

## A COMPUTER MODEL OF PARTICLE BALANCE IN ECR ION SOURCES

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The investigation of widespread model of particle balance and energy transport [1–5] for calculation of ion charge-state distribution (CSD) in electron cyclotron resonance (ECR) ion source [6] is given. The modification of this model that allows one to describe more precisely the confinement and accumulation processes of highly charged ions in ECR plasma for gas mixing case is discussed. The discussion of the new calculation technique for ions and electrons time confinement calculation based on the theory of Pastukhov [7, 8] is given, viz. calculation of confinement times during two-step minimization of special-type functionals. The preliminary results obtained by this approach have been compared with available experimental data.

В работе проанализирована широко распространенная модель уравнений баланса [1–5] для расчета зарядовых распределений ионов (ЗРИ) в ионном источнике на электронно-циклотронном резонансе (ЭЦР) [6]. Приводится модификация рассматриваемой модели, позволяющая более точно описывать процессы удержания и накопления тяжелых ионов в ЭЦР-плазме ионного источника в случае смеси газов. Обсуждается подход расчета времен удержания частиц (ионов и электронов) на основе теории Пастухова [7, 8], а именно: расчет времен удержания в процессе двухэтапной минимизации функционалов специального вида. Дается сравнение с экспериментальными результатами.

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### BALANCE EQUATIONS SET FOR CALCULATION OF ION CSD IN ECR ION SOURCE

The described model of ion CSD calculation is based on balance equations set for ion and electron densities in the ECR plasma of ion source. Inherently the balance equations technique is one of the methods for solving Boltzmann equation [9] applied for investigation of heavy charged ions accumulation in ECR ion source.

In compliance with some previous work [1, 2], the main set of the balance equations for ion and electron densities have been generalized for a case of multicomponent consideration of electron fraction in ECR plasma [3–5]. Also, the additional collision processes have been added into the set of balance equations; however, with the admission of cold electrons to the calculation we must include radiative recombination process which becomes significant at the higher charge states; also in recent years the importance of dielectronic recombination for reducing the charge state has become recognized and in this case this process was included too.

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The agreed notations for the set of Eqs. (1), (2) and for next describing formalism are:  $s, s'$  — ion species indices;  $z, z'$  — ion charge-state indices;  $m$  — process multiplicity index for single and double ionization and charge exchange processes and a simple index in case of radiative recombination  $m = 1$  or dielectronic recombination  $m = 2$ ;  $k, k'$  — electron component indices;  $\bar{u}_{s,0}$  — neutral velocity;  $V_{\text{ECR}}, S_{\text{ECR}}$  — volume confined by resonance surface and its area;  ${}^m\nu_{s,z \rightarrow z+m,k}^{\text{ion}}, {}^m\nu_{s,z \rightarrow z-m,k}^{\text{cx}}, {}^m\nu_{s,z \rightarrow z-m,k}^r$  — ionization, charge exchange and radiative rates from charge state  $z$  to  $z+m$  for ionization and from charge state  $z$  to  $z-m$  for charge exchange and recombination processes, correspondingly;  $n_{s,z}, n_{e,k}$  — ions and electrons densities;  $n_{s,0}, n_s$  — neutral density inside and outside of the source chamber;  $\tau_{s,z}, \tau_{e,k}$  — confinement times for ions and electrons;  $\tau_{e,k \rightarrow k'}^h$  — time heating for electron component with temperature  $T_{e,k}$  to  $T_{e,k'}$ , here  $k < k'$ ;  $T_{s,z}, T_{e,k}$  — ions and electrons temperatures;  $\nu^{s,z \setminus e,k}, \nu^{e,k \setminus s,z}$  — collision rates between ions and electrons and its contrary;  $\nu^{s,z \setminus s',z'}, \nu^{e,k \setminus e,k'}$  — ions and electrons collision rates, correspondingly.

