

Boundary conditions for the multi-ion magnetized plasma-wall transition

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Abstract

Properties of the multi-ion magnetized plasma-wall transition (PWT) are investigated. The corresponding boundary conditions are derived for the case when different ions species have similar gyro-radii.

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1. Introduction

Particle and heat fluxes to the wall are strongly influenced by plasma conditions in the so-called ‘plasma-wall transition (PWT)’, a narrow layer in front of the wall. This makes the PWT an important subject for investigation. Major efforts in this field are concerned with boundary conditions (BCs) at some suitable position inside the PWT. There are two reasons for doing this. First, these BCs can be directly used to calculate particle and heat fluxes to the wall, thus yielding estimates of plasma–surface interaction processes, and second, they are necessary for fluid codes simulating edge plasmas [1].

From the practical point of view, one of the most important cases is the PWT in fusion plasmas, which can be divided into the three parts: The Debye sheath (DS), the magnetic presheath (MP) and the collisional

(or geometrical) presheath (CP) [2]. The above-mentioned BCs are then formulated at the MP–CP transition, which is usually called the MP entrance (MPE). While for a single-ion PWT the corresponding BCs have been formulated about 20 years ago [3], up to now no proper investigation has been made for the multi-ion case, which is the one most relevant to fusion plasmas. Rather, in this case a trivial generalization of the Bohm–Chodura BC (GBC) is used, which consists in applying the Bohm–Chodura BC for each ion species [3,4]. Another approach has been used in [5], assuming (without any self-consistent derivation) that in a highly collisional limit the different ions have the same velocity satisfying some special condition at the MPE. We also mention papers [6–8] on the unmagnetized PWT, where the sheath-singularity condition has been used to define the DS entrance. This condition represents just one condition for all (N) ion species and cannot be used as a boundary condition even in the unmagnetized-plasma case, when N conditions are needed (one condition for each ion species).

In this work we re-discuss the BCs for magnetized multi-ion plasmas and present results of self-consistent

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kinetic (PIC) simulations. We show that the correct BCs can differ from the GBCs used before.

In what follows we assume that the PWT can still be divided into a collisionless DS and MP, and a CP. In other words, we assume that the inequalities $\lambda_D \ll \rho \ll l_{\text{mfp}}$ are satisfied, where λ_D is the Debye length, ρ is the largest ion gyro-radius of all given ion species, and l_{mfp} is the smallest mean free path.

2. Theory

First of all, let us clarify which are the quantities used for the formulation of BCs at the MPE [4]. These are: the potential drop between the MPE and the wall, $\Delta\phi_{\text{MP}}$, the normal (to the wall surface) components of the ion fluid velocities at the MPE, $V_{z,i}^0$, and the electron and ion sheath heat transmission coefficients, $\gamma_{e,i}$. The latter are defined as $\gamma_{e,i} = \frac{\Theta_{e,i}}{T_{e,i}I_{e,i}}$, where $\Theta_{e,i}$, $\Gamma_{e,i}$ and $T_{e,i}$ are the normal (to the wall surface) energy and particle fluxes, and the temperatures, respectively. We consider the case when the PWT consists of electrons and positive ions.

The classical model of the one-dimensional MP neglects gradients parallel to the wall surface and assumes a cut-off Maxwellian distribution for the electrons at the MPE [3], which results in

$$\gamma_e = \frac{2}{1 - G_e} + \frac{e\Delta\phi_{\text{MP}}}{T_e^0} \quad (1)$$

where G_e is the effective secondary electron emission coefficient [9]. Here and below the superscript '0' will define the MPE.

Using the expression for the current density at the MPE, we obtain after simple transformations

$$\Delta\phi_{\text{MP}} = \frac{T_e^0}{e} \ln \left(\frac{V_T^0 \sin \alpha}{\sqrt{2\pi}} \frac{1 - G_e}{\sum_{i=1}^N s_i^0 Z_i V_{z,i}^0 - I/en_e^0} \right), \quad (2)$$

where N is the number of ion species, n_e and $V_T^0 = \sqrt{T_e/m_e}$ are the electron density and thermal velocity, Z_i and s_i are their charge state and concentration, respectively. α is the angle between the magnetic field and the wall surface, and I is the current density to the wall.

