2D Reactor Model - Mechanisms and Algorithms

Langmuir Project Documents

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Contents

Introduction **3**

Reactor Model 2D - ICP Field Equation **4**

Reactor Model 2D - Plasma Fluid Equation **10**

Reactor Model 2D - Transport Equation **22**

Introduction

This document introduces and discusses the mechanims and algorithms for 2-D reactor model.

Reactor Model 2D - ICP Field Equation

Inductively coupled E-field induced by RF coil currents is calculated.

ICP Field Eq. Derivation

Monday, August 24, 2020 4:57 PM

$$\nabla \cdot \mathbf{E} = \cancel{\frac{\rho}{\varepsilon_0}}$$

Charge neutrality in plasma
Charge is ignored in sheath

$$\xrightarrow{\quad} \nabla \cdot \vec{E} = 0$$

Electrostatic field, E_s, is solved separately

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \cancel{\mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}}$$

Displacement current is small and ignored in good conductor (plasma and metal)

$$\xrightarrow{\quad} \nabla \times \vec{B} = \mu_0 \vec{J}$$

Displacement can be found in dielectric and is ignored for ICP_v1.0

Introduce Vector Potential, $\vec{B} = \nabla \times \vec{A}$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \rightarrow \nabla \times \vec{E} = -\frac{\partial}{\partial t}\cancel{\nabla}(\times \vec{A}) \rightarrow \vec{E} = -\frac{\partial \vec{A}}{\partial t}$$

$\vec{E} = \vec{E}\exp(i\omega t + \phi)$
$\vec{A} = \vec{A}\exp(i\omega t + \phi)$

$$\vec{E} = -i\omega\vec{A}$$

Solve in frequency domain

$$\nabla \times \vec{B} = \mu_0 \vec{J}_{tot} \rightarrow \nabla \times \nabla \times \vec{A} = \mu_0 \vec{J}_{tot}$$

use math formula $\nabla \times \nabla \times \vec{A} = \cancel{\nabla(\cdot \vec{A})} \nabla^2 \vec{A}$

$$\cancel{\nabla(\cdot \vec{A})} \nabla^2 \vec{A} = \mu_0 \vec{J}_{tot}$$

$\nabla \cdot \vec{A} = \frac{i}{\omega} \nabla \cdot \vec{E} = 0 \leftarrow$ *charge neutrality*

$\nabla^2 \vec{A} = -\mu_0 \vec{J}_{tot}$ has an analytic solution

$$\boldsymbol{A} = \frac{\mu_0}{4\pi'} \int \frac{\boldsymbol{J}_{coil}(r,t') + \boldsymbol{J}_{ind}(r',t')}{|r - r'|} \mathrm{d}v'$$

$$\boxed{\nabla^2 \vec{A} = -\mu_0 \vec{J}_{tot}} \quad where\ \vec{J}_{tot} = \vec{J}_{coil} + \vec{J}_{plasma} + \vec{J}_{mater}$$

- $\vec{J}_{coil}$ *is the external current, taken as input parameter*
- $\vec{J}_{mater} = \sigma_m \vec{E}$, *where* σ_m *is the material conductivity, specified by the material properties*
- $\vec{J}_{plasma} = \sigma_p \vec{E}$ *, assuming plasma is collissional, Ohm's law is valid in plasma.*

  σ_p *depends on the electron and ion collision frequency, which* *is determined by the cross section and energy distribution. (plasma conductivity will be discussed in details later.)*

Vector potential has only tangential component, in azimuthal direction

$$\boldsymbol{A} = (0, A_\theta, 0)$$

$$\nabla^2 A_\theta - A_\theta/r^2 = -\mu_0(J_{coil} + J_{ind})$$

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{\partial^2}{\partial z^2}$$

Once A_θ is obtained, the EM field can be obtained by the following relations:

$$E_\theta = -\mathrm{i}\omega A_\theta$$

$$\mu_0 H_z = \frac{1}{r}\frac{\partial}{\partial r}(r A_\theta)$$

$$\mu_0 H_r = -\frac{\partial}{\partial r}A_\theta.$$

In the coil	**In the plasma**	**In the vaccum**
$\nabla^2 A_\theta - A_\theta/r^2 = -\mu_0 J_{coil}$ $\nabla^2 A_{\theta R} - A_{\theta R}/r^2 = -\mu_0 J_{coil}$ $\nabla^2 A_{\theta I} - A_{\theta I}/r^2 = 0.$	$\nabla^2 A_\theta - (1/r^2 + \mathrm{i}\omega\mu_0\sigma)A_\theta = 0$ $\nabla^2 A_{\theta R} - (1/r^2)A_{\theta R} + \omega\mu_0\sigma A_{\theta I} = 0$ $\nabla^2 A_{\theta I} - (1/r^2)A_{\theta I} - \omega\mu_0\sigma A_{\theta R} = 0$	$\nabla^2 A_\theta - A_\theta/r^2 = 0$

Boundary conditions:

1. $\vec{A}$ is *0* at the metal surface, where the conductivity σ is assumed to be infinite.
2. When boundary is far enough from the COIL, $\vec{A}$ is *0* ,called far-field boundary condition.
3. At the interface, continuity is enforced for $\vec{A}$.
   a. For the boundary conditions at the interfaces between

different zones we assume continuity of the vector potentials cross the interfaces without jumping. This implies that the magnitude and the direction of $A\theta R$ and $A\theta I$ remain unchanged on both sides of the interfaces. Physically this is not necessarily consistent since a change in the dielectric properties of the material across the interface would result in a corresponding difference in the normal component of the electric field, and hence of the vector potential. It is difficult, however, in the FLUENT code to set different boundary conditions on the two sides of an interface. For the interfaces shown in figure 1 the electric field and, accordingly, the vector potential are parallel to the interfaces so that the continuity in the boundary conditions can be applied.

