}{2}.$$

The hydrodynamic equations are closed by the equations of state:

$$p_\alpha = A_\alpha^{(-1)} \rho_\alpha R_g T_\alpha, p_\beta = A_\beta^{(-1)} \rho_\beta R_g T_\beta$$

where  $R_g$  is the gas constant,  $A_\alpha$ ,  $A_\beta$  are the mean molecular weights of the ion and neutral components. The molecular weight of the ion component takes into account the contribution of electrons and is consistent with the chemical composition used in the calculation of the cooling function, neutrals are considered as pure hydrogen.

The transfer of energy and momentum between the components of the medium occurs due to collisional processes. To calculate the characteristic collision time  $\tau_{\alpha\beta}$ , we take a constant interaction cross section  $\sigma \sim 5 \cdot 10^{-15} \text{ cm}^2$  [4, 5]:

$$\tau_{\alpha\beta} = \frac{1}{n_0 \sigma_s (kT_\alpha / m_\alpha)^{1/2}},$$

then the friction force can be written as:

$$R_{\alpha\beta} = -\frac{m_\alpha n_\alpha}{\tau_{\alpha\beta}} (\mathbf{v}_\alpha - \mathbf{v}_\beta).$$

The transfer of energy in this case:

$$Q_\alpha = -\sum_\beta 3 \frac{m_\alpha}{m_\alpha + m_\beta} \frac{n_\alpha}{\tau_{\alpha\beta}} k_B (T_\alpha - T_\beta) - \sum_\beta \frac{m_\beta}{m_\alpha + m_\beta} (\mathbf{v}_\alpha - \mathbf{v}_\beta) \mathbf{R}_\alpha.$$

It also takes into account the heating due to the friction force  $R$ , which is necessary to maintain the energy balance.

The rates of energy loss by the ion component and the heating are written as

$$Q_{cool} = \Lambda(T) n_e n_H, \quad Q_{heat} = \Lambda(T_0) n_{e0} n_{H0},$$

where  $n_H$  is the hydrogen number density. The heating is constant and compensates the losses for the background parameters of the environment:  $T_0$  is the temperature of the environment and  $n_{H0}$  is the hydrogen number density in it, which allows the bow shock to propagate through an invariable medium.

In this paper, we consider a model that takes into account the effect of neutrals. They are added to the system as a second fluid that interacts with the ion component through collisions. The ionization and recombination processes are also taken into account. We use the coronal, which corresponds to the limiting case of low density. Such a situation occurs, for example, in the plasma of the solar corona.

The ionization equilibrium in this case is calculated by the formula:

$$\frac{N^{(z+1)}}{N^{(z)}} = \frac{\langle v\sigma_i \rangle}{\chi_v + \chi_d}$$

where  $N^{(z+1)}$ ,  $N^{(z)}$  is the density of  $X_z$  and  $X_{(z+1)}$  ions with atomic effective charge  $z$ ,  $\langle v\sigma_i \rangle$  is the excitation velocity,  $\chi_v$ ,  $\chi_d$  are the velocities of the radiative and dielectronic recombination.

To describe the radiation losses  $Q_{cool}$ , we use the cooling function  $\Lambda(T)$ , which describes the volume losses for the solar chemical composition [6] – see Fig.1. When calculating this function, the addition of a small fraction of heavier elements to hydrogen and helium, their ionization state and the corresponding transitions are taken into account. Thus, the ionization and recombination processes are also taken into account in the cooling.