In order to calculate γ_i we, without loss of generality, represent the ion distribution function at the MPE as the sum of a shifted Maxwellian (with the parallel shift velocity being $V_{\parallel,i}^0 = V_{z,i}^0/\sin \alpha$) and a kinetic correction function. Then, after simple calculations we obtain

$$\gamma_i = 2.5 + 0.5(V_{\parallel,i}^0/V_T^i)^2 + \Delta\gamma_i, \quad V_T^i = \sqrt{T_i^0/m_i}. \quad (3)$$

Unfortunately, the kinetic correction $\Delta\gamma_i$, which originates from the correction function, cannot be uniquely defined as it depends on the collisionality inside the CP and on the upstream plasma conditions. For the single-ion case it satisfies the condition [1] $-1.5 \leq \Delta\gamma_i \leq 0$.

From the expressions (1)–(3) it emerges that all BCs at the MPE (except $\Delta\gamma_i$) can be defined in terms of the ion velocities $V_{z,i}^0$. Of course, we assume that other quantities such as particle temperatures, ion concentrations and the current to the wall, are given. For the single-ion case (with $Z_i = 1$) we apply the Bohm–Chodura condition [3]

$$V_{z,i}^0 = C_s^0 \sin \alpha, \quad C_s = \sqrt{\frac{\chi_i T_i + T_e}{m_i}}, \quad (4)$$

so that the system (1)–(3) reduces to the well known BCs [4] (here we omit the index '0'):

$$\Delta\phi_{\text{MP}} = \beta \frac{T_e}{e}, \quad \beta = \ln \left(\frac{\sqrt{m_i/2\pi m_e}(1 - G_e)}{\sqrt{\chi_i T_i/T_e + 1} - I/en_e V_T^e \sin \alpha} \right),$$

$$\gamma_e = \frac{2}{1 - G_e} + \beta, \quad \gamma_i = 2.5 + 0.5 \left(\frac{T_e}{T_i} + \chi_i \right) + \Delta\gamma_i, \quad (5)$$

where χ_i is the adiabatic constant ($1 \leq \chi_i \leq 3$ [10]).

Thus, for formulating the BCs it is sufficient to find the ion velocities at the MPE, $V_{z,i}^0$. One can do this considering the MP, or the CP. In what follows we consider both possibilities.

The MP. We consider a half-bounded collisionless plasma (the MP), assuming the wall at $z = 0$ and the MPE at $z \rightarrow -\infty$. We assume that in the upstream part of the MP (i.e., near the MPE) the ion dynamics can be described by fluid equations, and follow the analysis presented in [11,12].

The ion particle and momentum conservation equations and the electron density are given by

$$\begin{aligned} \partial_z(V_{z,i}n_i) &= 0, \quad V_{z,i}\partial_z V_{x,i} = \Omega_z^i V_{y,i}, \quad i = 1, \dots, N, \\ V_{z,i}\partial_z V_{y,i} &= \Omega_x^i V_{z,i} - \Omega_z^i V_{x,i}, \quad \vec{\Omega}^i = \frac{eZ_i}{m_i}(B_x, 0, B_z), \\ V_{z,i}\partial_z V_{z,i} &= -\frac{eZ_i}{M_i}\partial_z \phi - \frac{1}{m_i n_i}\partial_z n_i T_i - \Omega_x^i V_{y,i}, \\ \sum_{j=1}^N Z_j n_j &= en_e = en_e^0 \exp(e\phi/T_e), \end{aligned} \quad (6)$$

where we have used the quasineutrality constraint and assumed Boltzmann-distributed electrons. In order to close the system (6) we assume that the pressure gradient can be described by a polytropic law $\partial_z(n_i T_i) = \chi_i T_i \partial_z n_i$. At the MPE the gradients vanish, so that the BCs for the system (6) take the form

$$V_{x,i}^0 = V_{\parallel,i}^0 \cos \alpha, \quad V_{y,i}^0 = 0, \quad V_{z,i}^0 = V_{\parallel,i}^0 \sin \alpha. \quad (7)$$