In the coil:

$$\nabla^2 A_\theta - A_\theta / r^2 = -\mu_0 J_{coil}$$

4. or

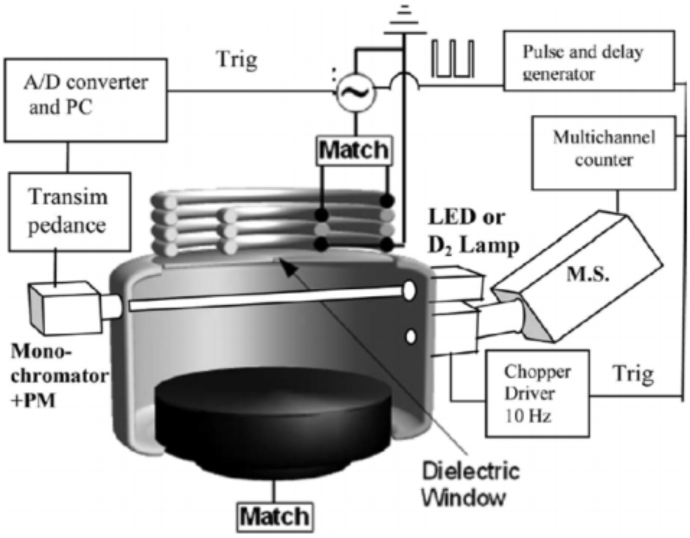
$$\nabla^2 A_{\theta R} - A_{\theta R} / r^2 = -\mu_0 J_{coil}$$

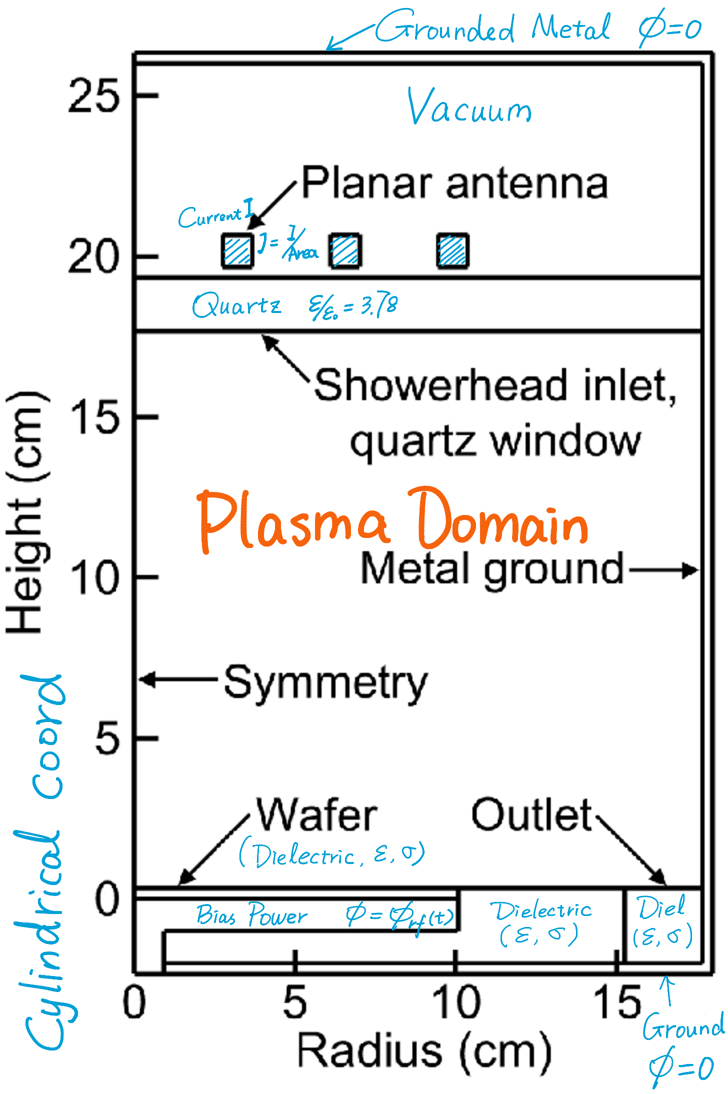
$$\nabla^2 A_{\theta I} - A_{\theta I} / r^2 = 0.$$

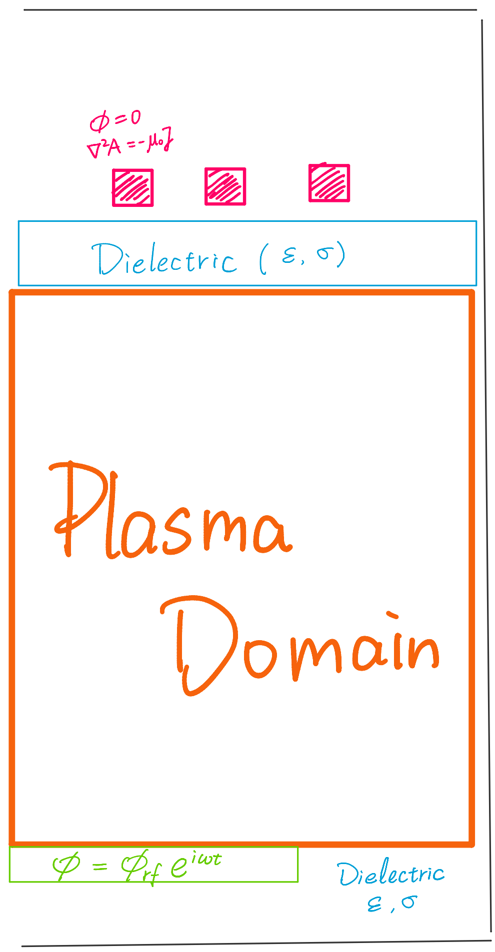
Here we have assumed that the electric conductivity of the coil is zero, which means $Jind$ in the coil is zero. $Jcoil$ = I/(π a2) is uniformly distributed over the cross section of the coil conductor.