The main equations set for ion densities generalized for a gas mixing case has the following form:

$$\begin{aligned} \frac{dn_{s,0}}{dt} = & \frac{\bar{u}_{s,0} S_{\text{ECR}}}{V_{\text{ECR}}} (n_s - n_{s,0}) + \sum_{m=1}^M \sum_{k=1}^K {}^m\nu_{s,1 \rightarrow 0}^r n_{e,k} n_{s,1} - \\ & - \sum_{m=1}^M \left( \sum_{k=1}^K {}^m\nu_{s,0 \rightarrow m,k}^{\text{ion}} n_{e,k} + \sum_{s'=1}^S \sum_{z=m+1}^{Z_{s'}} {}^m\nu_{s',z \rightarrow z-m}^{\text{cx}} n_{s',z} \right) n_{s,0}, \end{aligned}$$

$$\begin{aligned} \frac{dn_{s,1}}{dt} = & \sum_{k=1}^K \left( {}^1\nu_{s,0 \rightarrow 1,k}^{\text{ion}} n_{e,k} n_{s,0} + \sum_{m=1}^M {}^m\nu_{s,2 \rightarrow 1,k}^r n_{e,k} n_{s,2} \right) + \\ & + \sum_{s'=1}^S \left( \sum_{m=1}^M {}^m\nu_{s,m+1 \rightarrow 1}^{\text{cx}} n_{s,m+1} n_{s',0} + \sum_{z=2}^{Z_{s'}} {}^m\nu_{s',z \rightarrow z-1}^{\text{cx}} n_{s',z} n_{s,0} \right) - \\ & - \left( \sum_{m=1}^M \sum_{k=1}^K \left( {}^m\nu_{s,1 \rightarrow m+1,k}^{\text{ion}} n_{e,k} + {}^m\nu_{s,1 \rightarrow 0,k}^r n_{e,k} \right) + \frac{1}{\tau_{s,1}} \right) n_{s,1}, \end{aligned}$$

$$\begin{aligned} \frac{dn_{s,2}}{dt} = & \sum_{m=1}^M \sum_{k=1}^K \left( {}^m\nu_{s,2-m \rightarrow 2,k}^{\text{ion}} n_{e,k} n_{s,2-m} + {}^m\nu_{s,3 \rightarrow 2,k}^r n_{e,k} n_{s,3} \right) + \\ & + \sum_{s'=1}^S \left( \sum_{m=1}^M {}^m\nu_{s,m+2 \rightarrow 2}^{\text{cx}} n_{s,m+2} n_{s',0} + M \sum_{z=3}^{Z_{s'}} {}^2\nu_{s',z \rightarrow z-2}^{\text{cx}} n_{s',z} n_{s,0} \right) - \\ & - \left( \sum_{m=1}^M \sum_{k=1}^K \left( {}^m\nu_{s,2 \rightarrow m+2,k}^{\text{ion}} n_{e,k} + {}^m\nu_{s,2 \rightarrow 1,k}^r n_{e,k} \right) + \sum_{s'=1}^S {}^1\nu_{s',2 \rightarrow 1}^{\text{cx}} n_{s',0} + \frac{1}{\tau_{s,2}} \right) n_{s,2}, \end{aligned}$$

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### PLASMA NEUTRALITY AND LOSS FLOW CONSERVATION

Based of the main set of balance equations (1), (2), it is easy to show one of the important properties of this system, viz. conservation of the loss flow of charged particles from the ion source:

$$\frac{d}{dt} \left( \sum_{s=1}^S \sum_{z=1}^{Z_s} z n_{s,z} - \sum_{k=1}^K n_{e,k} \right) = \sum_{s=1}^S \sum_{z=1}^{Z_s} \frac{z n_{s,z}}{\tau_{s,k}} - \sum_{k=0}^K \frac{n_{e,k}}{\tau_{e,k}} = 0. \quad (3)$$

This indicates that the plasma neutrality (first part of this expression) is realised if the loss flow is conserved (second part of this expression). This fact is used for developing of new method for time confinement of charged particles trapped in minimum- $B$  magnetic field configuration of ECR ion source. This fact is valid for both of operating modes of ECR ion source working, i.e., stationary and dynamic.

### NEW METHOD FOR TIME CONFINEMENT CALCULATION

Using the dependence of ions time confinement on potential dip  $\tau_{s,z} = \tau_{s,z}(\Delta\phi)$  and of confinement time of cold electron components on plasma potential  $\tau_{e,0} = \tau_{e,0}(\phi)$ , the following functional was made:

$$F_1(\Delta\phi, \phi) = \left( 1 - \frac{\sum_{s=1}^S \sum_{z=1}^{Z_s} \frac{z n_{s,z}}{\tau_{s,z}(\Delta\phi)}}{\frac{n_{e,0}}{\tau_{e,0}(\phi)} + \sum_{k=1}^K \frac{n_{e,k}}{\tau_{e,k}}} \right)^2. \quad (4)$$

