AETHER: A simulation platform for inductively coupled plasma

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A B S T R A C T

An in-house code is developed to simulate the inductively coupled plasma (ICP). The model comprises the fluid, electromagnetic and transformer submodels. Fluid equations are solved to evaluate the plasma flow parameters, including the plasma and neutral densities, ion and neutral velocities, electron flux, electron temperature, and electric potential. The model relies on the ambipolar approximation and offers the evaluation of plasma parameters without solving the sheath region. The electromagnetic model handles the calculation of the electric and magnetic fields using the magnetic vector potential. The transformer model captures the effect of the matching circuit utilized in laboratory experiments for RF power deposition. The continuity and momentum equations are solved using finite volume method. The energy, electric potential, and magnetic vector potential equations are solved using finite difference method. The resulting linear systems of equations are solved with iterative solvers including Jacobi and GMRES. The code is written using the C++ programming language, it works in parallel and has graphical user interface. The model is applied to study ICP characteristics of a plasma confined within a cylindrical chamber with dielectric walls for two different power deposition cases. The results obtained from the developed model are verified using the plasma module of COMSOL Multiphysics. The model is also applied to a plasma source configuration, and it is demonstrated that there is an overall increase in the plasma potential when current is extracted from ICP with a biased wall electrode.

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1. Introduction

Numerical modeling of plasma is of crucial importance in understanding the underlying physics of ionized gases and in designing advanced engineering plasma devices. The field of plasma processing is focused on the utilization of RF heated plasma for industrial applications such as etching, deposition, and welding. RF plasma is classified as being in capacitive, inductive or helicon mode. Even though it may be misleading to generalize, most of the plasma processing reactors work in capacitive mode, whereas examples from electric propulsion devices predominantly work in the inductive mode.

The basic distinction between the capacitive and inductive RF discharges is the alignment of the electric field with respect to the chamber walls. If the electric field induced by RF coils is parallel to the walls, the plasma is called inductively coupled, whereas if the electric field is perpendicular to the walls, the plasma is called capacitively coupled. The model we introduce here is capable of simulating the inductively coupled case.

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Models for low density plasmas utilize the kinetic approach using methods like PIC (Particle-In-Cell) [1], Hybrid-PIC [2], PIC-MCC (Monte Carlo Collisions) [3] or PIC-DSMC (Direct Simulation Monte Carlo) [4]. All these methods include the solution of the Boltzmann kinetic equation. Many variations relying on the kinetic approach are to be found in the literature. A detailed review of these methods is to be found in [4]. In this study the fluid model is utilized and plasma is assumed to be dense enough to be considered as a continuum. Fluid models deal with the equations derived from the Vlasov equation. Knudsen number, which is defined as the ratio of the mean free path for ion–neutral collisions to the characteristic length of the domain, is the dimensionless number to decide whether the plasma medium can be considered as continuous and thus fluid approximation can be applied. The evaluation of Knudsen number for RF plasma devices is discussed in [5]. The criterion to apply the fluid approximation is:

$$Kn = \frac{\lambda_{mfp}}{L} < 0.4 \quad \lambda_{mfp} \equiv \frac{1}{n_i Q_{in}}$$

where \(\lambda_{mfp}\) is the mean free path for ions, \(L\) is the characteristic length of the discharge chamber, \(n_i\) is the neutral number density, and \(Q_{in} = (8.28072 \times 10^{-16})/c_i\) is the ion–neutral scattering cross-section where \(c_i = \sqrt{16kT_i/(\pi m_i)}\) is the relative thermal velocity between ions and background neutrals. The Knudsen number is evaluated for ions, since they are not affected by any confinement mechanism. On the other hand, electrons are confined to a certain degree within the discharge chamber because of the sheath region that repels them from the walls.

There are various thruster concepts for in-space propulsion applications, which are based on different types of plasmas. RF ion thruster is one of those thruster types where the ICP plasma is sustained within a cylindrical discharge chamber and the plasma ions are accelerated out of the chamber through the use of parallel electrostatic grids separated by a small gap [6]. A 2D fluid model for ICP in RF ion thruster discharge chamber is presented in [5]. That model requires input from experiments to simulate a thruster design properly. An analytical model presented in [7] is very successful in predicting ion thruster performance but fails to provide the spatial distribution of plasma flow parameters. A comprehensive 2D modeling [8] of the ICP in RF ion thrusters is carried out with the model presented in this paper.

There are various examples of codes that have been developed to simulate different types of plasma. For example, the PEGASUS code [9] simulates astrophysical plasma using the hybrid-PIC approach. Object–plasma interactions are investigated in DEMOCRITUS [10] also using the PIC approach. QUICKPIC [11] has been developed to study the wakefield acceleration in plasmas. TOKAM-3D [12] and BOUT++ [13] are examples for platforms that are used to perform Tokamak plasma edge simulations. Most of the relevant work has been performed in the field of plasma processing. A comprehensive fluid model, which accounts for the sheath through analytical formulations, is developed for capacitively coupled plasma (CCP) dynamics for plasma reactors [14]. A recent study [15] employs the fluid model for plasma and solves for the flow parameters in 2D axisymmetric domain focusing on the reactants and surface reaction kinetics during the etching process. For the modeling of the charged particles in the plasma, using drift-diffusion approximation for flux evaluation is a widely encountered technique [16]. This approach has been generally applied to model weakly ionized atmospheric pressure plasma reactors [17,18].