Boundary condition and geometry

Tuesday, September 22, 2020 9:37 AM







1. Poisson equation is solved in the whole domain.
   a. Ground metal, $\phi = 0$, for most boundaries
   b. Bias power, with assigned potential boundary, $\phi = \phi(t)$
   c. At $r = 0, \vec{E} = 0, \frac{\partial \phi}{\partial r} = 0$
2. Fluid equations are solved in the plasma domain.
   a. Lossy boundary at all surfaces. When particle

density get to the surfaces, $n_{e,i}$ is enforced to be 0.

b. At $r = 0$, $\frac{\partial n_{e,i}}{\partial r} = 0$.

Reactor Model 2D - Plasma Fluid Equation

Basic plasma fluid equations are introduced here.

ICP Fluid Equation - Organized

Tuesday, September 1, 2020 12:01 PM

Continuity Eq.

$$\frac{\partial n_e}{\partial t} = -\nabla \cdot \vec{\Gamma_e} + S_e$$

Two terms unknown

Source Term

1. $S_e = 0$, no source term (no ionization), plasma will decay
2. $S_e = k_e(T_e)n_g n_e$, simple ionization term, is determined by T_e and n_e , n_g can be seen as constant unless n_g is updated through flow caculation
3. $S_e = k_e(f(\varepsilon))n_g n_e$, ionization term is determined by EEDF (Electron Energy Distribution Function), which is computed from EEDF module

Flux Term

1. $\vec{\Gamma_e} = -D_e \nabla n_e - e\mu_e n_e \nabla \phi$, Drift-Diffusion Approximation, electron flux is assumed to be diffusion term + drift term
2. $\vec{\Gamma_e}$, uses Schaffeter–Gummel fluxes which is essentially an auto-selecting upwind differentiation technique, still under Drift-Diffusion Approximation
3. $\frac{\partial \vec{\Gamma}_e}{\partial t} = \frac{e n_e \nabla \phi}{m_e} - \frac{\nabla p}{m_e} - v_{coll}\vec{\Gamma}_e$, momentum equation
4. Momentum equation + Energy equation

$\frac{\partial n_e}{\partial t} = \nabla \cdot (D_e \nabla n_e + e\mu_e n_e \nabla \phi)$, $n_e(t + \Delta t)$ is determined by $n_e(t)$, electrostatic potential $\phi(t)$.

Diffusion Coefficient, $D_e = \frac{k_B T_e}{m_e v_{coll}}$; Mobility, $\mu_e = \frac{e}{m_e v_{coll}}$;

Unknown term is $\phi(t)$, which is determined by the Poisson's Equation:

$\nabla(\epsilon \nabla \phi) = -(\Sigma n_i - n_e)$,

Poisson's Equation is determined by all charged species including ions, so ion densities need to be solved simultaneously.

Ion densities can be solved following the same routine as electrons

$\frac{\partial n_i}{\partial t} = \nabla \cdot (D_i \nabla n_i + e\mu_i n_i \nabla \phi)$, $n_i(t + \Delta t)$ is determined by $n_i(t)$, electrostatic potential $\phi(t)$.

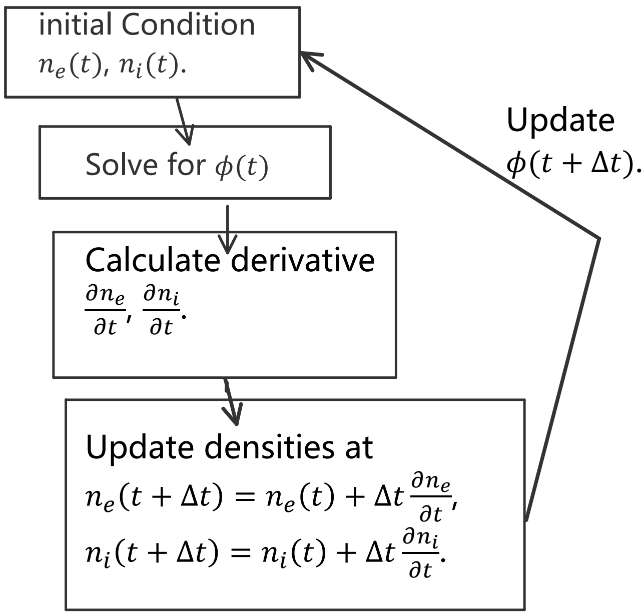
Diffusion Coefficient, $D_i = \frac{k_B T_i}{m_i v_{coll,i}}$; Mobility, $\mu_i = \frac{e q_i}{m_i v_{coll,i}}$;

Now we have,

$\frac{\partial n_e}{\partial t} = f_1(n_e(t), \phi(t))$,

$\frac{\partial n_i}{\partial t} = f_1(n_i(t), \phi(t))$,

$\nabla(\epsilon \nabla \phi(t)) = -(\Sigma n_i(t) - n_e(t))$,



Since at the surface/b.c., time step Δt, is limited by the dielectric relaxation time for explicit method.

