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FLUID MODELS OF INDUCTIVELY COUPLED PLASMA SOURCES FOR NEGATIVE HYDROGEN ION SOURCES*

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Abstract

Negative hydrogen ion sources are widely used to produce neutron beams via spallation both for neutron science in its own right, and as neutron sources for fusion devices. Numerical modeling is a useful tool for trying to optimize negative hydrogen ion sources. However there are significant numerical and computational challenges that have to be overcome, including code performance and resolution of separation of time scales between ion and electron motions. One method is to utilize fluid models to simulate inductively coupled ion sources (ICPs).

We have been developing algorithms to simulate negative hydrogen production in high-power, external-antenna ICP sources. We present simulation results using the USim [1, 2] framework to model plasma chemistry that produces negative hydrogen , and model the effects of electron temperature on overall negative hydrogen production rates. The numerical plasma chemistry models include processes of ionization, dissociation, recombination, as well as reactive dissociation of vibrationally resolved states and de-excitation of atomic hydrogen. We benchmark our plasma chemistry model results using plasma parameters relevant to experiments being carried out at the D-Pace Ion Source Test Facility.

We have also been developing fluid-based drift/diffusion models for multi-component plasmas, such as those in negative hydrogen sources. These simulation results demonstrate enhancement of the effective diffusion rates in plasmas that contain both electrons and negative ions.

INTRODUCTION

It has long be recognized that there are significant numerical and computational challenges involved in modeling ion sources using kinetic models, including code performance and resolution of separation of time scales between ion and electron motions. Due to the vast differences between ion and electron masses, detailed simulations that resolve electron motions are typically not feasible for long time scale models of plasma evolution in ICPs.

One method is to utilize fluid models to simulate ICPs. We have been developing algorithms to consistently simulate negative hydrogen production in both rf-driven and continuous-wave (CW) ion sources. Fluid models can be appropriate in regimes where the collisional mean-free-path is small, but the assumptions on electron distributions that are required to develop fluid models typically break down for low density, high-temperature plasmas, and in cases where the electrons are clearly not Maxwellian, such as in plasma sheaths. We have focussed on developing full plasma chemistry models for the production of negative hydrogen , and coupling these models with a fluid-based drift-diffusion model. The overall goal here is to provide numerical models that will predict negative hydrogen and ultimately heavier negative ion production rates in rf-driven ICP and CW sources.

We perform simulations using the USim[1, 2] fluid plasma modeling framework. USim is a flexible and parallel code for solving a variety of continuum equations in general geometries including fluids and plasmas and electromagnetics using finite volume and discontinuous Galerkin techniques. It is unique in that it can solve problems from weakly ionized plasma to high temperature and strongly magnetized regimes including free space electromagnetics. We have successfully coupled models of plasma chemistry with USim, which we discuss in detail below.

PLASMA CHEMISTRY MODELS FOR VOLUME NEGATIVE HYDROGEN PRODUCTION

In order to estimate the equilibrium densities of plasma species in an ICP source, we employ a global model to first determine the subset of plasma chemistry reactions that are important for volume negative hydrogen production. We have integrated a new version of the Global Enhanced Vibrational Kinetic Model (GEVKM)[3], with our fluid-based models, that down-selects the most relevant reactions based on the operational parameters for a specific ion source. We apply these models to nominal ion source parameters for production-level negative hydrogen sources under development at the D-Pace Ion Source Test Facility [4]. Namely, we model sources with a neutral H_2 gas pressure of ~ 30 mTorr, corresponding to an initial H_2 gas number density of approximately 1.0×10^{21}#/m^3, and we use an initial electron density in the range $1.0 \times 10^{17} - 1.0 \times 10^{20}$#/m^3.