It is easy to see the relation between the two last expressions (3) and (4). The result of minimization problem for the first functional (4) is two values potential dip  $\Delta\phi$  and plasma potential  $\phi$  and this entire forms the first stage of the new method for time confinement calculation. The second stage of the developed method regards to correction of the time confinement that comes from the first stage. Use the following functional:

$$F_2(\tau_{1,1}, \tau_{1,2}, \dots, \tau_{1,Z_1}, \dots, \tau_{S,1}, \tau_{S,2}, \dots, \tau_{S,Z_S}, \tau_{e,0}, \tau_{e,1}, \dots, \tau_{e,K}) = \left( 1 - \frac{\sum_{s=1}^S \sum_{z=1}^{Z_s} \frac{z n_{s,z}}{\tau_{s,z}}}{\sum_{k=0}^K \frac{n_{e,k}}{\tau_{e,k}}} \right)^2 \quad (5)$$

and minimize it, the new confinement time in this case is more proper, but of course it is a problem for discussion.

The above two-stage minimization scheme involves the Pastukhov theory for charged particle confinement in the open magnetic trap [7] with modification by Rognlien and Cutler [8]:

$$\begin{aligned}\tau_{s,z}(\Delta\phi) &= \left( RL \sqrt{\frac{\pi m_{s,z}}{2 k_B T_{s,z}}} + \frac{G \left( \frac{z e \Delta\phi}{k_B T_{s,z}} \right)^2}{\left( \frac{1}{2} + \frac{z e \Delta\phi}{k_B T_{s,z}} \right) \nu_{s,z}} \right) \exp \left( \frac{z e \Delta\phi}{k_B T_{s,z}} \right), \\ \tau_{e,1}(\phi) &= \left( RL \sqrt{\frac{\pi m_e}{2 k_B T_{e,0}}} + \frac{G \left( \frac{e \phi}{k_B T_{e,0}} \right)^2}{\left( \frac{1}{2} + \frac{e \phi}{k_B T_{e,0}} \right) \nu_{e,0}} \right) \exp \left( \frac{e \phi}{k_B T_{e,0}} \right), \\ \tau_{e,k} &= \frac{1.48 \left( \ln R + \sqrt{\ln R} \right)}{\nu_{e,k}}, \quad G = \frac{\sqrt{\pi} (R+1) \ln(2R+2)}{2R}.\end{aligned}\tag{6}$$

Here  $R$  — mirror ratio;  $L$  — effective mirror-to-mirror length;  $e$  — electron charge.

On the first stage the expressions (6) was used in order to determine  $\Delta\phi$  and  $\phi$  values. These values and formalism (6) were used on the second stage but only like starting point for minimization problem of second functional (5).

The Spitzer formalism [10] was used for calculation of partial rates  $\nu^{s,z \setminus e,k}$ ,  $\nu^{e,k \setminus s,z}$ ,  $\nu^{s,z \setminus s',z'}$ ,  $\nu^{e,k \setminus e,k'}$  and total collision rates  $\nu_{s,z}$  and  $\nu_{e,k}$ , i.e.,

$$\nu^{\alpha \setminus \beta} = 1.8 \cdot 10^{-19} \frac{\sqrt{m_\alpha m_\beta} z_\alpha^2 z_\beta^2 n_\beta \lambda^{\alpha \setminus \beta}}{\sqrt{(m_\alpha T_\beta + m_\beta T_\alpha)^3}}, \quad \nu^{\alpha \setminus \beta} = \sum_\beta \nu^{\alpha \setminus \beta}.\tag{7}$$

Here  $\alpha, \beta$  — ion or electron species indices;  $\lambda^{\alpha \setminus \beta}$  — Coulomb logarithm. For more detailed information, see [10, 11].

We also note here that the developed approach (first minimization stage) can be used to compare plasma potential and dip with available experimental data.

## DEFINITION OF VOLUME CONFINED BY RESONANCE SURFACE AND ITS AREA

The volume  $V_{\text{ECR}}$  confined by resonance surface and its area  $S_{\text{ECR}}$  are parameters in the first equation in the set of balance equations (1), (2). Previous works use numerical estimation [1] of volume confined by ECR surface and its area or some assumption about resonance surface shape [2–5] that supposes the analytical calculation of these two values, e.g., ellipsoidal shape.

Based on the approximation of minimum- $B$  field configuration produced by ECR ion source magnetic system it is possible to find the implicit equation of ECR resonance surface:  $F = F(x, y, z)$ .