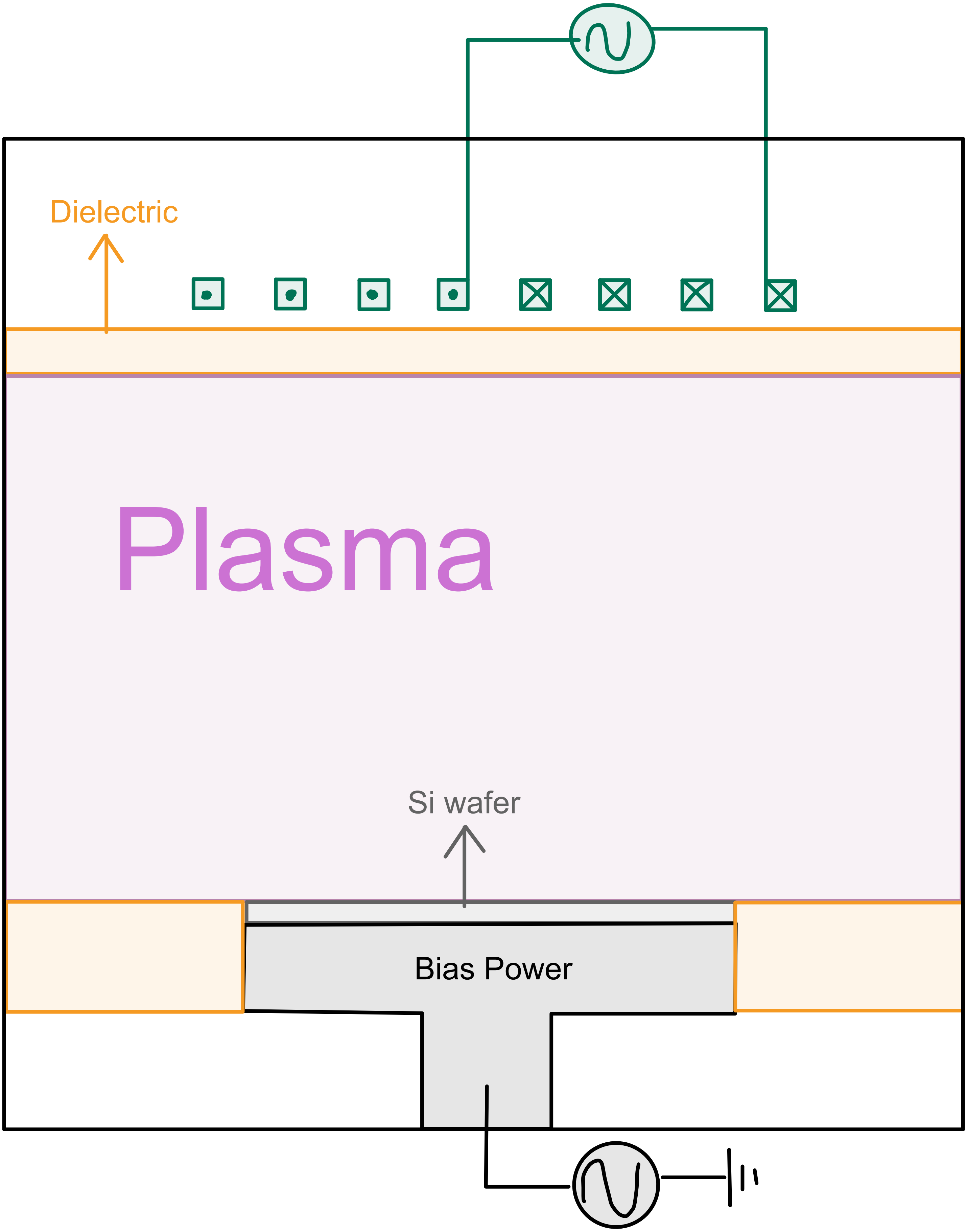
$$\Delta t < \frac{\epsilon_0}{\sigma_m}.$$

σ_m is the conductivity of the materials.
An implicit coupling method is needed.