The code presented in this study, AETHER, is able to simulate ICP for different types of boundary conditions by handling the coupling between the plasma parameters and electromagnetic fields. Two of the configurations that can be solved using AETHER are demonstrated in Fig. 1. The first configuration in this figure shows a dielectric chamber with RF coils wrapped around. In this configuration the RF current passes through the coils, whose winding count and effective length are determined by the user. The desired power to be deposited \((Q_{RF})\) is given as input to the software and the necessary current for this amount of power is determined within the model. The second configuration represents the case with no RF power deposition, but an external uniform or regional power deposition \((Q_{ext})\) with a biased auxiliary electrode is placed on one of the walls. The boundary conditions for this case are clarified in Section 2.2.1. This configuration is investigated to simulate plasma sources similar to the one developed in [19]. It is also possible to simulate various types of plasma sources if the amount and region of the power deposition are known beforehand. An example of such a study is presented in [20]. Efforts on simulating plasma sources with quasineutral plasma models can be found in literature. For example, a microwave plasma source is modeled with a quasineutral hybrid-PIC model [21]. There is also an attempt to model RF controlled hollow cathode design using a fluid model for plasma [22].

The structure of this article is as follows: Section 2 lists the equations to be solved and explains how the plasma fluid model developed for this study utilizes the ambipolar flow approximation and incorporates this approximation into
the equations. Section 3 details the numerical methods employed to solve the model equations. Section 4 describes the algorithm implemented for self-consistent solution of the model equations. The components of the software like the user interface and the graphics engine are elaborated in Section 5. The results for a benchmark case and verification are presented in Section 6. Conclusion and future work are discussed in Section 7.

2. Model equations

The model equations are elaborated under three main components: Fluid model, electromagnetic model and transformer model. The electromagnetic (EM) model equations are Maxwell’s equations to evaluate the EM fields. The fluid model equations are modified Euler equations to capture the effect of the electromagnetic fields and collisions on plasma transport. The transformer model is developed to set the power to be deposited by the RF waves by modeling the matching circuit at laboratory experiments.

2.1. Electromagnetic model

Electromagnetic model consists of the solution of Maxwell’s equations. Utilizing the axially symmetric geometry that the presented study employs, the magnetic vector potential, \( A \), which is defined as follows [23], is introduced:

\[
\nabla \times A = \mathbf{B}
\]

\[
\nabla \cdot A = 0
\]

where \( \mathbf{B} \) is the magnetic field. Introducing the magnetic potential formulation to Maxwell’s equations yields:

\[
\nabla^2 A = \mu_0 \sigma \left( \nabla \phi + \frac{\partial A}{\partial t} - \frac{\nabla P}{\epsilon_0 \epsilon_r} \right)
\]

where \( \mu_0 \) is magnetic permeability of free space and \( \sigma \) is the plasma conductivity. This model is developed for low temperature plasma where the electrons are not magnetically confined and plasma frequency is lower than electron–neutral collision frequency. In this case the plasma conductivity tensor reduces to the classical (or conventional) conductivity which is given as [24]:

\[
\sigma = \frac{n_e e^2}{m_e v_{\text{eff}}}
\]

where \( n_e \) is the electron number density, \( m_e \) is the electron mass, and \( v_{\text{eff}} \) is the effective collision frequency, which is equal to the sum of electron–ion and electron–neutral elastic collision frequencies, \( v_{\text{eff}} = v_{\text{ei}} + v_{\text{en}} \). Because of the axially symmetric 2D cylindrical solution domain, the magnetic vector potential comprises only of the azimuthal component, which reduces (4) to:

\[
\nabla^2 A_\theta - \frac{A_\theta}{r^2} = \mu_0 \sigma \frac{\partial A_\theta}{\partial t}
\]

Boundary conditions for the dielectric wall discharge chamber boundaries are evaluated analytically using the Biot–Savart law. The formulas evaluated for the boundary conditions are identical to those given in [23]:

\[
A_\theta(r, z) = \frac{\mu_0 I_{\text{coil}}}{2\pi} \sum_{i=1}^{\text{coil}} \sqrt{\frac{r_c}{r}} G(m_i) + \frac{\mu_0}{2\pi} \sum_{\text{element}} \sqrt{\frac{r_i}{r}} j_{\theta, i} S_i G(m_i)
\]

where \( I_{\text{coil}} \) is the current supplied to the coils, \( r_c \) denotes the coil radius, \( r_i \) denotes the element radial position, \( S_i \) is the azimuthal element surface area, \( j_{\theta, i} \) is the current density in azimuthal direction. The function \( G(m_i) \) is evaluated as:

\[
G(m_i) = \frac{[(2 - m_i) K(\sqrt{m_i}) - 2 E(\sqrt{m_i})]}{\sqrt{m_i}} \quad m = \frac{4 r_c \tau}{(z - z_c)^2 + (r + r_c)^2}
\]

where \( K \) and \( E \) are the complete elliptic integrals of the first and second kind, respectively [25]. The boundary conditions for the magnetic vector potential equation in case of the dielectric walls are evaluated with the formula given above.

2.2. Fluid model

Fluid model solves for the plasma flow parameters assuming that the plasma behaves as a compressible gas. The pressure term is approximated by using the ideal gas relation \( P = n k T \). In this relation \( n \) is the number density, \( k \) is Boltzmann’s constant and \( T \) is temperature in Kelvins. For the charged particles, namely ions and electrons, the Lorentz force term is added as body force to momentum equations. The fluid model consists of continuity and momentum equations for ions and neutrals, energy equation for electrons, and the plasma potential equation.
Quasi-neutrality holds in the bulk plasma, such that \( n_i = n_e \) throughout the domain. The plasma sheath, which is on the order of few Debye lengths and where the quasi-neutrality does not hold any more, is excluded from the computational domain. The electric potential is calculated using the ambipolar flow approximation as elaborated below.

