Implementation of a plasma-neutral model in NIMROD

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Outline

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- Fluid description
- NIMROD FEM
- Code implementation
- Reaction rates
- Continuity test case
- Momentum test case
- Energy conservation test case

Motivation for a reacting plasma-neutral model

- Implementing a computationally viable model to study the primary effects of plasma-neutral interactions
- Using the established NIMROD code as a well known platform
- Study different application areas in fusion science, including:
  - Startup in pulsed experiments
  - Charge-exchange transport
  - Tokamak boundary
  - Gas/pellet refueling
  - Massive Gas Injection disruption mitigation

Description of the plasma-neutral model

- Physical model is derived by E. Meier and U. Shumlak*
- The model is a generalization of Braginskii, in which a single fluid MHD plasma reacts and interacts with a gas-dynamic neutral fluid.
- It accounts for ionization, recombination, and charge exchange collisions:

$$e^- + n \rightarrow i^+ + 2e^- - f_{ion}$$

$$e^- + i^+ \rightarrow n + hn$$

$$i^+ + n \rightarrow n + i^+$$

- Further Assumptions:
  - Single ionization and overall charge neutrality
  - Negligible electron mass
  - No bound excited states
  - Effective ionization energy included
  - Optically thin plasma / neutral fluid

* E.T. Meier and U. Shumlak, Phys. Plasmas (2012)

Fluid model is derived by taking the moments of Boltzmann equation

- Distribution function for each species is given by Boltzmann equation

$$\frac{\partial f_a}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_a + \frac{q_a}{m_a}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{v}} f_a = \left.\frac{\partial f_a}{\partial t}\right|_{collisions} = C_a^{scattering,reacting}$$

- Moments of the reaction collision operators are required to derive the governing equations for fluid model, e.g.

$$\int C_n^{ion}\, d\mathbf{v} \approx \Gamma_n^{ion} \equiv -\int f_n(\mathbf{v}')\int f_e(\mathbf{v})\,\sigma_{ion}(v_{rel})\,v_{rel}\, d\mathbf{v}d\mathbf{v}' = -n_e n_n \langle \sigma_{ion} v_e \rangle$$

- Simplistic closures are used for stress tensors and heat flux

$$\Pi_n = -\xi_n\left[\nabla\mathbf{v}_n + \left(\nabla\mathbf{v}_n\right)^T\right]$$

$$\mathbf{h}_n = -\kappa_n \nabla T_n$$

- Mass, momentum and energy are conserved

Two-component plasma-neutral model

- Continuity

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = \Gamma_i^{ion} - \Gamma_n^{rec}$$

$$\frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{v}_n) = \Gamma_n^{rec} - \Gamma_i^{ion}$$

- Momentum

$$\frac{\partial}{\partial t}(m_i n \mathbf{v}) + \nabla \cdot (m_i n \mathbf{v}\mathbf{v} + p\mathbf{I} + \Pi) = \mathbf{j} \times \mathbf{B} + \mathbf{R}_i^{in} + \mathbf{R}_e^{en}$$
$$+ \Gamma_i^{ion} m_i \mathbf{v}_n - \Gamma_n^{rec} m_i \mathbf{v} + \Gamma^{cx} m_i (\mathbf{v}_n - \mathbf{v}) + \mathbf{R}_{in}^{cx} - \mathbf{R}_{ni}^{cx}$$

$$\frac{\partial}{\partial t}(m_i n_n \mathbf{v}_n) + \nabla \cdot (m_i n_n \mathbf{v}_n \mathbf{v}_n + p_n \mathbf{I} + \Pi_n) = - \mathbf{R}_i^{in} - \mathbf{R}_e^{en}$$
$$- \Gamma_i^{ion} m_i \mathbf{v}_n + \Gamma_n^{rec} m_i \mathbf{v} - \Gamma^{cx} m_i (\mathbf{v}_n - \mathbf{v}) - \mathbf{R}_{in}^{cx} + \mathbf{R}_{ni}^{cx}$$