The following approximation of the magnetic field map was applied [12]:

$$\mathbf{A}(\rho, \theta, z) = \begin{pmatrix} 0 \\ A_\theta \\ A_z \end{pmatrix}.\tag{8}$$

Here  $A_\theta = A_\theta(\rho, z)$  — azimuthal component and  $A_z = A_z(\rho, \theta)$  — longitudinal component of vector potential  $\mathbf{A} = \mathbf{A}(\rho, \theta, z)$ :

$$A_\theta(\rho, z) = J_1 \left( \rho \frac{d}{dz} \right) \Phi(z), \quad \Phi(z) = B_1 + z^2 B_2, \quad A_z(\rho, \theta) = \frac{\rho^3 B_0 \sin 3\theta}{3R_0^2}. \quad (9)$$

Here  $B_0/R_0^2$ ,  $B_1$ ,  $B_2$  are numerical coefficients;  $B_0$  is a pole tip magnet field and  $R_0$  is a lens radius. The dimension of a quantity  $B_0/R_0^2$  is G/cm<sup>2</sup>, and dimension of quantities  $B_1$ ,  $B_2$  is G. The magnetic field  $\mathbf{B} = \mathbf{B}(\rho, \theta, z)$  is defined as

$$\mathbf{B} = \nabla \times \mathbf{A}. \quad (10)$$

After conversion (9) to Cartesian coordinate system and definition of the magnetic field absolute value  $B = B(x, y, z)$ , for  $F(x, y, z)$  we have

$$\begin{aligned} F(x, y, z) &= B(x, y, z) - B_{\text{res}}, \\ B(x, y, z) &= \sqrt{B_x^2(x, y, z) + B_y^2(x, y, z) + B_z^2(z)}, \\ B_x(x, y, z) &= (x^2 - y^2) B_0 - x z B_2, \\ B_y(x, y, z) &= -y (2 x B_0 + z B_2), \quad B_z(z) = \Phi(z). \end{aligned} \quad (11)$$

Here  $B_{\text{res}}$  — resonance value of the magnetic field in Gauss and coefficient of  $B_0/R_0^2$  here was redefined as  $B_0$ . The volume can be defined as

$$V_{\text{ECR}} = \iiint_{\Omega} dV, \quad dV = dx dy dz, \quad \Omega = \{(x, y, z) : F(x, y, z) < 0\}, \quad (12)$$

and resonance surface area is

$$\begin{aligned} S_{\text{ECR}} &= \oiint_S \mathbf{n} \cdot d\mathbf{S}, \quad d\mathbf{S} = \mathbf{n} dS, \quad dS = dx dy, \\ S &= \{(x, y, z) : F(x, y, z) = 0\}. \end{aligned} \quad (13)$$

Using the Ostrogradsky–Gauss theorem, we reduce the last expression, i.e.,

$$\begin{aligned} \oiint_S \mathbf{n} \cdot d\mathbf{S} &= \iiint_{\Omega} \nabla \cdot \mathbf{n} dV, \quad S_{\text{ECR}} = \iiint_{\Omega} \nabla \cdot \mathbf{n} dV, \\ \mathbf{n} &= \mathbf{n}(x, y, z), \quad \mathbf{n}(x, y, z) = \frac{\nabla B(x, y, z)}{|\nabla B(x, y, z)|}. \end{aligned} \quad (14)$$

The formalism (11), (13) for calculation of  $V_{\text{ECR}}$  and  $S_{\text{ECR}}$  was applied using Monte Carlo method and tested for surfaces with analytical expression for volume and area, i.e., sphere with given radius and ellipsoid with given semiaxis.

For more detailed description of this calculation, see [13].

## ECR HEATING PHENOMENON

Assuming the expression  $\nu_{e,k}$  for total electron collision rate well-known, the time heating can be determined as follows [9]:

$$\tau_{e,k \rightarrow k'}^h = \sqrt{\frac{2m_e(T_{e,k'} - T_{e,k})}{e^2 E^2}}. \quad (15)$$

Here  $E$  — magnitude of the external super high frequency (SHF) field;  $m_e$  — electron mass. The dependencies of external SHF field power  $P_s \sim E^2$  can be found in [6].

## PROCESSES RATES CALCULATION

The values  ${}^m\nu_{s,z \rightarrow z+m,k}^{\text{ion}}$ ,  ${}^m\nu_{s,z \rightarrow z-m}^{\text{cx}}$ ,  ${}^m\nu_{s,z \rightarrow z-m,k}^r$  in balance equations set (1), (2) describe the transfer rates of ions from charge state  $z$  to  $z+m$  for ionization and from charge state  $z$  to  $z-m$  for charge exchange and recombination processes, correspondingly.