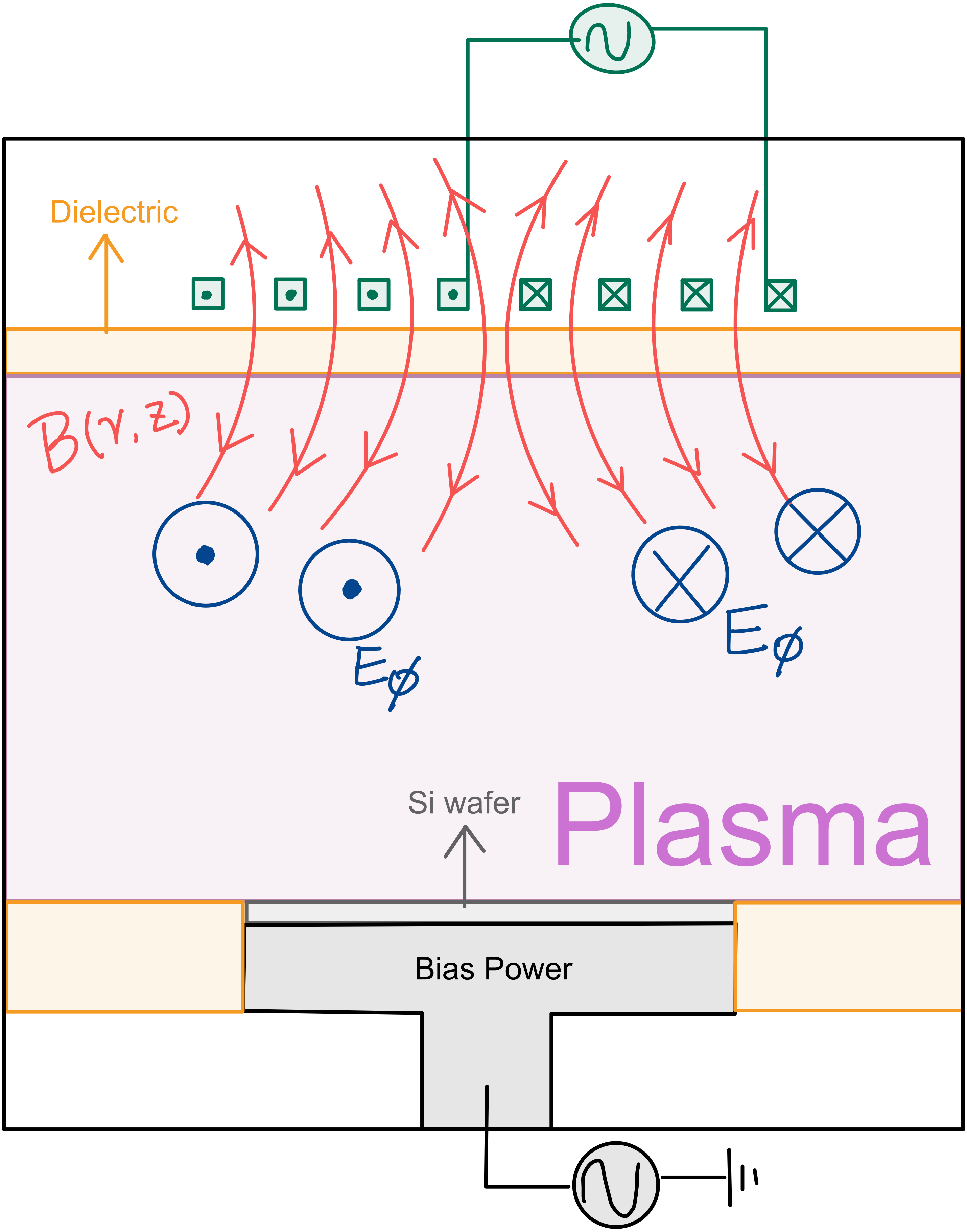
Boundary Condition

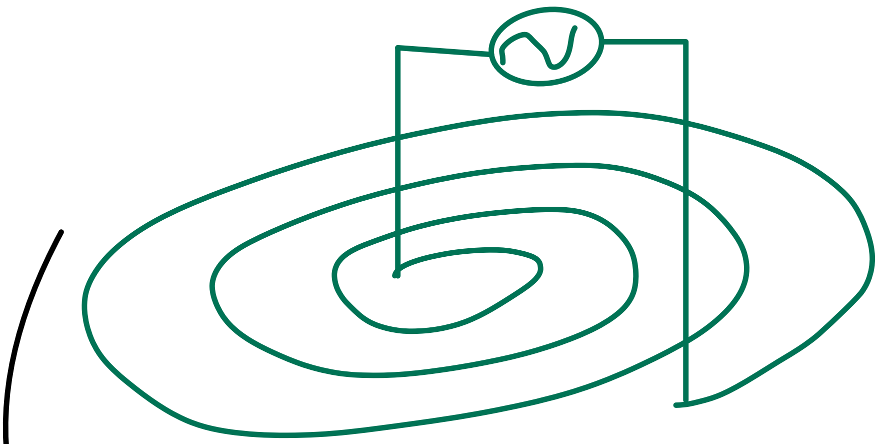
Cartesian	Cylindrical
$n_{e,i} = 0$, at non-plasma b.c.	$\vec{\Gamma}_{e,i}\ in\ \vec{r}$, at $r = 0$
$\phi = \phi_0\|_{b.c.}$, at domain b.c.	$\nabla\phi = 0\ in\ \vec{r}$, at $r = 0$