Continuity equations are formulated as:

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v}_i) = \dot{R} \tag{9}
\]

\[
\frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{v}_n) = -\dot{R} \tag{10}
\]

where \( \dot{R} \) denotes the ion generation through ionization collisions and is formulated as \( \dot{R} = n_i n_e (v_e Q_{ion}) \). The term in angled brackets is the ionization reaction rate obtained from [26] for xenon or argon depending on the application. Ion momentum equation is formulated as:

\[
m_i n_i \left( \frac{\partial \mathbf{v}_i}{\partial t} + \mathbf{v}_i \cdot \nabla \mathbf{v}_i \right) + k \nabla (n_i T_i) = e n_i \mathbf{E} + e n_i \mathbf{v}_i \times \mathbf{B} - m_i n_i v_{in}(\mathbf{v}_i - \mathbf{v}_n) - m_i n_i v_{ei}(\mathbf{v}_i - \mathbf{v}_e) \tag{11}
\]

where the first two terms on the right hand side are Lorentz force terms and the remaining two terms denote the collisions between the ions and the other species. Similarly, neutral momentum equation is as follows:

\[
m_n n_i \left( \frac{\partial \mathbf{v}_n}{\partial t} + \mathbf{v}_n \cdot \nabla \mathbf{v}_n \right) + k \nabla (n_n T_n) = -m_n n_i v_{in}(\mathbf{v}_n - \mathbf{v}_i) - m_n n_i v_{en}(\mathbf{v}_n - \mathbf{v}_e) \tag{12}
\]

As compared to the ion momentum equation, neutral momentum equation does not include Lorentz force terms since neutrals do not possess any charge.

The electron momentum equation is formulated very similar to the ion momentum equation [8]. For the sake of completeness, this equation is given as below:

\[
m_e n_e \left( \frac{\partial \mathbf{v}_e}{\partial t} + \mathbf{v}_e \cdot \nabla \mathbf{v}_e \right) + k \nabla (n_e T_e) = -e n_e \mathbf{E} - e n_e \mathbf{v}_e \times \mathbf{B} - m_e n_e v_{en}(\mathbf{v}_e - \mathbf{v}_n) - m_e n_e v_{ei}(\mathbf{v}_e - \mathbf{v}_i) \tag{13}
\]

The solution of this equation would be computationally very expensive because of the high speed of electrons. To capture the electron motion fully, the mesh would have to be much finer (on the order of Debye length) and the time step would be much smaller. To overcome this challenge, the drift diffusion approximation is applied. In the scope of this approximation inertia terms are neglected and it is assumed that the ion and neutral velocities are negligible compared to electron velocity, so that these terms are neglected for the collision terms. The equation after these approximations takes the form:

\[
m_e n_e (v_{ei} + v_{en}) \mathbf{v}_e = -k \nabla (n_e T_e) - e n_e \mathbf{E} - e n_e \mathbf{v}_e \times \mathbf{B} \tag{14}
\]

Calling \( \nu_{eff} = v_{ei} + v_{en} \), formulating \( \mathbf{E} = -\nabla \phi - \partial \mathbf{A}/\partial t \), and dividing each side with \( m_e \nu_{eff} \) yield the final form of the drift-diffusion approximation equation:

\[
I_{\phi} = n_e \mathbf{v}_e = -\frac{k \nabla (n_e T_e)}{m_e \nu_{eff}} + \frac{e n_e}{m_e \nu_{eff}} \left( \nabla \phi + \frac{\partial \mathbf{A}}{\partial t} - \nu_{e,\phi} \times \mathbf{B} \right) \tag{15}
\]

where \( \phi \) is the plasma electric potential, and \( \nu_{e,\phi} \) is the azimuthal component of the electron velocity. The electric field is formulated as the gradient of the electric potential on \( r-z \) plane and the time rate of change of the magnetic vector potential.

The electric potential term is evaluated using the ambipolar approximation by imposing the divergence-free current constraint:

\[
\nabla \cdot \mathbf{j} = \nabla \cdot (e n_i \mathbf{v}_i - e n_e \mathbf{v}_e) = 0 \tag{16}
\]

where \( \mathbf{j} \) denotes the current density. This equation can be used to evaluate the electric potential by inserting the electron flux from drift-diffusion approximation equation (15). The resulting expression is as follows:

\[
\nabla \cdot (\sigma \nabla \phi) = e \nabla \cdot (n_i \mathbf{v}_i) + \nabla \cdot \left( \frac{ek}{m_e \nu_{eff}} \nabla (n_e T_e) \right) + \nabla \cdot (\sigma (\nu_{e,\phi} \times \mathbf{B})) \tag{17}
\]

The solution of this equation gives the electric potential for the floating wall case. The boundary condition is zero, so that the plasma potential is evaluated with respect to the presheath boundary. The sheath potential drop is calculated with the floating wall condition, i.e. the net current reaching the wall is zero [5]:

\[
n_i u_B = \frac{1}{4} n_e v_{th} \exp \left( -\frac{e \Delta \phi_{sheath}}{kT_e} \right) \tag{18}
\]

which results in the expression for the sheath potential drop by inserting the formulas for the Bohm velocity and electron thermal velocity:
\[ \Delta \phi_{\text{sheath}} = \frac{kT_e}{e} \ln \left( \sqrt{\frac{m_i}{2\pi m_e}} \right) \]  

(19)