## 2. Cooling function

Volumetric energy losses due to irradiation processes can be simply treated as a sink term in the energy equation:

$$\partial_t(\rho e) + \partial_i(\rho v_i e) + p \partial_i v_i = -\Lambda(T) n_e n_H, \quad (10)$$

where  $e$  is a specific internal energy per unit mass,  $n_e$  and  $n_H$  are number densities of electrons and hydrogen, respectively,  $\Lambda(T)$  is a cooling function (CF) usually normalized by  $n_e n_H$ . But, if we use cooling function with assumption of CIE, electron concentration  $n_e$  could be included into  $\Lambda$ . So, for hydrodynamic simulations we can use cooling function normalized by  $n_H^2$  or even  $\rho^2$ , since hydrogen fraction is constant

$$\Lambda_H(T) = \frac{\Lambda(T) n_e}{n_H}, \quad \Lambda_\rho(T) = \Lambda(T) n_e \left( \frac{n_H}{\rho} \right).$$

For equation (10) the implicit scheme was implemented, which is described in [7]. It increases robustness of the scheme and eliminates ambiguity of the solution. In simulation we can use a tabulated CF like in [6], which corresponds to equilibrium plasma with solar metallicity, or calculate our own CF using data for radiative processes.

### 1.1. Calculation of cooling function

As we need cooling function for certain ion composition, we can't use well-known tabulated cooling functions for solar abundances, so we calculate our own CF using data for several radiative processes. To obtain CF for some chemical element composition, at first, we find ion and electron concentrations in ionization equilibrium for the range of temperatures. The coronal approximation is used to determine ionization equilibrium as in hydrodynamical simulation for consistency. Obtained ion and electron concentrations then used to calculate cooling rate due to several radiative processes which include:

- Bremsstrahlung

Total emissivity due to Coulomb scattering of electrons by a mixture of ions in a plasma of electron temperature  $T$  is given by

$$\frac{dE_{ff}}{dt dV} = C_{ff} \sqrt{T} N_e \sum_{Z,z} N_{Z,z} z^2 g_{ff}(T) \text{ [erg} \cdot \text{cm}^{-3} \cdot \text{s}^{-1}], \quad C_{ff} = 1,426 \cdot 10^{-27} \text{ [cm}^5 \cdot \text{s}^{-3} \cdot \text{K}^{-1/2} \cdot \text{g}],$$

where  $N_e$  is the electron density,  $N_{Z,z}$  the density of ions with atomic number  $Z$  and effective charge  $z$ , which is defined by

$$z = n_0 \left( I_{Z,z-1,n_0} / I_H \right)^{1/2},$$

$I_H$  is hydrogen ionization energy,  $I_{Z,z-1,n_0}$  is the ionization energy from ground state with principle quantum number  $n_0$  in the previous ion,  $g_{ff}(T)$  is the free-free gaunt factor (in code we use values from [8]).

- Radiative recombination

Total energy emitted per unit volume and time interval by the captures of electrons in the bound states  $n$  is given by [9]

$$\frac{dE_{fb}}{dtdV} = \frac{C_{ff}}{k\sqrt{T}} N_e \sum_{Z,z,n} g_{fb} N_{Z,z,n} \left( \frac{\zeta_{Z,z,n}}{n} \right) \frac{I_{Z,z-1,n}^2}{I_H} [\text{erg}\cdot\text{cm}^{-3}\cdot\text{s}^{-1}],$$

where  $\zeta_{Z,z,n}$  is the number of free positions in the  $n$ -th shell to be occupied by the captured electron. The free-bound gaunt factor  $g_{fb}$  can be taken as 1.

- Spectral lines emission

This category refers to bound-bound electron transitions with emission of one photon. Emissivity from transitions from level  $k$  to  $j$  with energy  $E_{kj} = E_k - E_j$  is given by

$$\frac{dE_{kj}^i}{dtdV} = N_e N_i E_{kj} \frac{8.629 \cdot 10^{-6}}{T_e^{1/2}} \exp(-E_{kj} / kT_e) \Omega_{kj}^{eff}.$$

Approximation for  $\Omega_{kj}^{eff}$  can have an exponential form or fit simple power law, see [10]. We take into account about several hundred main lines for most abundant elements.