Plasma Fluid Model V1.0



Plasma Fluid Model V1.0



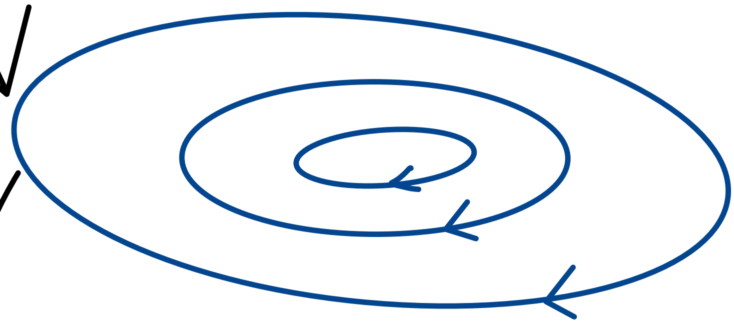


$$\vec{J} = J_0 e^{i\omega t}$$

Current in coils

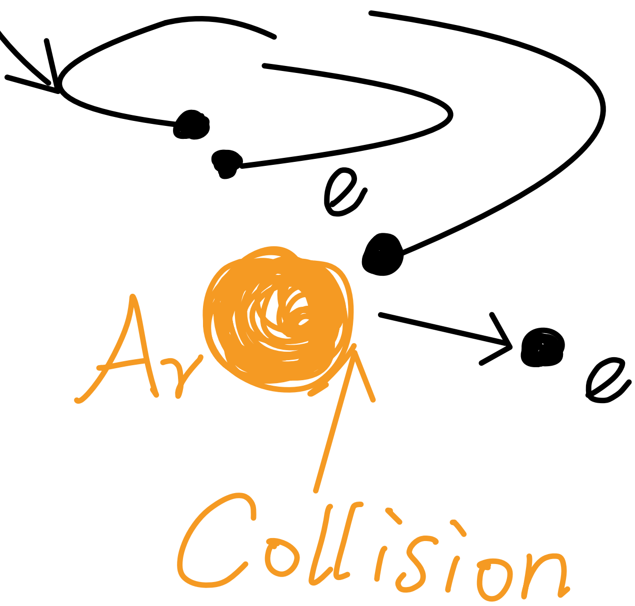
$$\vec{B} = B_0 e^{i\omega t}$$

$\vec{B}$ field in chamber



$$\vec{E} = E_\phi e^{i\omega t}$$

$\vec{E}$ field in plasma



$$a_\phi = \frac{q_e E_\phi e^{i\omega t}}{m_e}$$

steady state,

$$v_\phi = \mu_e E_\phi e^{i\omega t}$$

$\vec{J} \rightarrow \vec{B} \rightarrow \vec{E} \rightarrow \vec{v}$

$J_\phi \rightarrow B_{r,z} \rightarrow E_\phi \rightarrow v_\phi$

All B and E fields are the intermediate steps from current to velocity. As long as velocity is obtained, B and E fields are discarded.

Velocity $\vec{v}$

External J_ϕ

$(n_i - n_e)$ Self induced

$$v_\phi = \mu_e E_\phi$$

$$v_{r,z} = -D_e \frac{\nabla n_e}{n_e} - \mu_e E_{r,z}$$

$$v_\phi \xrightarrow{\text{Collisions}} v_{r,z}$$

Collision Process can be very complicated.
Instead, we solve for electron temperature, Te.

$$D_e, \mu_e = D_e(T_e), \mu_e(T_e)$$

Diffusion coefficient and mobility

$$\Gamma_e = -D_e \nabla n_e - \mu_e n_e \vec{E}$$

$$D_e = \frac{kT_e}{m_e \nu_{coll}} \qquad \mu_e = \frac{|e|}{m_e \nu_{coll}}$$

$$\nu_{coll} = \nu_{coll}(T_e)$$

Continuity Eq. for electron

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \vec{\Gamma}_e = S_e$$

$$S_e = S_e(T_e)$$

1D Maxwellian velocity distribution

$$f(v) = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mv^2}{2kT}\right)$$

m — mass of particle

k — Boltzmann's constant

T — particle temperature, width of the Maxwellian distribution

1D average kinetic energy

$$\mathcal{E}_{mean} = \frac{\int \frac{1}{2} m v^2 f(v)\, dv}{\int f(v)\, dv} = \frac{1}{2} kT$$

3D mean energy $\mathcal{E}_{mean} = \frac{3}{2} kT$

With the assumption of MaxWellian distribution

$\mathcal{E}$ is equivalent to T

In plasma physics, we usually use temperature instead of energy and velocity

Energy equation

Continuity Eq. for electron

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \vec{\Gamma}_e = S_e$$

Energy Eq. for electron

$$\frac{\partial}{\partial t}(n_e \varepsilon_e) + \nabla \cdot \vec{Q}_e = P_{in} - P_{Coll\text{-}Loss}$$

$n_e \varepsilon_e = \frac{3}{2} n_e k T_e$ — Electron Energy Density

$\vec{Q}_e = \frac{5}{2} k T_e \vec{J}_e - k_e \nabla T_e$ — Energy Flux

$P_{in} = \boxed{\vec{J}_e \cdot \vec{E}}$ — Joule/Ohm/collision Heating

$$P_{coll\text{-}loss} = P_{momentum\text{-}Loss} + P_{reaction\text{-}Loss}$$

$$= 3\frac{m_e}{M} n_e k \nu_m (T_e - T_g) + n_e N \sum_j k_j(T_e) \Delta \varepsilon_j$$

Local heating vs. Non-local heating

Local Heating — Fluid Model
collision freq is sufficient high
Energy is balanced Locally

$$P_{in} = \vec{J}_e \cdot \vec{E} = \boxed{J_\phi E_\phi} + \boxed{J_r E_r + J_z E_z}$$