Using (6) and (7), we obtain after some transformations [11,12]

$$\begin{aligned} V_{y,i}^2 &= -(V_{z,i} - V_{z,i}^0)^2(1 + \tan \alpha) + 2\tan^2 \alpha (V_{z,i} - V_{z,i}^0)\Pi \\ &\quad - 2V_{z,i}^0 \Pi + 2\Gamma - \tan^2 \alpha \Pi^2, \quad i = 1, \dots, N, \\ \Pi &= \int_{V_{z,i}^0}^{V_{z,i}} C_i^2 \frac{dV_{z,i}}{V_{z,i}^2}, \quad \Gamma = \int_{V_{z,i}^0}^{V_{z,i}} C_i^2 \frac{dV_{z,i}}{V_{z,i}}, \end{aligned} \quad (8)$$

where

$$C_i^2 = \frac{\chi_i T_i + Z_i s_i T_e \partial_z n_e / \partial_z n_i}{m_i} = C_{s,i}^2 - \Delta_i, \quad (9)$$

$$C_{s,i} = \sqrt{\frac{\chi_i T_i + Z_i T_e}{m_i}}, \quad \Delta_i = \frac{Z_i T_e}{m_i} \frac{\partial_z \ln s_i}{\partial_z \ln n_i}.$$

$C_{s,i}$ the i th ion species.

Expanding the right-hand sides of the Eq. (8) near the MPE in series of $V_{z,i} - V_{z,i}^0$, we obtain after a simple transformation

$$V_{y,i}^2 = (V_{z,i} - V_{z,i}^0)^2 \left(\frac{C_i^{02}}{V_{z,i}^0} - 1 \right) \left(1 + t g^2 \alpha \left(1 - \frac{C_i^{02}}{V_{z,i}^0} \right) \right) + \mathcal{Q} \left((V_{z,i} - V_{z,i}^0)^3 \right),$$

$$C_i^0 \equiv C_i|_{z \rightarrow -\infty}. \quad (10)$$

From this expression we immediately obtain the set of conditions

$$\left(\frac{C_i^{02}}{V_{z,i}^0} - 1 \right) \left(1 + t g^2 \alpha \left(1 - \frac{C_i^{02}}{V_{z,i}^0} \right) \right) \geq 0, \quad (11)$$

yielding the following BCs for the ion speed at the MPE:

$$C_i^0 \sin \alpha \leq V_{z,i}^0 \leq C_i^0, \quad i = 1, \dots, N. \quad (12)$$

An important consequence of (9) and (12) is the set of conditions

$$\sqrt{\chi_i \frac{T_i}{m_i}} < V_{\parallel,i}^0, \quad i = 1, \dots, N. \quad (13)$$

Note that, contrary to the single-ion case, the conditions (12) are less informative. First of all, C_i^0 depends not only on local parameters ($T_{i,e}$ and s_i), but also on local derivatives ($|\partial_z \ln s_i / \partial_z \ln n_i|_{z \rightarrow -\infty} = \partial_{\ln n_i} \ln s_i|_{z \rightarrow -\infty}$). Another disadvantage of the conditions (12) is that even if one of them is satisfied marginally this will not guarantee that the other conditions are also satisfied marginally. Thus, the corresponding ion velocities cannot be explicitly defined. Still, these conditions deliver useful information: they indicate (i) the maximum allowed velocity at the MPE for which a monotonic MP can still develop, and (ii) that the generalized Bohm–Chodura condition (used probably in all multi-ion fluid codes), $C_{s,i}^0 \sin \alpha \leq V_{z,i}^0$, $i = 1, \dots, N$, can be satisfied only in the special case $\partial_{\ln n_i} \ln s_i|_{z \rightarrow -\infty} = 0$, $i = 1, \dots, N$.

As we will see below, it is useful to derive a BC which is independent of the local derivatives. After some transformations we obtain from (12)

$$\sum_{i=1}^N \frac{Z_i^2 s_i^0}{m_i V_{\parallel,i}^{02} - \chi_i T_i^0} \leq \frac{1}{T_e}. \quad (14)$$