The electron temperature is evaluated by solving the power balance for electrons:

\[ \frac{3}{2} \frac{\partial}{\partial t} (n_e e T_e) + \nabla \cdot \mathbf{Q}_e = -e \mathbf{E}_d \cdot \mathbf{I}_e + P_{\text{dep}} - P_{\text{coll}} \]  

(20)

where the first term denotes the time rate of change of thermal energy, the second term on the left hand side is the heat flux due to conduction, which is formulated as given in [14]:

\[ \mathbf{Q}_e = \frac{5}{2} \Gamma_e e T_e - \frac{5}{2} n_e e^2 T_e \nabla T_e \]  

(21)

The first term on the right hand side is the ambipolar cooling term, where \( \mathbf{E}_d = -T_e \nabla n_e / n_e \) is the ambipolar electric field. \( P_{\text{dep}} \) is power deposited into the plasma and \( P_{\text{coll}} \) is the heat loss due to collisions. Power deposition is formulated as:

\[ P_{\text{dep}} = \sigma |\mathbf{E}|^2 \]  

(22)

If RF field is disabled and a uniform power deposition is given as input, this term is replaced by the uniform power deposition term. Power loss due to collisions include both elastic and inelastic collisions. This term is calculated as:

\[ P_{\text{coll}} = n_e n_i e (v_e Q_{\text{ion}}) U_{\text{ion}} + n_e n_i e (v_e Q_{\text{exc}}) U_{\text{exc}} + \sum_h \frac{2m_e}{m_h} \frac{3}{2} k(T_e - T_h) v_{eh} n_e \]  

(23)

where, \( U_{\text{ion}} \) is the first ionization energy, \( U_{\text{exc}} \) is the average excitation energy, and the terms in angled brackets represent the reaction rates directly computed from the Maxwellian averaged product of electron velocity and collision cross-section. First ionization energy and the average excitation energy for xenon are taken to be 12.1 eV and 8.32 eV, respectively, whereas for argon the ionization energy is 15.80 eV, and the average excitation energy is 11.50 eV. The last term denotes the energy lost to elastic collisions with heavy species, which are ions and neutrals.

The solution domain extends up to the presheath region next to the boundaries, which means that quasineutrality is valid throughout the domain and ions leave the domain with the Bohm velocity. This is the boundary condition for the ion velocity applied in the model. For the temperature boundary condition, electrons are assumed to deposit energy equal to \( 2kT_e \) to the walls. Walls are modeled as outlets for ions, whereas they are formulated as inlets for the neutrals. Ions that reach the wall go back into the computational domain as neutrals. Therefore, \( \Gamma_n = -\Gamma_i \) condition is imposed at boundaries.

2.2.1. Case with DC bias (auxiliary electrodes)

In some applications, the plasma is confined within metal walls and a bias potential can be applied at some portions of the boundaries. An example of such an application is RF plasma source, where an auxiliary electrode, which is biased positively with respect to the plasma, is placed at the wall and it acts as an anode that extracts current. The grounded walls in return collect ions and current balance is laid out between the auxiliary electrode and the walls.

The current balance to be applied on this case is investigated in previous studies from literature [20,27]. The current balance can be expressed as follows:

\[ I_{e, w} + I_{e, AE} = I_{i, w} + I_{i, AE} \]  

(24)

where \( I_{e, w} \) denotes the electron current to the wall, \( I_{e, AE} \) denotes the electron current to the auxiliary electrode, \( I_{i, w} \) denotes the ion current to the wall and \( I_{i, AE} \) denotes the ion current to the auxiliary electrode.

The current collection to an auxiliary electrode mostly depends on the ratio of the electrode area \( (A_{AE}) \) to the wall area \( (A_w) \). The ratio of these parameters is denoted with \( \alpha = A_{AE} / A_w \). Depending on this ratio, the structure of the sheath incident on the auxiliary electrode changes. The sheath incident on the electrode can either be monotonic ion sheath, monotonic electron sheath, or double sheath [27]. Most of the recent RF plasma source designs [19,28] satisfy the following condition:

\[ \alpha \geq 1.7 \mu \]  

(25)

which corresponds to monotonic ion sheath configuration. Also the term \( \mu \) is calculated as:

\[ \mu \approx \sqrt{\frac{2.3 m_e}{m_i}} \]  

(26)

The ratio of the areas for an operating gas is determined according to the specific chamber geometry. In literature a formula is laid out to calculate the plasma potential [27]:

\[ \phi_p = -\frac{T_e}{e} \ln \left[ \frac{A_w + A_{AE}}{A_w} \mu - \frac{A_{AE}}{A_w} \exp \left( -\frac{e \Delta \phi_{AE}}{T_e} \right) \right] \]  

(27)
where $\phi_p$ is the electric potential of the plasma and $\phi_{AE}$ is the electric potential of the auxiliary electrode.

The electric potential boundary conditions for dielectric walls and biased walls are implemented differently. For the case with dielectric walls, the electric potential boundary condition is applied as 0 V at all boundaries and the sheath potential drop is calculated using (19). For the biased walls configuration, the electric potential in front of the biased electrode is calculated using the formula presented in (27). After this potential is applied, the net current is calculated by evaluating the electron and ion flux values incident on the electrode. The calculated net electron current on the electrode must be equal to the net ion current on the walls (24). It is assumed that this net ion current is distributed uniformly to the walls. The electron flux incident on the walls is modified to satisfy this condition and sheath potential drop is adjusted accordingly.

2.3. Transformer model

Transformer model is implemented to be able to model the power deposition into the plasma by the RF coils. To our knowledge, the leading study that models the inductively coupled plasma as the secondary of an air core transformer is presented in [29]. This model is then improved with other works in literature [30,31]. The equations used in this model are explained elsewhere [5] and used in a previous study [32].