The GEVKM global model for these parameters determines a set of twenty four species that are important for negative hydrogen production. These include the neutral heavy species hh2, H, positively charge heavy species H^+, H_2^+, H_3^+, fifteen resolved vibrational states of molecular hydrogen, two excited states of neutral hydrogen, and of course negative hydrogen . In addition, we also track electrons and photons produced by de-excitation of neutral H. The GEVKM model generates reaction rates based on bulk ion source parameters, that are fit to Arrhenius rates of the form

$$k(T) = \sigma_0 T^{\alpha} \exp(-E_a/T). \quad (1)$$

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In addition to kinetic ionization and dissociation reactions, we identified over 900 dissociative attachment reactions involving vibrationally-resolved reactions important in the production of negative hydrogen . Numerical values for these reaction rates, in exponential polynomial forms, are reported in [5]. Rate coefficients in the GEVKM global model have been updated recently based on benchmarking with another global model GMNHIS [6]. In total, we calculate reaction rates for 970 different reactions involving the 25 model species.

Our model integrates the local ODE equations using a Bulirsch-Stoer [7] integration scheme, as implemented in the BOOST C++ Library [8]. Care is taken to set the integration time step to a value small enough so that the integrator can converge over the large range of reaction rates and species densities in these models.

PLASMA CHEMISTRY MODELS RESULTS

We used the GEVKM global model to reduce the primary reaction paths down to 970 reactions. Of those, approximately 930 reactions involve higher order vibrational kinetics. Although their reaction rates are typically orders of magnitude smaller than electron-induced processes like ionization, recombination, and dissociation of heavy species, vibrational reactions have large rates of H^- production due to reactive dissociation of neutral H_2. Not including vibrational reaction kinetics reduces the predicted H^- densities by up to a factor of 6-10 in our simulations.

Figure 1 compares the time evolution of number density for the different model species for electron temperatures of 0.1 eV (top) and 3.0 eV (bottom). After a μs of simulation time, the species densities have generally reached a steady concentration. Small changes are observed due to the gradual depletion of the H_2 density. However, in actual ion sources the H_2 gas is replenished by continuous inflow. The lines labeled *de-excitation* in Fig. 1 correspond to photon production through relaxation of electronically excited states. The general effect of higher electron temperatures is to decrease the long-term H^- density, all other parameters held constant. For example, the H^- density is approximately 9 times lower at a plasma temperature of 3.0 eV than at 0.1 eV.

DRIFT-DIFFUSION FLUID MODELS FOR NEGATIVE ION PLASMAS

We have developed models to address the unique features of a multi-component plasma. A main feature of negative ion plasmas is that, while the plasma must remain overall quasi-neutral, the presence of a heavy negative species means that the light electron species may not have sufficient density to neutralize all the positive ions [9]. For example, in the limit where negative ions have the same density as the positive ions, quasi-neutrality implies there will be no electron density at all. The effect of this multi-component nature to the plasma is that diffusion rates and other transport

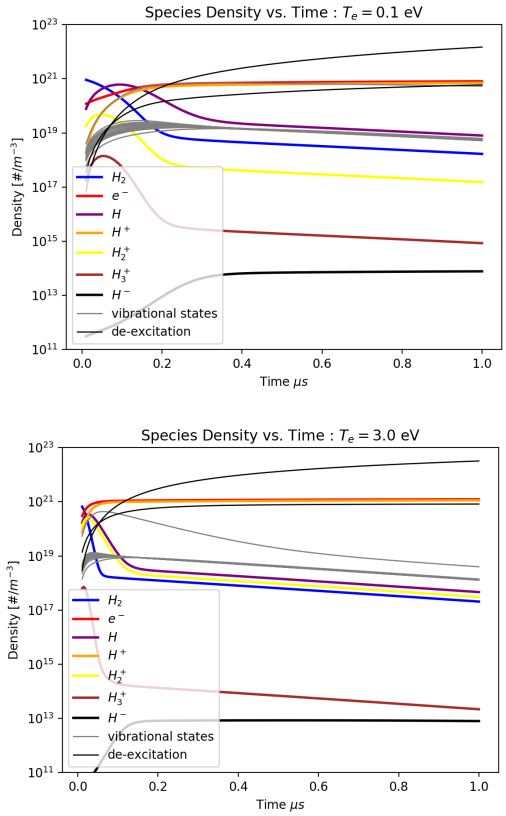

Figure 1: Species number density evolution for a system with plasma temperatures of 0.1 eV (top) and 3.0 eV (bottom).

properties can be significantly different than in a standard two-component ion-electron plasma.