Ionization/Recombination

Elastic Neutral Collisions

Charge Exchange Collisions

Γ - Density production rate

$\mathbf{R}$ - Frictional force

Q - Collisional heat exchange

Two-component plasma-neutral model

- Energy

$$\frac{\partial e}{\partial t}+\nabla\cdot\left[e\mathbf{v}+\mathbf{v}\cdot\left(p\mathsf{I}+\mathsf{P}\right)+\mathbf{h}\right]=\mathbf{j}\cdot\mathbf{E}$$

$$+\mathbf{v}\cdot\mathbf{R}_i^{in}+\mathbf{v}_e\cdot\mathbf{R}_e^{en}+Q_i^{in}+Q_e^{en}+\Gamma_i^{ion}\left(\frac{1}{2}m_i\mathbf{v}_n^2-f_{ion}\right)+Q_n^{ion}-\Gamma_n^{rec}\frac{1}{2}m_i\mathbf{v}^2-Q_i^{rec}-Q_e^{rec}$$

$$+\Gamma^{cx}\frac{1}{2}m_i\left(\mathbf{v}_n^2-\mathbf{v}^2\right)+\mathbf{v}_n\cdot\mathbf{R}_{in}^{cx}-\mathbf{v}\cdot\mathbf{R}_{ni}^{cx}+Q_{in}^{cx}-Q_{ni}^{cx}$$

$$\frac{\partial e_n}{\partial t}+\nabla\cdot\left[e_n\mathbf{v}_n+\mathbf{v}_n\cdot\left(p_n\mathsf{I}+\mathsf{P}_n\right)+\mathbf{h}_n\right]=$$

$$-\mathbf{v}_n\cdot\left(\mathbf{R}_i^{in}+\mathbf{R}_e^{en}\right)+Q_n^{in}+Q_n^{en}-\Gamma_i^{ion}\frac{1}{2}m_i\mathbf{v}_n-Q_n^{ion}+\Gamma_n^{rec}\frac{1}{2}m_i\mathbf{v}^2+Q_i^{rec}+Q_e^{rec}$$

$$-\Gamma^{cx}\frac{1}{2}m_i\left(\mathbf{v}_n^2-\mathbf{v}^2\right)-\mathbf{v}_n\cdot\mathbf{R}_{in}^{cx}+\mathbf{v}\cdot\mathbf{R}_{ni}^{cx}-Q_{in}^{cx}+Q_{ni}^{cx}$$

- Faraday's law

$$\frac{\partial\mathbf{B}}{\partial t}=\nabla\times\left[\mathbf{v}\times\mathbf{B}-\frac{1}{qn}\left(\mathbf{j}\times\mathbf{B}-\nabla\cdot\mathsf{R}_e-\mathbf{R}_i^{ie}+\mathbf{R}_e^{en}\right)\right]$$

NIMROD finite element code*

- **N**on-**I**deal **M**agnetohydrodynamics with **R**otation, **O**pen **D**iscussion
- NIMROD is a 2D Finite Element code in poloidal plane and employs Fourier expansion in 3rd dimension
  - It is commonly used for toroidal or linear geometry with arbitrary mesh shaping
- NIMROD expands the primary variables into equilibrium and perturbation parts as

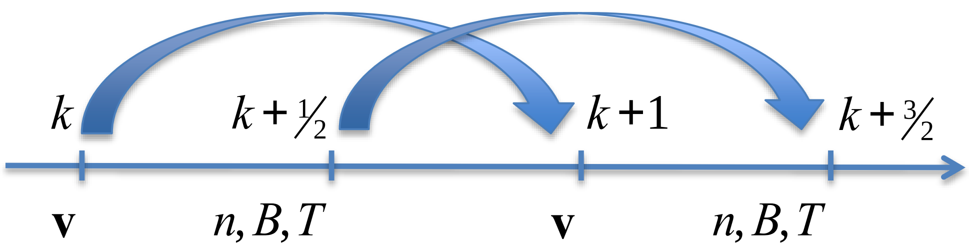
$$q = q_{eq} + \tilde{q} = q_{eq} + \sum_{n=-N}^{+N} q_n \left(R, Z\right) e^{ik_n \Phi}$$

- It is able to solve linearized or non-linear equation sets.
- All the equations are solved for the perturbed part.

* C. R. Sovinec et. al., JCP (2004)

NIMROD implicit leap-frog time integration

- NIMROD adopts an implicit leap-frog time integration scheme, in which flow velocity is staggered in time from the other fields.