**Electron Impact Ionization.** The electron impact ionization is the main process for the ions production in ECR plasma.

There are a lot of experimental data for electron impact ionization for neutral atoms and low charged ions in the literature, and also different theoretical models are used to calculate ionization cross sections for highly charged ions, as well as for low charged ions and neutrals. Lotz's formalism [14, 15] is one of the most useful for calculating ionization cross sections of neutral atoms and ions by electron impact.

The multiple ionization rate of an ion from charge state  $z$  to  $z+m$  by electrons impact of energy  $E_{e,k}$  was calculated assuming thermal equilibrium for the electrons and average over Boltzmann distribution  $f_{e,k}$  of temperature  $T_{e,k}$ . The cross section for this calculation was taken from [14, 15].

**Charge Exchange Process.** As opposed to electron impact ionization, charge exchange processes reduce the mean charge of ions, increase the total ion number in the plasma and can be considered as a very undesirable process in ECR ion source.

The cross section of the charge exchange process for low collision energies does not depend on the energy, has a strong dependence on the ionic charge state and ionization potential of the neutral atom and can be estimated, for example, from the well-known empirical formula of Müller and Salzborn [16, 17]. Assuming that the plasma is close enough to thermal equilibrium to use the Boltzmann distribution  $f_{s,z}$  and formalism [16, 17], the multiple charge exchange rates were calculated.

**Recombination.** Electron capture into an excited state of an electron shell with simultaneous emission of a photon is radiative recombination. Sometimes this process is important for highly charged ions in plasma of cold electrons. Another process is electron capture into a fixed excited state of an electron shell with a simultaneous transition of one electron of the shell at the excited level. This is dielectronic recombination, a resonant process negligible for electron energy in the keV range.

The radiative rates have been calculated in compliance with reference [1].

### NUMERICAL EXAMPLES FOR SERSE ION SOURCE

The developed method has been applied for extracted current calculation of currents from superconducting ECR ion source (SERSE 18 GHz, INFN-LNS) in stationary operating regime [18].

The Cauchy problem for system of nonlinear differential equations (1), (2) of particles balance in dynamic operating regime of ion source was posed.

The solution in dynamic case is used as first iteration for densities of nonlinear algebraic equations set based on (1), (2) which describes a stationary operating regime of ion source working.

The confinement times of charged particles trapped in ion source are found due to two-stage minimization of special-type functionals (4) and (5) created with flow equation (3).

The fitted magnetic field parameters  $B_0$ ,  $B_1$ ,  $B_2$  (8)–(11) are

$$B_0 = 333.7 \text{ G} \cdot \text{cm}^{-2}, \quad B_1 = 5373.8 \text{ G}, \quad B_2 = 42.5 \text{ G} \cdot \text{cm}^{-2}, \quad B_{\text{res}} = 6425.9 \text{ G}. \quad (16)$$

For these parameters (16) the volume  $V_{\text{ECR}}$  confined by resonance surface and its area  $S_{\text{ECR}}$  (12)–(14), we have

$$S_{\text{ECR}} = 210 \text{ cm}^2, \quad V_{\text{ECR}} = 260 \text{ cm}^3. \quad (17)$$

The dimensions of SERSE ion source working chamber are

$$D = 13 \text{ cm}, \quad L = 48 \text{ cm}. \quad (18)$$

An approach commonly adopted for the determination of the extracted currents was proposed by West [1]. It takes into account the confinement losses, but not the limitations due to the space charge effects. In order to consider them, we normalize the currents following the  $\sqrt{z}$  law, characteristic of the Child–Langmuir formula [19]. Therefore,

$$J_{s,z} = \sqrt{\frac{z}{Z_s}} \frac{eV_p a z n_{s,z}}{2S_p \tau_{s,z}}. \quad (19)$$

