Development of a fluid code for rapid simulation of high-density ECWR plasmas

S. Sfikas\textsuperscript{1}, E. Amanatides\textsuperscript{1}, D. Mataras\textsuperscript{1,2}, and D. Rapakoulias\textsuperscript{1}

\textsuperscript{1}Plasma Technology Laboratory, Department of Chemical Engineering, University of Patras, Greece
\textsuperscript{2}email: dim@plasmatech.gr

Abstract: A fluid model of electron cyclotron wave resonance (ECWR) Argon discharges is presented. The application of a predetermined set of boundary conditions for the magnetic potential and a modified effective electron collision frequency that includes plasma non-uniformities were found to be essential parameters, leading to very satisfactory agreement of the rapidly converging fluid code to experimental data and other simulation results.

Keywords: Electron cyclotron wave resonance, ECWR, fluid model, RF discharges.

1. Introduction

Plasma simulation is nowadays an attractive alternative to diagnostic techniques in controlling various plasma material processing parameters. On the other hand, the development of time-effective computer codes in order to realistically reproduce plasma properties is still a challenging task [1].

The main target in developing the fluid code presented in this work is to gain rapid and reliable insight into the complicated physicochemical processes that take place during plasma treatment and deposition using inductively coupled RF plasma sources within a weak DC magnetic field (namely ECWR plasma sources). Sources of this type have attracted important technological interest, due to the high dissociation degree of the precursor gases and the production of reactive species suitable for surface treatment and material deposition [2, 3]. The resonance-like increase in plasma density during the ECWR phenomenon was first reported by H. Neuert [4] and can be described as the formation of a standing wave pattern within the source coil, by adjusting the plasma refractive index and hence the wavelength via the superimposed static magnetic field. Most of the experimental work performed on ECWR’s can be reasonably well explained by the theory of modified skin effect and electron cyclotron wave propagation in plasma sheaths which was first introduced by B. Pfeiffer [5, 6].

The fluid model that was developed to simulate ECWR Argon discharges is briefly described in the next section. The simulation results for a low pressure plasma slab (1-dimensional model) are checked against the particle in cell/Monte Carlo (PIC/MC) simulation results by Krimke et al. [7] and are also compared against the analytical theory and experimental data by B. Pfeiffer [5, 6]. Moreover, the results for a 1-mTorr cylindrical ECWR reactor (2-dimensional model) are compared to the simulation results by Krimke et al. [8] and the experimental data of E. P. Szuszczechwicz et al. [9]. As a final point, preliminary results for the diffusion of Argon plasma generated from a cylindrical ECWR source in the processing chamber at 5 mTorr are compared with the experimental findings of V. Vartolomei et al [10].

2. Model description

In the 1-dimensional model of a slab reactor geometry [6, 7], a set of predefined boundary conditions [11] were applied for the high frequency (27.12 MHz) magnetic potential, which were extracted from the integration of published analytic solutions for the $h^f$ magnetic field [5]. A similar approach was used for the 2-dimensional case (cylindrical reactor geometry [8, 9]), where Szuszczechwicz’s approach [12] was adopted for the refractive index of the right hand polarized (RHP) wave that is responsible for electron heating. In this configuration, the RHP $h^f$ magnetic field was reproduced using Bessel functions as boundary conditions for the magnetic potential.

A simplified chemistry of Argon discharge including two species (Ar and Ar$^+$) and three gas phase reactions (ionization, momentum transfer and ion-electron recombination) was incorporated in the model. The reactions’ rate constants were calculated from JILA database [13] cross-sections assuming Maxwellian energy distributions. Additionally, the electron effective collision frequency $v_{\text{eff}}$ was properly modified [11, 14, 15] as in Eq. (1) in order to include the effect of spatial in-homogeneity in plasma conductivity and electron mobility and diffusivity.

\[
v_{\text{eff}} = 1 + \left( \frac{\omega_c}{N_{\text{RES}}} \right)^2 \nu
\]  

For the specific set of conditions [6] used in the slab geometry, $\omega_c$ is the electron cyclotron frequency (3.956x10$^8$ sec$^{-1}$), $N_e$ the electron density, $N_{\text{RES}}$ the electron density in resonant conditions ($10^{17}$ m$^{-3}$) and $\nu$ is the electron collision frequency as in [15].

The system of equations [11] resulting from the cou-
pling of Poisson’s (electrostatic field) with Boltzmann’s moment equations is implemented in the commercial code CFD-ACE+. The high frequency electromagnetic field and electrons energy input were calculated from Maxwell’s equations given the prearranged conditions for the magnetic potential at the boundaries. As a final remark, the drift-diffusion approximation for ions was not sufficient at this low pressure range (15 mTorr) and the momentum equation had to be resolved.

The model’s predictions for basic plasma properties in an ECWR source can be used as a starting point for the modeling of plasma expansion from the source to a processing chamber and grounded surfaces. A tempting approach for a rapid simulation is the numerical solution of the system [11] without RF power input. This approach was also followed in the present case, where a 2-dimensional model of a cylindrical ECWR source expansion without static magnetic field [10] was developed for a 20 cm in diameter chamber. The values referred in [10] for the plasma temperature and density in the center of the ECWR plasma source, were implemented as a constant temperature/density inlet of the domain.

3. Results and discussion

Simulation results for a 15 mTorr Argon discharge in a d=7 cm plasma slab under resonance conditions are presented in the next two figures: In Fig. 1 the distribution of electron density in the slab is in good agreement with the calculation of PIC/MC results [7], which are also included in the figure together with Schottky theory prediction. The maximum value of $N_e$ is almost $10^{17}$ m$^{-3}$, which is equal to the value used in the analytical calculations of Ref. [5].