- By employing this scheme equations are decoupled and evolved separately, giving the following advantages:
  - sequential solution of governing equations
  - smaller matrices
  - less memory
  - quicker runs

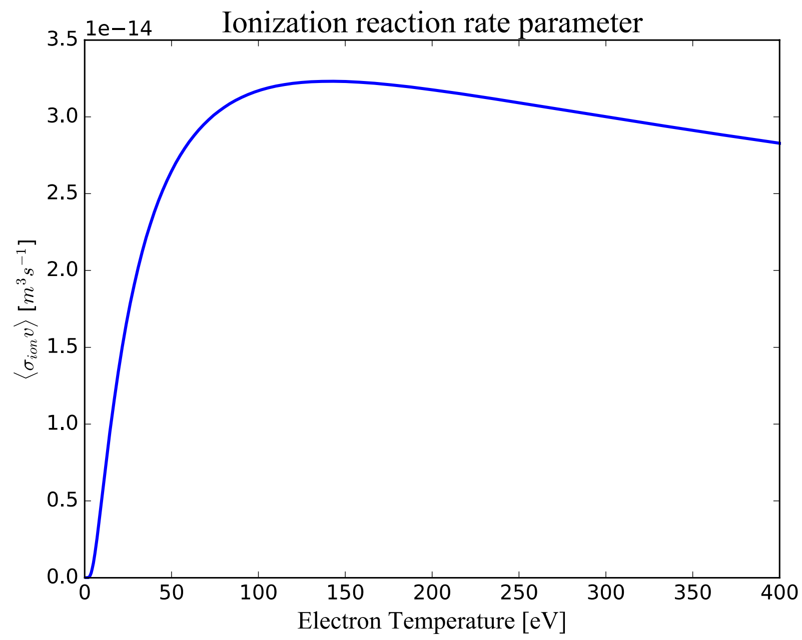
Ionization reaction rate coefficient

- Ionization rate depends on plasma and neutral number densities as well as averaged ionization reaction rate.

$$G_i^{ion} = \langle s_{ion} v_e \rangle n n_n$$

- The ionization reaction rate is a function of temperature*.

$$\langle s_{ion} v \rangle = \frac{0.291 \times 10^{-13}}{0.232 + 13.6 / T_e} \left(\frac{13.6}{T_e} \right)^{0.39} \exp\left(-\frac{13.6}{T_e} \right) \; [m^3 s^{-1}]$$



*G. S. Voronov, Atomic Data Nucl. Data (1997)

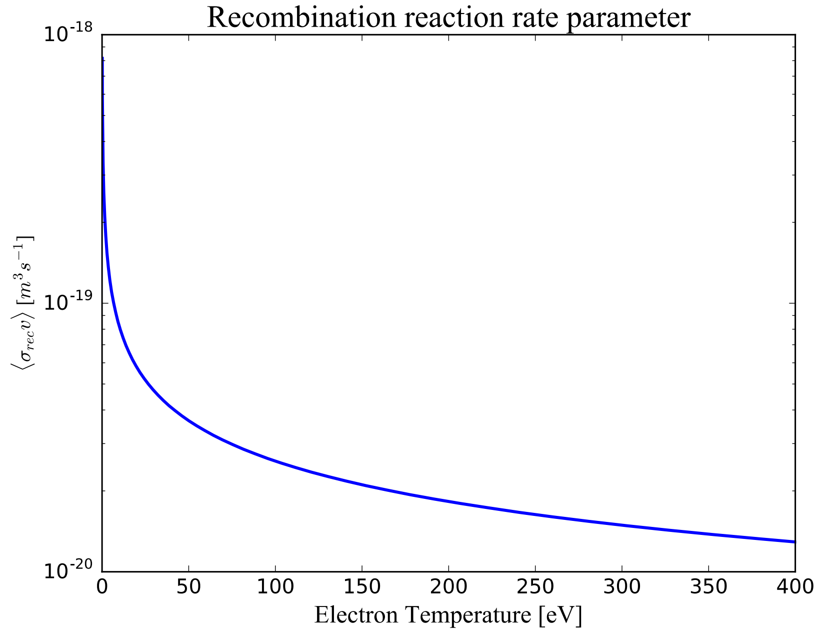
Recombination reaction rate coefficient

- Also recombination rate depends on plasma number density as well as recombination reaction rate coefficient.

$$\Gamma_n^{rec} = \langle \sigma_{rec} v_e \rangle n^2$$

- Likewise, the recombination reaction rate is a function of temperature*.

$$\langle \sigma_{rec} v \rangle = 0.7 \times 10^{-19} \left(\frac{13.6}{T_e} \right)^{1/2} \quad [m^3 s^{-1}]$$



*R. W. P. McWhirter (1965)