In this model the matching circuit used in laboratory experiments is represented. The model updates the current supplied to the RF coil. The ICP inside the discharge chamber is approximated as the secondary coil of an air core transformer.

In the scope of this model, plasma is treated as a medium where the electrons can flow through. The circuit representation of plasma and the transformer model is depicted in Fig. 2. In this figure C denotes the capacitance of the matching circuit, $R_c$ is the coil resistance, and $L_c$ is the coil inductance. Plasma is assigned a resistance and an inductance value which are denoted with $R_p$ and $L_p$, respectively. These values are calculated as follows [5]:

$$L_p = 0.002\pi (D_p \times 100) \left[ \ln \left( \frac{4D_p}{L} - \frac{1}{2} \right) \right] \times 10^{-6} + \left( \frac{R_p}{v_{\text{eff}}} \right)$$

(28)

where $D_p$ is the plasma winding diameter, $L$ is the chamber length, $v_{\text{eff}}$ is the effective elastic collision frequency and $R_p$ is the plasma resistance which is formulated as:

$$R_p = \frac{2\pi R}{\sigma L \delta}$$

(29)

where $R$ is the radius of the discharge, $\sigma$ is the plasma conductivity as given in (5), $\delta$ is the skin depth which is formulated as $\delta = \sqrt{2/(\omega \mu_0 \sigma)}$. Plasma winding diameter is taken as $2/3$ of the chamber diameter as suggested by [5]. From the plasma resistance equation, it can be seen how the plasma is attributed the characteristics of a conductor. The transformed plasma inductance and resistance become:

$$L_2 = \frac{-\omega^2 L_m^2 L_p}{R_p^2 + (\omega L_p)^2} \quad R_2 = \frac{\omega^2 L_m^2 R_p}{R_p^2 + (\omega L_p)^2}$$

(30)

where $L_m$ is the mutual inductance, which is formulated as:

$$L_m = 0.0095N \frac{(100D_p)^2}{\sqrt{(100D_w)^2 + (100L_c)^2}}$$

(31)

where $D_w$ is the coil winding diameter, $N$ is the number of coil windings, and $l_c$ is the axial length the coil covers. The total impedance of the system is calculated using the standard transformer calculations and the coil current is evaluated as described in [32]:

$$Z = \frac{Z_1 Z_2}{Z_1 + Z_2} = \frac{(1/j\omega)(R_c + R_2 + j\omega L_c + j\omega L_2)}{(1/j\omega) + (R_c + R_2 + j\omega L_c + j\omega L_2)}$$

(32)

The peak and coil currents are calculated using the total impedance value:

$$I_{\text{peak}} = \sqrt{2} Z_0 P_{\text{forward}} \left( 1 - \frac{Z - Z_0}{Z + Z_0} \right) \quad I_{\text{coilm}} = \left| I_{\text{peak}} \left( \frac{Z_1}{Z_1 + Z_2} \right) / \sqrt{2} \right|$$

(33)

where $Z_0$ is the source impedance. The resulting coil current value is transferred to the electromagnetic model and the boundary condition for the magnetic vector potential equation is calculated with this current value.
3. Numerical method

The equations described in Section 2 are discretized with the finite volume method. The details of this procedure are followed from [33]. The basis of the algorithm employed in this study, namely the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm, is explained in [34]. The modifications for the compressible gas case presented in [35] are adapted to the case presented in this study, where the species are assumed to behave as ideal gas.

Finite volume method is applied to the continuity ((9), (10)) and momentum ((11), (13)) equations. In the scope of the application of finite volume method to the Navier–Stokes equations, the continuity equation is used as the pressure correction equation. In this study, the continuity equations are handled as number density correction equations and the evaluated number density correction is used to update the velocity components. The nonlinear convective term in the momentum equation is linearized by equating the fluxes of the transported parameters ($u$ and $v$) at the boundaries around the control volume. Fluxes are evaluated with the parameters coming from the previous iteration. For example, the transient and convective terms of the momentum equation in axial direction are discretized as follows:

$$
mn\frac{u - u^0}{\Delta t} \Delta V + (mn^*u^*uA)_e - (mn^*u^*uA)_w - (mn^*v^*uA)_n - (mn^*v^*uA)_i
$$

where $u^0$ denotes the axial velocity of the previous time step, $n^*$, $u^*$ and $v^*$ denote number density, axial and radial velocity values from previous iteration, respectively. The subscripts $e$, $w$, $n$ and $i$ denote the east, west, north and south faces of the control volume, respectively. The use of the subscripts indicates that the parameters inside the brackets are evaluated at these locations. After the momentum equation is solved the number density correction equation is solved to evaluate $n'\rho$, which denotes the number density correction. Following the guidelines presented in [35], the flux term of number density correction equation (9) is discretized as:

$$(nruA)_e - (nruA)_w + (nrvA)_n - (nrvA)_i$$

(35)

where the unknown parameters in this discretization are extended as:

$$
(nruA) = (n^* + n')ru^*A = n^*ru^*A + n^*ru^*A + n'ru^*A + n'ru^*A
$$

(36)

where $n'$ is the number density correction, and $u'$ and $v'$ are axial and radial velocity corrections, respectively. The equation is solved for $n'$. The last term in the equation above, which contains the multiplication of number density and velocity corrections, is neglected assuming that this term is small [35]. The expression given above requires the formulations of velocity corrections which are formulated for ions as:

$$
u' = \left( n' \nabla \phi + en'wBz - kT_i \nabla n' + mn'v_{in}u_A \right) \frac{\Delta V}{a_v}$$