- Two-photon processes

Last type of processes we take into account is electron transitions in H-like and He-like ions with emission of two photons. Emissivity from two-photon processes given by [9]

$$\frac{dE_{2\gamma}}{dtdV} = \frac{C_{2\gamma}}{\sqrt{T}} N_e \sum_{Z,z} N_{Z,z} f_{Z,z} \bar{g}_{Z,z} \exp\left(\frac{-e_{Z,z}}{kT}\right) [\text{erg}\cdot\text{cm}^{-3}\cdot\text{s}^{-1}].$$

where  $e_{Z,z}$  is the energy of 1s-2s transition,  $f_{Z,z}$  is the absorption oscillator strength,  $\bar{g}_{Z,z}$  is the Gaunt factor.

All formulas for emissivities above applicable for a very low density only (the coronal approximation). Finally, total cooling function given by sum over all ions and processes

$$\Lambda(T) = \sum_i \Lambda_{ff,i}(T) + \Lambda_{fb,i}(T) + \Lambda_{2\gamma,i}(T) + \Lambda_{lines,i}(T),$$

where  $\Lambda_{*,i}$  are energy loss rates by one of the mentioned processes normalized by  $n_e n_i$ .

### 1.2. Example of cooling function

For a demonstration that our code correctly calculates cooling functions we obtained common CF for solar abundances to compare with results from other works, see Fig.1. Resulting cooling curve is in a rather good agreement with previous results

## 3. Dynamic of a supernova remnant

Let us consider the application of this model for calculating the dynamics of a supernova remnant. In the calculation, ions are given using the equation:  $p_i = (Z+1)n_i kT_i$ .

The average charge number  $Z = 1.0732$  and the average atomic mass  $A = 1.2189$ , calculated according to the table from [6]. Neutrals are hydrogen. The system of equations is supplemented by the equation:  $p_n = n_n k T_n$ .

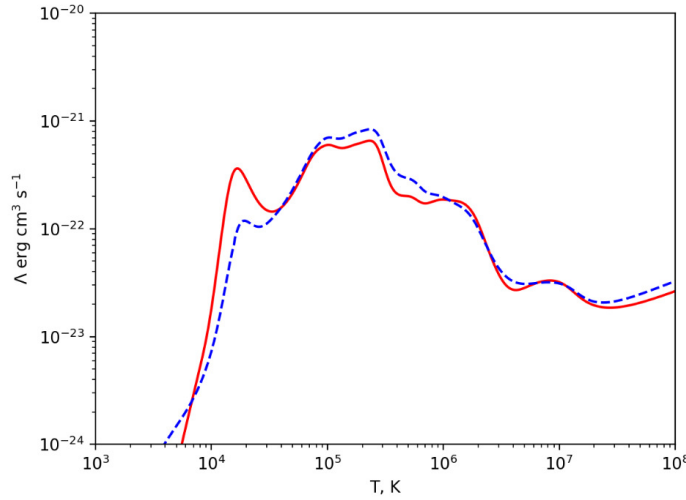


Fig.1. Cooling function for solar abundances obtained with our code (solid line) and CF from work [6] (dashed line).

At the initial moment, the medium is filled with homogeneous ionic and neutral components. The release of energy from the ionic component  $E_i = 1.28 \cdot 10^{51}$  erg occurs instantly in the center of the region  $R = 4pc$ . The ambient temperature outside the region of energy release for ions and in the entire region for neutrals  $T_i = T_n = 8000$  K. Comparisons were made with the neutral component and taking into account ionization-recombination processes, and calculations with only the ionic component.

The calculations were carried out on a grid of  $100 \times 100$  cells.