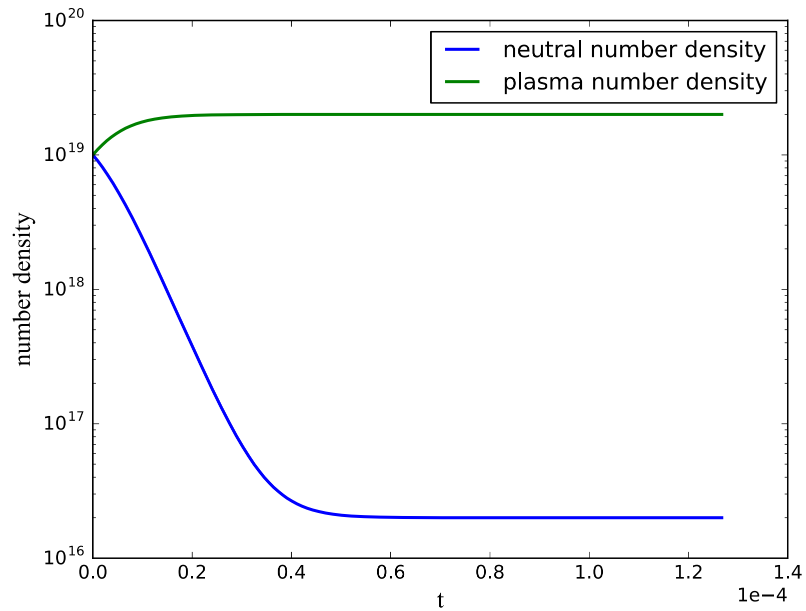
Coronal equilibrium test case shows the equilibration of electron impact ionization and radiative recombination

- Interaction between static plasma and neutral fluids is solely because of ionization and recombination.
- Electron impact ionization results in sink for neutral density and source for plasma density.
- Radiative recombination term grows until reaches an equilibrium with ionization term.
- Theoretical solution to this problem is given as:

$$\frac{\partial n}{\partial t} = +\langle \sigma_{ion} v \rangle n n_n - \langle \sigma_{rec} v \rangle n^2 = 0$$

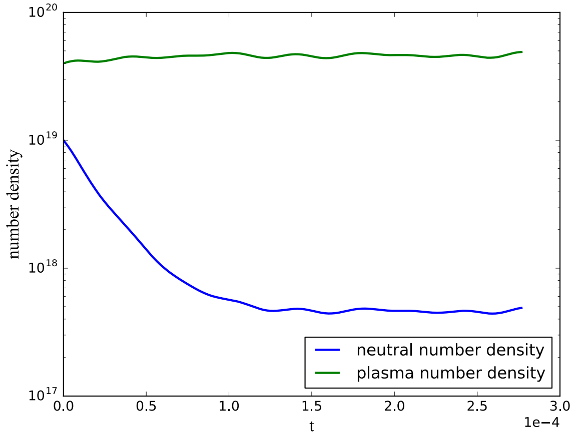
$$\frac{\partial n_n}{\partial t} = -\langle \sigma_{ion} v \rangle n n_n + \langle \sigma_{rec} v \rangle n^2 = 0$$

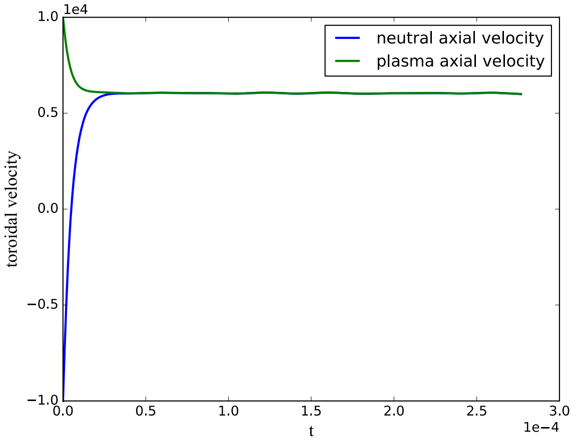
$$\Rightarrow \left. \frac{n_n}{n} \right|_{eq} = \frac{\langle \sigma_{rec} v \rangle}{\langle \sigma_{ion} v \rangle}$$