(37)

$$
u' = \left( en' \nabla \phi + en'wBz - kT_i \nabla n' + mn' \frac{w^2}{r} + mn'v_{in}u_A \right) \frac{\Delta V}{a_v}$$

(38)

where $a_u$ and $a_v$ are central coefficients of the momentum equations, which are formed according to the guidelines presented in [33]. These corrections are plugged into the number density correction equation and the equation is solved. Accordingly, the number density and velocity components are corrected at each iteration after solving the number density correction equation:

$$n = n^* + n'$$

$$u = u^* + u'$$

$$v = v^* + v'$$

(39)

In the finite volume method utilized in this study, central differencing is applied on the transported parameters. The conventional finite volume method requires the utilization of a staggered grid for easier implementation of the flux terms [33]. Velocity and number density components are calculated at different nodes at the staggered grid. The alignment of these parameters on the staggered grid is given in Fig. 3. In cylindrical coordinate system, volume of each cell changes with the radial position of the cell. The wedge-shaped finite volume cell is presented in Fig. 4.

The energy equation and also the electric potential equation are solved self-consistently with the continuity and momentum equations at every time step. The discretization of these two equations is done using the finite difference method [36]. For these equations finite difference discretization is chosen over the finite volume method for the sake of simplicity during the implementation. An interpolation scheme is developed to interpolate the values evaluated on the finite difference grid to the staggered grid, which is used in the finite volume method. Electron temperature and electric potential values are evaluated on the same nodes with the number densities through this interpolation process.

Additional to the flow parameters, the electromagnetic fields are evaluated on the grid as well. As it is the case with the energy and electric potential equations, finite differences with second order central differencing is applied on the magnetic vector potential equation (6). Since the electromagnetic model is developed separately from the fluid model, the nodes that
the equation is solved are different than the fluid equations that utilize the staggered grid. As depicted in Fig. 3, the square shaped nodes denote the nodes that the magnetic vector potential equation is solved.

A structured, rectangular grid is employed in this study to facilitate the implementation process. A 50 × 50 grid is observed to be sufficient to capture the quasineutral plasma flow parameters. In the scope of the finite volume method, ghost nodes are implemented to apply the desired boundary conditions. With the appropriate time step selection, this mesh size allows for the rapid solution of model equations. The boundary conditions for velocity are of Dirichlet type, so that constant velocity values are assigned for both ions and neutrals. Ions flow out from the system with Bohm velocity, whereas neutrals come back into the system with the same flux as ions leave the system. Since velocity boundary conditions are given as Dirichlet type, the number density correction equations have Neumann type boundary conditions.

Time-dependence of the equations is handled in the following way: In the scope of electromagnetic model, the magnetic vector potential equation can be solved either explicit or implicit in time. Fluid equations are solved implicit in time. The time step for the magnetic vector potential equation for the explicit solution is determined according to the general stability criterion [23]:

\[ \Delta t \leq \frac{1}{2} \frac{(\Delta r)^2}{\alpha} \quad \omega \Delta t \ll 1 \]

where \( \Delta r \) is the smallest mesh size, \( \alpha \) is the general diffusivity term, and \( \omega \) is the RF frequency. The general diffusivity term in this case is determined as:

\[ \alpha = \frac{1}{\mu_0 \sigma} \]  \hspace{1cm} (41)

where \( \sigma \) denotes the plasma conductivity. Since the electron motion is not resolved in time and evaluated using the drift-diffusion approximation, the time step of the plasma fluid equations can be larger without causing any inconvenience. For 2 MHz of RF frequency, the time step for the magnetic vector potential equation for explicit solution is determined to be 1.5E–11 seconds, whereas for the fluid equations the time step is determined to be 4.8E–08 seconds. If implicit solution is enabled for the electromagnetic equations, it is experienced that the solver marches faster in time. The time step for the magnetic vector potential equation for 2 MHz becomes 3.0E–10 seconds for the implicit solution.

For 2D axially symmetric domain, the second order finite volume and finite difference discretizations result in a banded matrix structure for each equation. This banded structure consists of five diagonal entries and zeros everywhere else, as depicted in Fig. 5. The preferred sparse matrix storage scheme is compressed diagonal storage (CDS) and it is implemented
as described in [37]. To solve these linearized systems, the utilization of an iterative solution scheme is mandatory. Jacobi, Gauss–Seidel [38], GMRES [39] and ILU preconditioned GMRES [40] methods are implemented in the software framework as solvers. These solvers are implemented considering the matrix storage scheme used. All equations are solved successively and residual is reduced below a predetermined threshold for all equations.

4. Algorithm

The equations presented in Section 2 are solved with the methods described in Section 3 in a self-consistent manner. The three submodels, the electromagnetic model, the fluid model and the transformer model are executed in accordance. The communication diagram between these submodels and the transferred parameters between each submodel are shown in Fig. 6. All the submodels are connected to each other by transferring parameters to provide the self-consistent solution.

Before starting to solve the model equations, AETHER needs some input parameters from the user. Some of these parameters must be given (or calculated) to perform the simulation. These input parameters for the dielectric wall configuration are listed as below:

- RF coil frequency
- Physical length of the domain in both axial and radial directions
- Number of coil windings around the chamber
- Coil radius
- Effective length of the coils
- Number of mesh nodes in radial and axial directions
- Time step for fluid and EM models

For the biased wall configuration, instead of the RF settings listed above, the auxiliary electrode size and applied voltage should be given as input. In addition, the external power deposition should be entered. The power deposition field can either be uniform or distributed on the grid according to the particular problem setting.