The CP. As we have shown, treatment of the MP did not yield all the information necessary for formulating

the BCs at the MPE. Let us now consider the CP [13]. As was done for the MP, we assume a constant magnetic field and neglect gradients parallel to the wall surface. Then the corresponding BCs can be formulated as a singularity condition at the MPE. Here we follow the multi-ion CP analysis presented in [6–8] for unmagnetized plasmas. We consider a half-bounded collisional plasma (the CP) assuming the MPE at $z = 0$ (this corresponds to the limit $\rho \rightarrow 0$). Then for the one-dimensional CP (i.e., a CP uniform along the directions parallel to the wall surface) the ion particle and parallel momentum conservation equations and the electron density can be written

$$\partial_z (V_{\parallel,i} n_i) = S_i, \quad \sum_{j=1}^N Z_j n_j = e n_e = e n^0 \exp(e\phi / T_e),$$

$$V_{\parallel,i} \partial_z V_{\parallel,i} = -\frac{e Z_i}{m_i} \partial_z \phi - \frac{\chi_i T_i}{m_i n_i} \partial_z n_i - \frac{R_i}{m_i}, \quad (15)$$

where $S_i \geq 0$ and $R_i \geq 0$ represent the effective particle source and friction force, respectively. The explicit form of these terms is not important; they can originate from ionization, turbulence, friction due to charge-exchange collisions, etc. As for the MP case we consider Boltzmann-distributed electrons and use the polytropic law for the ions. In addition we assume that in the CP we have $V_{z,i} = V_{\parallel,i} \sin \alpha$ and $\partial_{\parallel} = \partial_z \sin \alpha$, where ∂_{\parallel} denotes the derivative along the magnetic field. As in [7,8] we assume the $V_{\parallel,i}$'s to be monotonically increasing towards the wall.

Using simple transformations we obtain from the system (15)

$$Z_i \partial_z n_i = \frac{Z_i^2 s_i}{m_i V_{\parallel,i}^2 - \chi_i T_i} T_e \partial_z n_e + Z_i \frac{m_i V_{\parallel,i} S_i + n_i R_i}{m_i V_{\parallel,i}^2 - \chi_i T_i}. \quad (16)$$

Summing over i and taking into account the quasineutrality constraint, we get

$$\left(1 - T_e \sum_{i=1}^N \frac{Z_i^2 s_i}{m_i V_{\parallel,i}^2 - \chi_i T_i} \right) \partial_z n_e = \sum_{i=1}^N Z_i \frac{m_i V_{\parallel,i} S_i + n_i R_i}{m_i V_{\parallel,i}^2 - \chi_i T_i}. \quad (17)$$

This equation exhibits a singularity when

$$\sum_{i=1}^N \frac{Z_i^2 s_i}{m_i V_{\parallel,i}^2 - \chi_i T_i} = \frac{1}{T_e}. \quad (18)$$

It is easy to check that the singularity condition (18) is satisfied between each two neighboring points where two ion velocities $V_{\parallel,i}$ are passing the corresponding $\sqrt{\chi_i T_i / m_i}$ (between these points the left-hand side of (18) varies from $+\infty$ to $-\infty$). As was mentioned in [7,8], these singularities are unphysical and can be removed (i.e. in this points the right hand side of the expression (17) vanishes). Now we can use the inequalities obtained for the MPE from the MP side. The set of

inequalities (13) guarantees that before reaching the MPE all $V_{\parallel,i}$ will pass the corresponding $\sqrt{\chi_i T_i / m_i}$. When the last $V_{\parallel,i}$ passes the corresponding value, the left-hand side of (18) starts to decrease from $+\infty$ and according to (14) will satisfy somewhere the singularity condition (18). This singularity cannot be removed as for these velocities the right-hand side of Eq. (17) is positively definite. Thus, the conditions (13) and (18) correspond to the ‘sheath singularity’ ($\partial_z \rightarrow \infty$), which defines the MPE. Using Eq. (16) it is easy to check that at the sheath singularity point we have $V_{\parallel,i} = C_i$. These analyses help in drawing the following conclusions.