External Field

Induced Field

$$J_{coil} \rightarrow B \rightarrow E_\phi$$

$$\nabla^2 \phi = -\frac{e}{\varepsilon_0}(n_i - n_e)$$

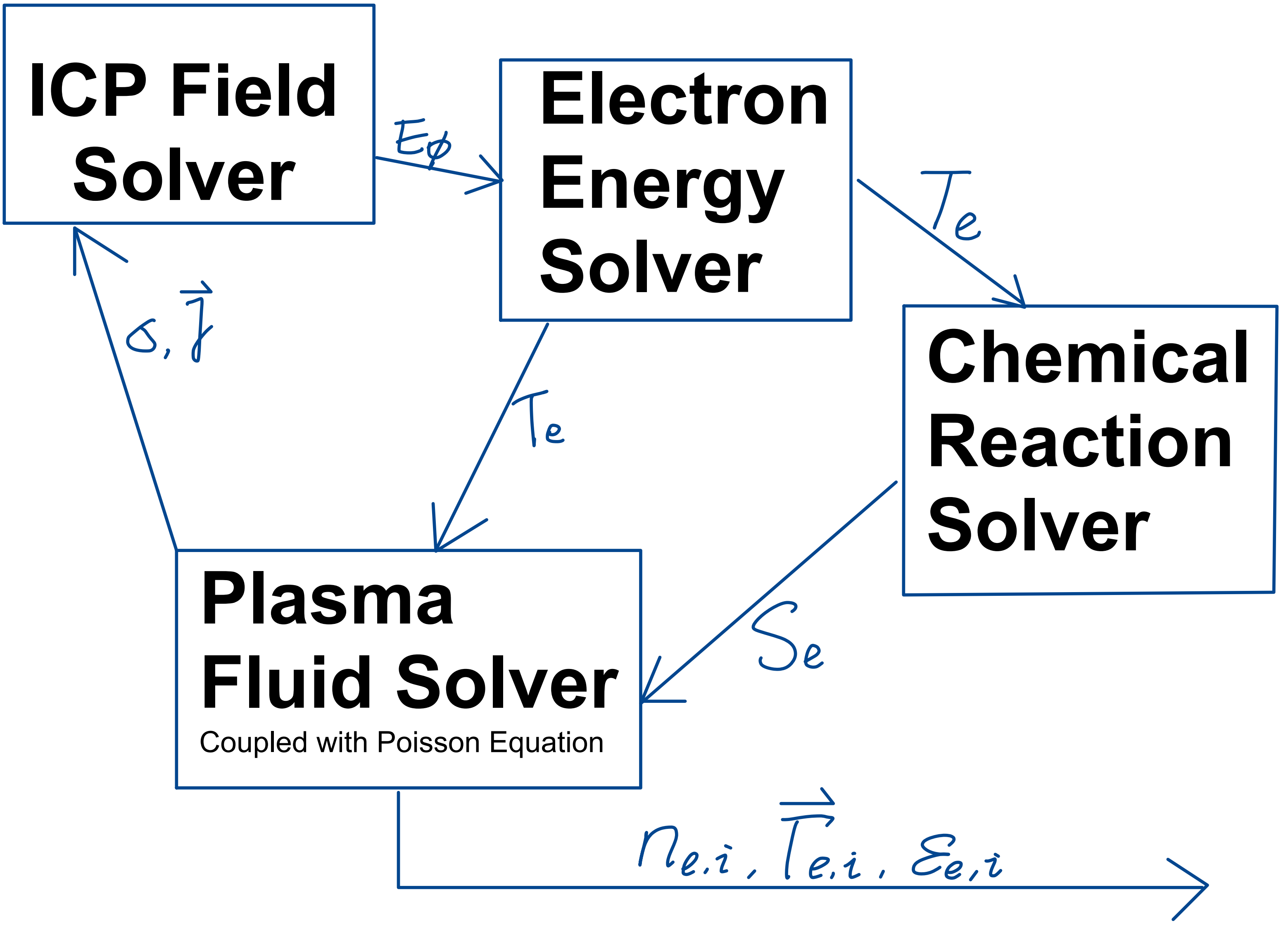
$$J_\phi = \sigma E_\phi$$

$$J_{r,z} = \sigma E_{r,z}$$

Ohm's Law
Assume plasma is homogeneous
σ is same for all directions

$$\sigma = \frac{n_e e^2}{m_e \nu_{coll}}$$

$$\nu_{coll} = \nu_{coll}(T_e)$$


ICP Field Solver
E_ϕ
Electron Energy Solver
T_e
Chemical Reaction Solver
S_e
T_e
$\sigma, \vec{J}$
Plasma Fluid Solver
Coupled with Poisson Equation
$n_{e,i}, \vec{\Gamma}_{e,i}, \varepsilon_{e,i}$

Reactor Model 2D - Transport Equation

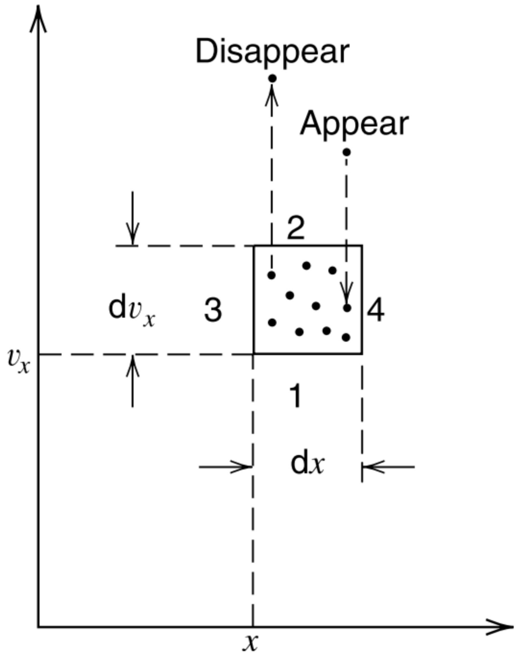
Transport equation is discussed here.

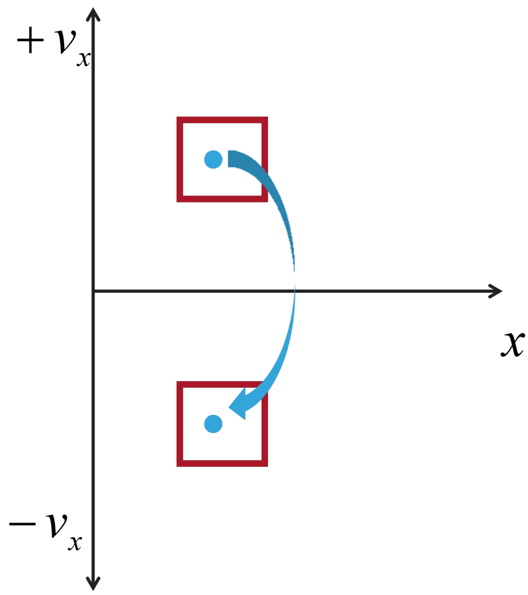
Drift-Diffusion Equation

Tuesday, October 13, 2020 10:38 AM

Diffusion and Mobility

$f(\mathbf{r}, \mathbf{v}, t)\mathrm{d}^3 r\, \mathrm{d}^3 v =$ number of particles inside a six-dimensional phase space volume $\mathrm{d}^3 r\, \mathrm{d}^3 v$ at $(\mathbf{r}, \mathbf{v})$ at time t