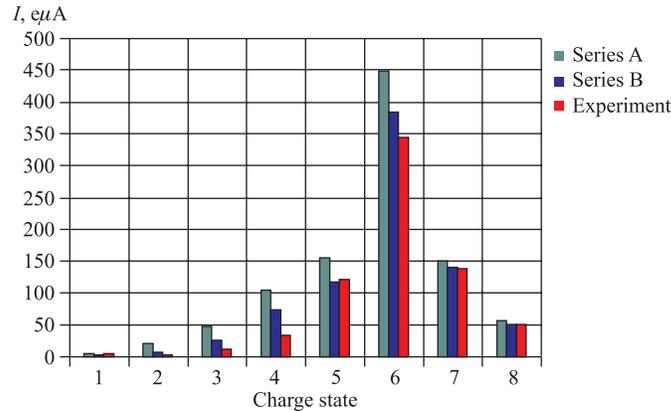


Fig. 1. Comparison of different current models. Heating times:  $\tau_{e,0 \rightarrow 1}^h = 10^{-7}$  s,  $\tau_{e,1 \rightarrow 2}^h = 10^{-8}$  s; series A:  $n_e = 2.3 \cdot 10^{12} \text{ cm}^{-3}$ ,  $T_{e,0} = 100 \text{ eV}$ ,  $T_{e,1} = 5 \text{ keV}$ ,  $T_{e,2} = 15 \text{ keV}$ ,  $P_s = 1466.2 \text{ W}$  (current model corresponds to [1]); series B: the same parameters sets, but current model corresponds to (19) [19]; experimental result,  $P_s = 1400 \text{ W}$

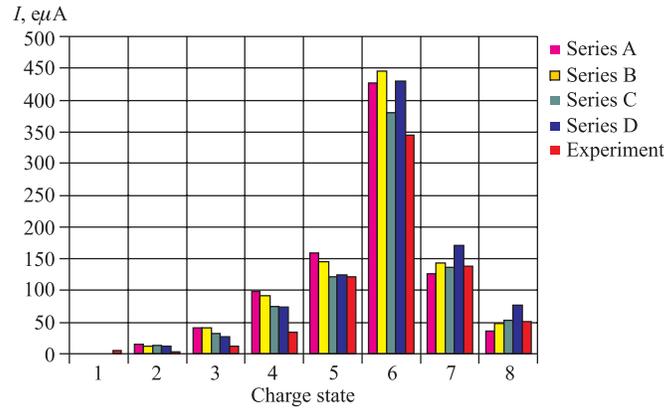


Fig. 2. Comparison of different time heating and different electron temperatures. Heating times:  $\tau_{e,0 \rightarrow 1}^h = 10^{-7}$  s,  $\tau_{e,1 \rightarrow 2}^h = 10^{-8}$  s; series A:  $n_e = 1.8 \cdot 10^{12}$  cm $^{-3}$ ,  $T_{e,0} = 100$  eV,  $T_{e,1} = 5$  keV,  $T_{e,2} = 8$  keV,  $P_s = 937.8$  W; series B:  $n_e = 2.1 \cdot 10^{12}$  cm $^{-3}$ ,  $T_{e,0} = 100$  eV,  $T_{e,1} = 5$  keV,  $T_{e,2} = 10$  keV,  $P_s = 1157.8$  W; series C:  $n_e = 2.3 \cdot 10^{12}$  cm $^{-3}$ ,  $T_{e,0} = 100$  eV,  $T_{e,1} = 5$  keV,  $T_{e,2} = 15$  keV,  $P_s = 1466.2$  W; heating times:  $\tau_{e,0 \rightarrow 1}^h = 10^{-9}$  s,  $\tau_{e,1 \rightarrow 2}^h = 10^{-10}$  s; series D:  $n_e = 2.5 \cdot 10^{12}$  cm $^{-3}$ ,  $T_{e,0} = 100$  eV,  $T_{e,1} = 5$  keV,  $T_{e,2} = 15$  keV,  $P_s = 1852.8$  W; experimental result,  $P_s = 1466.2$  W

Comparison of experimental and calculated data of extracted currents of oxygen-18 is shown in Figs. 1 and 2.

## CONCLUSION

The presented approach of the balance equations set (1), (2) in stationary regime has been considered on the superconducting ECR source (SERSE 18 GHz, INFN-LNS), determining plasma potential and potential dip by the special-type minimization procedure (4), (5) based on the charge flows conservation (3). A formula taking into account the limitations due to the space charge effects was used for the extracted ions currents, following the Child–Langmuir principle. The presented approach to the problem of the ions source modelling is versatile and can describe the main working principles of the source quantitatively, i.e., impact ionization of ions, ions charge exchange on neutrals of working gas, charged particles confinement by minimum- $B$  configured magnetic field and ECR heating phenomenon (15). The preliminary calculated results properly correspond to experimental data.

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