Definition. The MPE for the N (positive) ion magnetized PWT is defined as the point where the following condition is satisfied

$$\sum_{i=1}^N \frac{Z_i^2 s_i}{m_i V_{\parallel,i}^2 - \chi_i T_i} = \frac{1}{T_e}, \quad V_{\parallel,i} > \sqrt{\frac{\chi_i T_i}{m_i}}. \quad (19)$$

There the ion velocities satisfy the BCs

$$\begin{aligned} V_{z,i}^0 &= C_i^0 \sin \alpha, \\ C_i^0 &= \frac{1}{m_i} \left(\chi_i T_i^0 + \frac{Z_i T_e^0}{1 + (\partial_{\ln n_e} \ln s_i)^0} \right). \end{aligned} \quad (20)$$

As we see, the definition of the MPE as a sheath singularity point in the CP is much more precise than the one obtained from the MP side. Still it leaves out the supersonic case. It can happen that the ion velocities entering the CP from the plasma bulk side are already ‘supersonic’ and satisfy the condition

$$\sum_{i=1}^N \frac{Z_i^2 s_i}{m_i V_{\parallel,i}^2 - \chi_i T_i} < \frac{1}{T_e}, \quad V_{\parallel,i} > V_{\parallel,i} > \sqrt{\frac{\chi_i T_i}{m_i}}. \quad (21)$$

In this case there exists no sheath singularity, but the MP can still develop if these velocities are not too large (see Eq. (12)), $V_{\parallel,i} < C_i / \sin \alpha$, $i = 1, \dots, N$. This supersonic case will be considered elsewhere.

Now we can complete the set of BCs at the MPE. Using (2), (3) and (20) we obtain

$$\begin{aligned} \Delta \phi_{\text{MP}} &= \frac{T_e}{e} \ln \left(\frac{V_T^e}{\sqrt{2\pi}} \frac{1 - G_e}{\sum_{i=1}^N s_i^0 Z_i C_i^0 - I / en_e^0 \sin \alpha} \right), \\ \gamma_i &= 2.5 + 0.5 \left(\chi_i + \frac{Z_i T_e^0}{T_i} \frac{1}{1 + (\partial_{\ln n_e} \ln s_i)^0} \right) + \Delta \gamma_i. \end{aligned} \quad (22)$$

The system (22) together with (1) and (20) represents the full set of BCs at the MPE. Introducing the ‘screening temperature’ for the electrons [2], $T_e = \frac{en_e}{\partial_{\ln n_e}}$, one can generalize these BCs (except for (1)) for any electron distribution. Moreover, in our analysis we do not use the condition $\chi_i = \text{const}$, so that all above obtained results are applicable for any case by substituting in the BCs (20) and (22) $\chi_i = 1 + (\partial_z \ln T_i / \partial_z \ln n_i)^0$.

Let us consider some examples. *Single-ion case.* The BCs then reduce to the ones from (5). *Two-ion case.* For

simplicity we assume monotonic profiles ($\partial_z n_e = \partial_z(n_1 + n_2) < \partial_z n_1 < 0$) and $\chi_{1,2} = Z_{1,2} = 1$, $I = G_e = 0$. Then the BCs are given by (we omit the index ‘0’)

$$\begin{aligned} V_{z,1} &= \sqrt{\frac{T_1}{m_1} \left(1 + \frac{T_e}{T_1} \frac{1}{1 + \xi} \right)} \sin \alpha, \\ V_{z,2} &= \sqrt{\frac{T_2}{m_2} \left(1 + \frac{T_e}{T_2} \frac{s_1 - 1}{s_1(\xi + 1) - 1} \right)} \sin \alpha, \\ \Delta \phi_{\text{MP}} &= \beta \frac{T_e}{e}, \\ \beta &= -\ln \left(\sqrt{\frac{2\pi m_e}{m_1}} \left(s_1 \sqrt{\frac{T_1}{T_e} + \frac{1}{1 + \xi}} \right. \right. \\ &\quad \left. \left. + (1 - s_1) \sqrt{\frac{m_1}{m_2} \left(\frac{T_2}{T_e} + \frac{s_1 - 1}{s_1(\xi + 1) - 1} \right)} \right) \right), \\ \gamma_e &= 2 + \beta, \quad \gamma_1 = 3 + \frac{T_e}{T_1} \frac{0.5}{1 + \xi} + \Delta \gamma_i, \quad \xi = \partial_{\ln n_e} \ln s_1, \\ \gamma_2 &= 3 + \frac{T_e}{2T_2} \frac{s_1 - 1}{s_1(\xi + 1) - 1} + \Delta \gamma_i, \quad -1 < \xi < \frac{1}{s_1} - 1. \end{aligned} \quad (23)$$

Note that, depending on the concentration gradient ξ , the BCs can strongly deviate from the GBC.