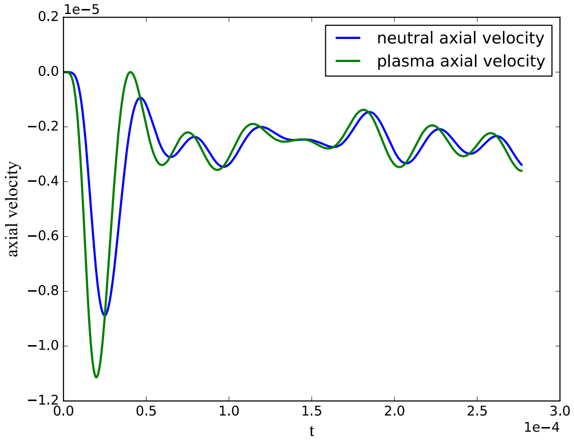


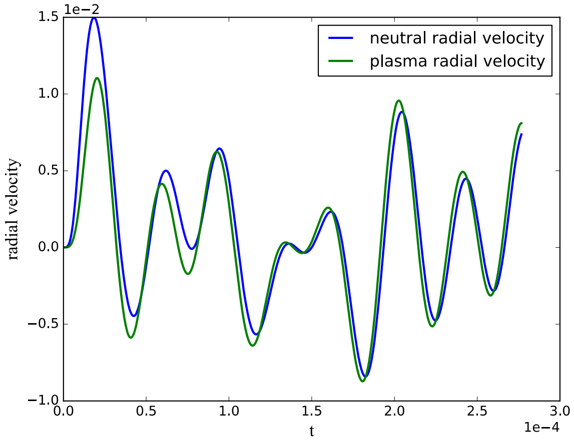
Resonant charge exchange collisions drive plasma and neutral momentum into an equilibrium state

- Resonant charge exchange reaction rate is almost always bigger than ionization/recombination rates.
- Therefore, momentum exchange between plasma and neutral fluids are mostly influenced by CX.
- All the charge exchange related source terms are a function of relative velocity as well.



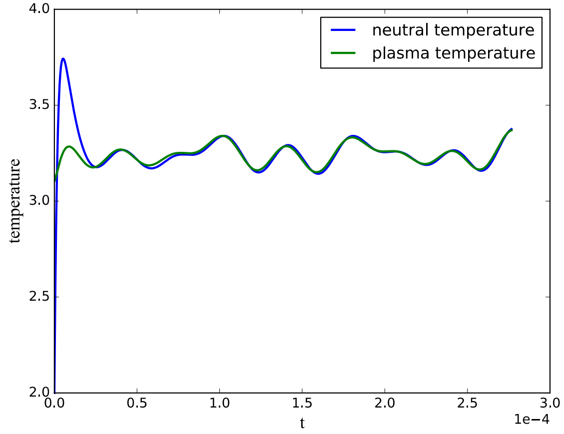


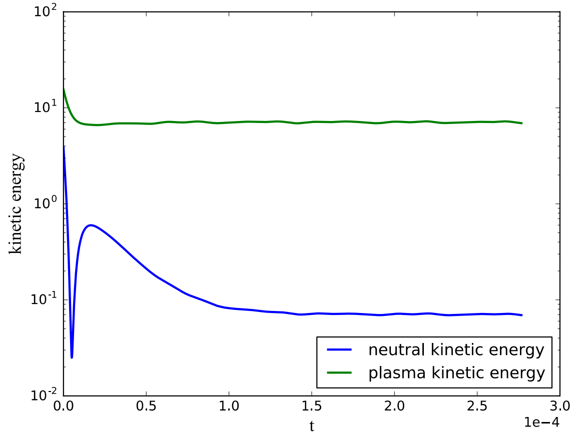


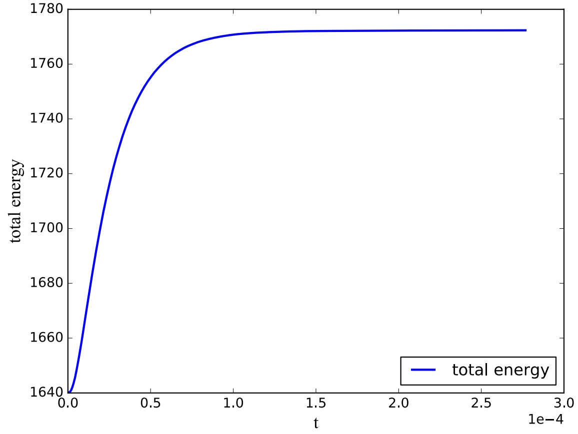


Total energy is almost conserved in plasma-neutral model

- Ionization, recombination and charge exchange cause the energy transfer between plasma and neutral species.
- Energy required for ionization and multiple excitations in neutrals are considered as effective ionization energy (which in this test case is assumed to be zero).
- Radiation energy due to recombination is ignored and lost from the system.







Summary

- The main motivation for this research is implementing a computationally tractable model to study plasma-neutral interactions.
- A generalized model is described based on Boltzmann equation and using Braginskii approach.
- Fluid representation of the model is derived by taking the moments of Boltzmann equation.
- NIMROD finite element code is used as a well known platform to implement the reacting plasma-neutral model.
- Ionization and recombination reaction rate coefficients are of great importance in the model and they both depend on temperature.
- The implemented code is tested against different problems to prove the conservation of number density, momentum and energy.