The solution starts with the initial uniform electron temperature, plasma density and conductivity fields, and an initial RF coil current value. First, the electromagnetic model is solved and the resulting electric and magnetic fields are transferred to the fluid model. These electromagnetic fields are used in evaluating the Lorentz force terms and the equations in the fluid model are solved in time. The resulting flow parameters are used to calculate the plasma conductivity and this value is transferred to the electromagnetic model, hence completing the coupling between the fluid and electromagnetic models.

In addition to this coupling, there is also an input to transformer model from the fluid model. Transformer model requires the flow parameters to evaluate the plasma resistance and inductance. Transformer model calculates the plasma impedance, and RF coil current is calculated and transferred to the electromagnetic model. The new current value is used in electromagnetic model to solve for the electromagnetic fields and the cycle is completed. The view of this scheme is presented in Fig. 7.
Because of the difference in the time steps of electromagnetic and fluid models, fluid equations are solved at predetermined time step intervals. For the ICP simulations presented in this study, one fluid time iteration is performed between each 200 electromagnetic time iterations. Each fluid time step consists of inner iterations that last until all the equations have residuals that lie below the tolerance value assigned before starting the solution. In the beginning of each time step, linear solvers yield high residual values for equations. As the number of inner iterations increases, these residual values decrease and eventually fall below the tolerance value, which is assigned as 1.0E-04 for this study. After the residuals fall below the tolerance, preferred solutions are written to files and then copied as previous time step’s solutions for the next time step. Plasma conductivity is recalculated to be sent to the electromagnetic model. Afterwards simulation continues with the solution of electromagnetic model. Users can either input the number of RF cycles or time steps for the simulation before initiating the calculations, or can end the simulation as desired.

5. Software components

The software developed in the scope of this work, AETHER, is built according to the model-view-controller design methodology [41] in C++ programming language. The user interface is developed using the WxWidgets [42] cross-platform user interface C++ library. The graphical user interface (GUI) of AETHER is shown in Fig. 8. The software has an OpenGL renderer for results visualization. The Visualization Toolkit (VTK) [43] is utilized for visualization purposes. The solvers and the mathematical calculations are implemented mostly parallel, providing 100% CPU utilization during the solution process. For the multi-core parallelization Microsoft’s Parallel Patterns Library [44] is utilized.

The implementation is performed using Microsoft Visual Studio 2010 Express C++. The runs are given on a dual processor 3.30 GHz Intel Xeon workstation.

6. Model results and verification

The model is used to solve a benchmark ICP configuration to verify the results with the Plasma Module of the commercial software COMSOL [45]. For the verification, the modeled geometry is a cylindrical discharge chamber with dielectric walls. The chamber is 7 cm long and has a diameter of 8 cm. RF power is deposited into the plasma through a 10 coil-winding antenna around the chamber, which extends 5 cm in the axial direction. Driving frequency is 13.56 MHz. ICP is generated using argon gas at an initial pressure of 20 mTorr, which corresponds to 3.0E+20 m\(^{-3}\) neutral density. The Knudsen number for the system is calculated to be 0.039 using the formulations presented in (1) and taking the cold gas temperature as 450 K. There is no neutral gas inlet to the system. All the ions that reach the wall go through a recomposition process and are directed back into the system as neutrals. The same configuration is also solved with COMSOL and the obtained results are compared. For comparison, two different power deposition values, that result in steady-state solutions, are chosen. These values are 3000 W and 6500 W.

The plasma density distribution obtained from AETHER at 0.1 milliseconds is shown in Fig. 9. It is seen that the plasma is confined at the center of the discharge chamber because of the losses to the walls. It is also seen that the plasma density
is slightly higher in the regions that are located below the coils (from origin to 0.050 m in axial direction) compared to regions that do not lie under RF coils (from 0.050 m to 0.070 m in axial direction).

The verification is performed by taking the data on two lines and comparing the electron number density values along these lines for different power deposition values. The first line, \( L_1 = |P_1 P_2| \), is the center line in radial direction, which starts at \( P_1 = (0.035, 0.000) \) and extends up to \( P_2 = (0.035, 0.040) \). The number density values along the line \( L_1 \) are presented in Fig. 10. The second line, \( L_2 = |P_3 P_4| \), is the center line in axial direction, which starts at \( P_3 = (0.000, 0.020) \) and extends up to \( P_4 = (0.070, 0.020) \). The number density values along the line \( L_2 \) are presented in Fig. 11.

As can be seen both from Fig. 10 and Fig. 11, solutions that come from AETHER match COMSOL’s Plasma Module results to a great degree with a little amount of overshoot. The plasma density is observed to be higher at the region below the RF antenna as expected.

Fig. 12 shows the electron temperature distribution inside the chamber, which is almost uniform, with the mean temperature value of 3.76 eV for 3000 W. This value is lower than the value evaluated by COMSOL Plasma Module, which is 4.47 eV.

The evaluated electric potential distribution is presented in Fig. 13. Here the potential at the boundaries of the domain, which is the presheath, is taken to be zero, and potential values are evaluated with respect to this sheath edge potential. The sheath potential is evaluated by equating the ion and electron fluxes to the wall, which is the zero current condition (18) that is valid for dielectric walls. It is also possible to assume that the walls are 0 V. If this is assumed, the plasma potential can be calculated by adding the sheath potential drop to the evaluated potential. According to the sheath potential drop formula (19), the sheath potential drop for the mean electron temperature of 3.76 eV is 19.81 V.

For the verification of the transformer model, a simple test case within AETHER is considered to be sufficient. Transformer model takes the power to be deposited into the plasma as one of the inputs. According to the desired input power value, it
Fig. 10. Comparison of number density results from AETHER and COMSOL along the line $L_1$ for 3000 W and 6500 W.