3. PIC simulations

In order to clarify kinetic effects and to find realistic values for the concentration gradients a set of high-accuracy (particle-in-cell) PIC simulations has been performed. We have used the 1d3v (one spatial and three velocity dimension) code BIT1 [12], which was developed on the bases of the XDPD1 code [14].

The simulation setup represents a bounded plasma between two walls, with a particle source in the middle of the system. During the simulation, Maxwellian distributed electrons and ions are injected into the source region, which is about 5 tritium gyro-radii wide. After a few ion transit times (system half size along the magnetic field over $V_{T,i}$) the system reaches a stationary state. The electron and ion motions are fully resolved and elastic and inelastic charged-neutral collisions are taken into account, so that the PWTs (on each side of the system) develop self-consistently. The neutrals constitute a fixed Maxwellian background with a given uniform density and temperature. Charged-neutral collisions are treated via the ‘null collision’ method [15]. For more details the interested reader is referred to [12,16].

Three sets of simulations have been run, with just a D plasma, a DT mixture (with different D and T concentrations), and a HDT mixture. The plasma parameters chosen are typical for fusion edge plasmas: $n^0 \approx 10^{18} \text{ m}^{-3}$,

Table 1
Mach numbers from theory and simulation

Ion and neutral concentration	D, D ₊ ^{50%} , T, T ₊ ^{50%}	D, D ₊ ^{75%} , T, T ₊ ^{25%}	H, H ₊ ^{20%} , D, D ₊ ^{40%} , T, T ₊ ^{40%}
PIC	$M_D = 0.99, M_T = 1.01$	$M_D = 0.99, M_T = 1.01$	$M_H = 0.96, M_D = 1.00, M_T = 1.02$
Analytic	$M_D = 1.03, M_T = 0.98$	$M_D = 1.03, M_T = 0.98$	$M_H = 1.08, M_D = 1.03, M_T = 0.96$

$T^0 \approx 20$ eV, $B = 1$ T and $\alpha = 5^\circ$. The differential cross-sections for elastic, excitation and ionization electron collisions with atomic H, D and T, as well as for elastic and charge-exchange collisions between atomic and ionic hydrogen isotopes have been taken from [17,18].

The relatively small difference in the masses and collisionalities of the hydrogen isotopes resulted in small concentration gradients ($|\partial \ln s_i / \partial \ln n_e|_0 \leq 0.2$), so that the BCs obtained from the PIC simulations, from our theory, and from GBC agree within an accuracy of a few percent. In Table 1 we give, as an example, Mach numbers, $M = V_{\parallel}^0 / C_s^0$, obtained from PIC simulations and from our theory. From Table 1 it emerges that, in spite of the very small difference, the analytical and PIC results show different tendencies. The analytic Mach numbers are subsonic for heavier ions and for lighter ones, while the PIC results show the opposite. The problem is the assumption of magnetized ions at the MPE (7) used in our and, probably, in all other fluid models of the magnetized PWT. These results indicate the limitations of our theory: if in the PWT there are different ion species with strongly different Larmor radius, ρ_i , then ones with large ρ_i can be unmagnetized at the MPE and the presented fluid theory fails.

4. Conclusion

The magnetized (positive) multi-ion PWTs can be divided into two classes. The first one corresponds to PWTs consisting of ions whose Larmor radii ρ_i do not differ significantly. In this case the theory presented above is applicable, i.e., one can derive the position of the MPE and the corresponding BCs. In the particular case of a PWT with hydrogen isotopes, considered by us, different isotopes have also similar collisionality and the ensuing BCs do not differ from the GBC. Thus, if the impurity concentration is negligibly small, the GBC is a very good approximation for hydrogen isotope PWTs. If there are different ions with similar ρ_i , but with the different collisionalities giving rise to a strong concentration gradient inside the PWT, then the GBC is not applicable any more and our model has to be used.

The second class of PWTs comprises those with a significant concentration of ion species with strongly different Larmor radii. In this case the ion species with larger

ρ_i will not be magnetized at the MPE (defined by condition (19)). Thus, the conditions used in our model can be violated and it cannot be applied. The corresponding study will be the topic of future work.

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