![Fig. 1](image1.jpg)  
**Fig. 1:** Plasma electron density $N_e$ as calculated in this simulation and compared to the simulation results of [7]. The Schottky diffusion profile is also indicated.

In Fig. 2, the plasma electrostatic potential $\Phi$ has a gradient profile and a maximum value of 14.85 V. Both the shape and the values of the electrostatic potential are identical to the results of Ref. [7], included in the figure. This agreement was possible only after the coupling of the Poisson’s relation to the fluid code i.e. the assumption of quasi-neutrality and ambipolarity led always to a strong underestimation of the electrostatic potential.

Extending the dimensionality of the model by properly defined boundary conditions for the magnetic potential, allowed the simulation of more realistic ECWR configuration: The simulation results for a 1 mTorr Argon discharge in a cylindrical ECWR reactor of diameter $d_{cyl}=9.75$ cm [8, 9] under resonance conditions are presented in Figs. 3 and 4.

Considering only an axial component for the $hf$ magnetic field, the modulus of the cross-sectional induced electric field resulting from the Szuszczywicz’s assumptions [12] for the RHP wave, is shown in the spatial map of Fig. 3: Two fields of dipole nature ($E_x$ and $E_y$ components) are superposed in $E_{RF}$ so that the quadrupolar

![Fig. 2](image2.jpg)  
**Fig. 2:** Electrostatic potential profile as calculated in this simulation and compared to the simulation results of [7].

![Fig. 3](image3.jpg)  
**Fig. 3:** Spatial map of the magnitude of the induced electric field, resulting from the specific boundary conditions used for the magnetic potential ($B_{st}$ indicates the static magnetic field).
character of the field revealed in [8] is still present—yet distorted. Nevertheless, the previous researchers have introduced a discharge model with predefined plasma properties within a static magnetic field (B\textsubscript{st}) of 2.55 mTesla, corresponding to β\textsubscript{res}=2.63 which is rather off the experimental value referred in [9].

In Fig. 4 we compare the results of our simulation for the electron density (spatial map with dark colored curves of constant density), with Szuszcze\l{}icz’s experimental findings [9] for N\textsubscript{RES} =10\textsuperscript{17} m\textsuperscript{-3}, β=2.0 (light colored curves: z=0, r =1.0, 2.0, 3.0, 4.0 cm). The alignment of the regions of maximum electron density in the simulation is in good agreement with experiment in the main volume of the discharge and the net result of the anisotropy in charged particle diffusion coefficient is closely reproduced. In ECWR sources, the electron density profile is a more steeply decreasing function of the radius r in the direction perpendicular to B\textsubscript{st} as resonance is approached, resulting in increasing inhomogeneity of the extracted ion beam [9].

This effect is demonstrated in figure 5 where electron density experimental data [9] collected in the center of the discharge along the diameter which is perpendicular to B\textsubscript{st} (β=0, 1.5, dotted lines) are compared to the simulation results (β=2.13589, straight lines). The normalized electron density radial profile (N\textsubscript{e}(x), β=2.13) along the static field is in fair agreement with the experimental data radial profile without the static field (N\textsubscript{e}(y), β=0) as it should due to the unaffected electron motion along the lines of force. The simulated electron density radial profile (N\textsubscript{e}(y), β=2.13) perpendicular to the static field is off the experimental values (N\textsubscript{e}(y), β=1.5); nevertheless the simulated N\textsubscript{e}(y) profile is sharper than the N\textsubscript{e}(x) profile. This deviation from the experimental findings can be attributed to the different plasma density symmetry properties at nonresonant values (β\textsubscript{res}>β=1.5) where the alignment of maximum density regions is along the static magnetic field [9].

Moreover, the model has been extended to include the plasma expansion into a diffusion region and towards the process chamber: Preliminary simulation results for a 5 mTorr ECWR plasma configuration (Copra 250CF shown in figure 6), are compared to the results of a spherical plasma expansion model [10] in figures 7 and 8.
The inlet (fixed $N_e=10^{17}$ m$^{-3}$ at $T_e=3.5$ eV) is located at the source bottom, resulting to a quasineutral plasma beam to the chamber. Perfectly conducting walls were considered in order to achieve a faster convergence. Even though the model nicely reproduces the rapid plasma degradation, electron density is overestimated close to the axis due to the assumption of grounded walls at $z=25$ cm. On the other hand, satisfactory agreement is found for plasma potential at axial distances $>10$ cm. Consideration of the chamber and source walls as dielectrics seems to give slightly better results but result also to much higher computational time.

Further work is in progress with modified inlet conditions and more complicated gas phase and surface chemistry in order to further validate and apply the fast convergence code in more complicated chemical systems.

4. Conclusion

A fluid model of low pressure ECWR Argon discharges, based on a modified effective collision frequency and predefined boundary conditions for the magnetic potential was developed. The model predictions are in good agreement with both experimental [6, 9] and PIC/MC [7] data, allowing for rapid estimation of basic plasma properties such as electron density, temperature and plasma potential. The simulation outputs can be used as inputs in a plasma diffusion model which seems to be in reasonable agreement with experimental data, and a spherical plasma expansion model [10].

The development of this fluid model is constantly under the perspective of its extension in complex chemical gas phase and surface processes used in ECWR material processing.

Fig. 7: Axial plasma density as calculated in the present simulation and compared to the spherical expansion model of [10].

Fig. 8: Axial plasma potential as calculated in the present simulation and compared to the spherical expansion model of [10].

References

[13]. ftp://jila.colorado.edu/collision_data/