Fig. 11. Comparison of number density results from AETHER and COMSOL along the line $L_2$ for 3000 W and 6500 W.

Fig. 12. Electron temperature distribution for the benchmark problem from AETHER.

arranges the current to be supplied to the RF coils. The transformer model can be verified if the power given as input to the model is equal to the power calculated using (22), which is evaluated with the plasma parameters that are independent of the transformer model. For the verification, a case of 400 W RF power deposition into the plasma is investigated. The change of the total power deposition with time is presented in Fig. 14. It is observed that after about 4 RF cycles, the amount of power deposited into the plasma becomes equal to the input given to the transformer model.

The verified plasma model can be used to simulate various plasma sources that utilize different modes of heating. The second configuration investigated in this study does not utilize RF heating and instead assumes an external power deposition source. The domain investigated is a 4.6 cm long, 4.0 cm diameter cylindrical discharge chamber, which has the same dimensions as the experimental RF plasma source studied in [28]. It is assumed that 50 W of power is deposited into the plasma. The auxiliary electrode is 4.0 mm in diameter. For this case, plasma is generated by xenon gas, since xenon
Fig. 13. Electric potential distribution for the benchmark problem from AETHER.

Fig. 14. Power deposition versus time from AETHER. Verification of the transformer model for $P_{dep} = 400$ W.

Fig. 15. Change of extracted electron current with the bias voltage applied to represent the auxiliary electrode.

is the conventionally used gas for electric propulsion applications. The simulation is performed until plasma reaches the steady state at around $t = 10$ ms.

Different bias voltages are applied to the auxiliary electrode to observe the change in extracted electron current and to understand the mechanism behind this change. The change in extracted electron current with varying bias voltage is depicted in Fig. 15. The net current is calculated by subtracting the electron current from the ion current incident on the electrode. The electron current is evaluated using the electron flux calculated from the drift-diffusion equation. The current increases with increasing bias voltage as expected. The relationship between the extracted electron current and the applied bias voltage is not linear. The curve follows the trend experimentally demonstrated in [19,28].

The applied bias voltage causes an increase in the overall plasma potential compared to the case when there is no bias voltage applied. The change in the electric potential is investigated by taking the data points on the axial line that starts from the 0 V left wall and ends at the center of the biased auxiliary electrode. The change in the electric potential on this line is shown in Fig. 16 for varying auxiliary electrode bias voltage values. It is observed from this figure that the current extracting mode causes an increase in the electric potential compared to the configuration when no bias voltage is applied.
7. Conclusion

A new simulation platform, AETHER, for inductively coupled plasma modeling is built within the scope of this work. The model is verified using the Plasma Module of the commercial COMSOL Multiphysics software. The model consists of three submodels that communicate with each other. It allows the prediction of plasma properties accordingly excluding the sheath region, which would require a much higher computational power. The main advantage of the model is that it allows for the less expensive calculation of the plasma parameters since the sheath is excluded. The conventional approach in low-temperature plasma simulations is to solve Poisson’s equation on the whole domain including the sheath region which requires very fine computational mesh to capture the drastic change in the electric potential. But the model presented in this study utilizes an electric potential solver that relies on the ambipolar flow of plasma and excludes the sheath region.

Another advantage of the model developed in this study is that it employs analytical boundary conditions for the magnetic vector potential equation which eliminates the need to extend the computational mesh outside of the discharge chamber to apply far-field boundary conditions.

The model developed in the scope of AETHER can be used for plasma simulations where the continuum approach is valid and ambipolar flow is dominant. AETHER utilizes the fluid model for plasma and performs the discretizations of the continuity and momentum equations according to the finite volume method. Electric potential and energy equations are discretized with the finite difference method. The implementation can be used to model axisymmetric discharge chambers.

The ICP model introduced here can be used to simulate RF ion thrusters with slight changes in the boundary conditions. RF ion thrusters have electrostatic accelerator grid system attached to the end of the discharge chamber, instead of a dielectric wall everywhere as investigated here. To represent the outflow of plasma, transparency values for ions and neutrals would be given as inputs, which denote the ratio of the species that leave the system out of incident particles to the grid. The perpendicular magnetic field component to the grid also becomes zero because the metallic grids have very high conductivity compared to the plasma. There is also a mass flow into the system on the order of a couple of standard cubic centimeters per minute (sccm). This configuration is investigated in detail and results obtained with AETHER are presented elsewhere [8].

Currently the model can handle systems with single positive ions as heavy charged species. Especially for plasma etching and processing applications, the model should include the handling of the negative ions, which is not one of the capabilities of our code. Also the code relies on the ambipolar flow approximation. To adapt for the applications that require the evaluation of directed plasma flows, Gauss’ Law should be solved in Poisson’s equation form to evaluate the spatial distribution of the electric potential.

The model and the implementation can currently handle structured grids with axially symmetric domains. We plan to extend the code in three dimensions to gain the capability of simulating wider scope of geometries. The code is also parallelized for shared memory structures, such as a multi-core system with single processor. It should be noted though that the code is parallelized for multi-thread processing in terms of testing whether the employed algorithms are parallelizable for large scale computations. Even though a huge effort is given to increase the code performance, it is to authors’ knowledge that more computationally optimized codes are available in the literature. Interested readers are suggested to look at [13], [46] and [47]. The distributed memory parallelization is planned to be performed with MPI (message passing interface) as future work.

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Fig. 16. Change of electric potential on the axial line that from the 0 V metallic left wall to the center of the axial electrode.
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