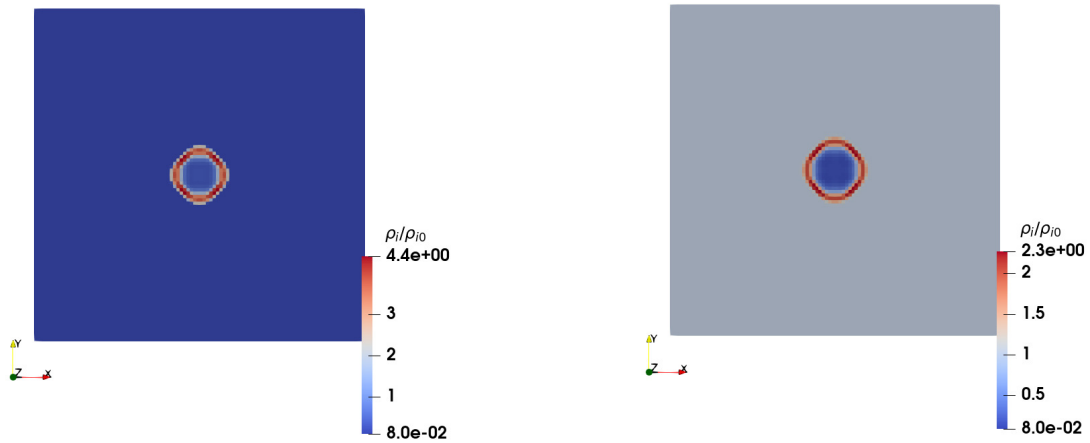


Fig.2. Normalized to the initial ionic density with ionization-recombination processes (left) and without (right) at the moment of time  $t = 10000$  years.

Due to the inclusion of the ionization and recombination processes, the total mass of the system is redistributed between ions and neutrals, as a result of which additional mass enters the ions (Fig.2).

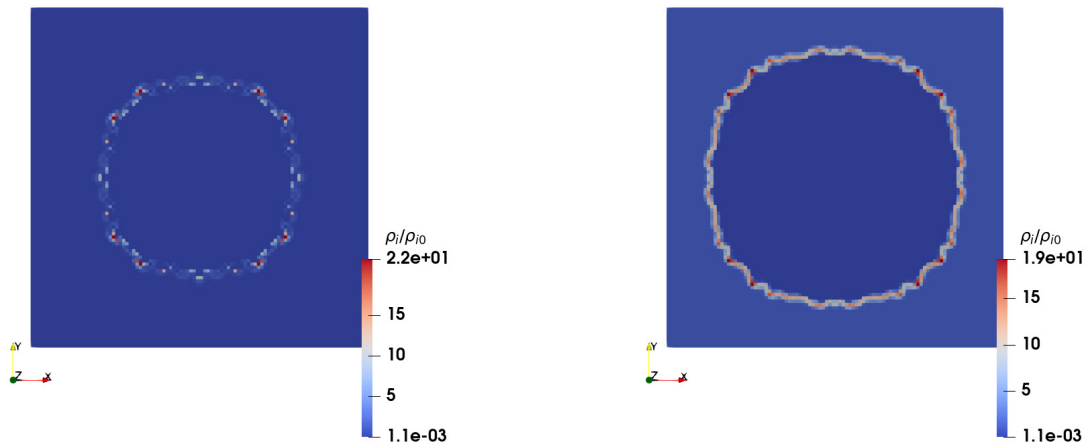


Fig.3. Normalized to the initial ionic density with ionization-recombination processes (left) and without (right) at the moment of time  $t = 350000$  years.

It was found that taking into account the ionization and recombination processes is not an obstacle to the emergence of instability. However, in current calculations, taking into account the ionization and recombination processes leads to the formation of a less continuous layer of ions with density perturbations on the surface of the layer itself and with a non-uniform density distribution over the azimuthal angle, which will affect the processes of particle acceleration and the glow of this layer (Fig.3).

#### 4. Conclusion

In this paper, we present a model of a partially ionized plasma, in which the ionic component is described by the MHD equations, the neutral component is described by nonmagnetic hydrodynamics, and the processes of ionization and recombination are taken into account using the coronal limit model. In this case, the components interact with each other through collisional processes.

As an example of the application of the model, the dynamics of the expansion of a supernova remnant into the environment is considered. The effect of taking into account the ionization and recombination processes on the formation and stability of a dense layer formed in this system was studied. Calculations show that taking into account the ionization and recombination processes affects the structure of the dense layer and the rate of its propagation.

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