$$\frac{df}{dt} = 0$$

$$\frac{\partial f}{\partial t} + \frac{\partial \vec{r}}{\partial t} \bullet \nabla_{\vec{r}} f + \frac{\partial \vec{v}}{\partial t} \bullet \nabla_{\vec{v}} f = 0$$

$$\frac{\partial f}{\partial t} + \vec{v} \bullet \nabla_{\vec{r}} f + \vec{a} \bullet \nabla_{\vec{v}} f = 0$$

$$\frac{\partial}{\partial t} f + \vec{v} \bullet \nabla_r f + \frac{\vec{F}}{m} \bullet \nabla_v f = collision\_term$$

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) + etc.$$

$$dN = f(\vec{r}, \vec{v}, t) d^3 \vec{r}\, d^3 \vec{v}$$

$$n(\vec{r}, t) = \iiint f(\vec{r}, \vec{v}, t) d^3 \vec{v}$$

$$\langle v(\vec{r}, t) \rangle = \frac{\iiint \vec{v} f(\vec{r}, \vec{v}, t) d^3 \vec{v}}{n(\vec{r}, t)}$$

$$n(\vec{r}, t) \langle v(\vec{r}, t) \rangle = \iiint \vec{v} f(\vec{r}, \vec{v}, t) d^3 \vec{v}$$

$$\boxed{mn \frac{\partial}{\partial t} \vec{u} = qn \vec{E} - \nabla p - mn\nu_m \vec{u}}$$

In a cold uniform plasma with an applied electric field, gives rise to a conductivity. The friction term, arising from collisions with a background species, also leads to diffusion in a nonuniform warm plasma.

Drift-Diffusion Approximation

At this point, we are only interested in steady-state solution, which results in $\frac{\partial u}{\partial t} = 0$

$$qnE - \nabla p - mnv_m u = 0$$

where we assume that the background species is at rest and that the momentum transfer frequency nm is a constant, independent of the drift velocity.

Taking an isothermal plasma, such that $\nabla p = kT\nabla n$, and solving equation above for u, we obtain

$$u = \frac{qE}{mv_m} - \frac{kT}{mv_m}\left(\frac{\nabla \mathrm{n}}{\mathrm{n}}\right)$$

$$nu = \frac{qnE}{mv_m} - \frac{kT\nabla n}{mv_m}$$

$$\Gamma = \pm\mu n E - D\nabla n$$
$$= Drift + diffusion$$

Where

$$\mu = \frac{|q|}{m v_m}\left(\frac{m^2}{V\ \cdot s}\right) = mobility$$

$$D = \frac{kT}{m v_m}\left(\frac{m^2}{s}\right) = diffusivity$$

$v_m = momentum\ collision\ frequency$

$Depends\ on\ Cross\ Section\ and\ Temperature$

Einstein Relation:

$$D = \frac{kT}{|q|}\mu$$

Ambipolar Diffusion

In the steady state we make the congruence assumption that the flux of electrons and ions out of any region must be equal, $\Gamma_e = \Gamma_i$, such that charge does not build up. This is still true in the presence of ionizing collisions, which create equal numbers of both species. Since the electrons are lighter, and would tend to flow out faster (in an unmagnetized plasma), an electric field must spring up to maintain the local flux balance. That is, a few more electrons than ions initially leave the plasma region to set up a charge imbalance and consequently an electric field.

$$-\mu_e n_e E - D_e \nabla n_e = \mu_i n_i E - D_i \nabla n_i$$

Note that drift is negative for electrons and positive for ions, where E-field drags electrons down and speed ions up to balance the fluxes. Assume $n_e \simeq n_i = n$

$$E = \frac{D_i - D_e}{\mu_i + \mu_e}\left(\frac{\nabla n}{n}\right)$$

Substituting this value of E into the common flux relation we have

$$\Gamma = \mu_i \frac{D_i - D_e}{\mu_i + \mu_e} \nabla n - D_i \nabla n = -\frac{\mu_e D_i + \mu_i D_e}{\mu_i + \mu_e} \nabla n$$

You can see the coefficient is symmetric, beautiful!
Define

$$D_{ambi} = \frac{\mu_e D_i + \mu_i D_e}{\mu_i + \mu_e}$$

$$\Gamma = -D_{ambi} \nabla n$$

$$\mu_e = \frac{|q|}{v_m}\left(\frac{1}{m_e}\right) \gg \mu_i = \frac{|q|}{v_m}\left(\frac{1}{m_i}\right), sine\ m_e \ll m_i$$

$$D_{ambi} \approx D_i + \frac{\mu_i}{\mu_e} D_e = D_i\left(1 + \frac{T_e}{T_i}\right)$$

Put it back to continuity equation.

$$\frac{\partial n}{\partial t} = D_{ambi} \nabla^2 n + S_e$$

Now the continuity equation becomes DIFFUSION equation, which is much easier to solve.

equation, which is much easier to solve.

When using Ambipolar Diffusion Approximation, we only calculate ion density n_i, and enforce charge neutrality, $n_e = n_i$.

Ambipolar E-field is ,

$$E = \frac{D_i - D_e}{\mu_i + \mu_e}\left(\frac{\nabla n}{n}\right)$$

Can be used for energy input for T_e.
Additionally, Poisson's Equation is avoided.

One of the main assumptions in the drift-diffusion model is that the background gas is dominant.