For a two-component plasma, the drift diffusion equation for the ions reads:

$$\frac{\partial n_p}{\partial t} = \nabla(n_p \mu_p e E + D_p \nabla n_p) \tag{2}$$

In the above, $n_p = n_e$ is the plasma number density, $\mu_p = 1/(m_i * \nu_{ii})$, and $D_p = \mu_p T_e(1 + T_i/T_e)$, where T_i and T_e are the ion and electron number density, m_i is the ion mass, and ν_{ii} is the ion-ion collision frequency. D_p is the diffusion coefficient. In the drift-diffusion limit, one can calculate an electric field from the electron force balance.

$$E = \frac{\nabla p_e}{n_e q} \tag{3}$$

and one can solve the above equations for plasma motion.

For the case of a plasma with negative ions in addition to positive ions, the situation is more complicated. For example, if a plasma had equal negative and positive ions (and thus no electrons), the plasma would evolve much more slowly than if the plasma had all electrons and positive ions. The lack of the more mobile, light electron species will slow the overall plasma evolution. The equation for electron diffusion in a three-component plasma becomes:

$$\frac{\partial n_e}{\partial t} = \nabla(D_{eff} \nabla n_e) \tag{4}$$

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where $D_{eff} = \mu_e T_e(2/(1-f) - 1 + T_i/T_e)$ and $f = n_n/n_p$ is the fraction of negative ions. The negative ion and electron densities maintain quasi-neutrality: $n_n + n_e = n_p$. We show in Fig. 2 the variation in the effective diffusion coefficient with relative negative ion density.

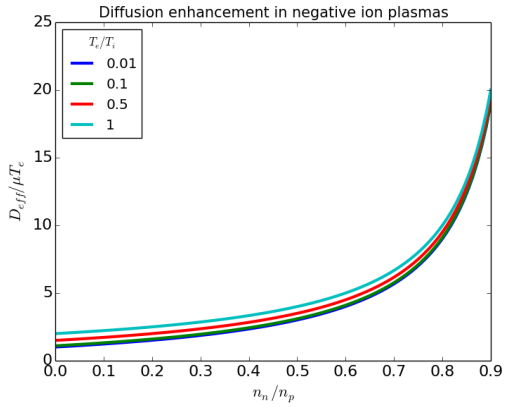

Figure 2: The diffusion enhancement v. fractional negative ion density for a negative ion plasma. The effective diffusion rate can be a factor of two enhanced for 30% negative ions and an order of magnitude enhanced for 80% negative ions.

Consider a model consisting of a one-dimensional plasma with a constant density gradient plus a small ripple (a linear perturbation). The initial densities of the three plasma components are shown in Fig. 3.

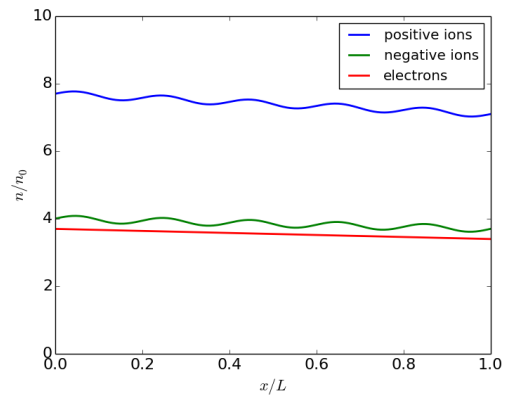

Figure 3: The densities of the three plasma components for our linear test problem with small perturbations.

As time evolves, the negative and positive ions drift in opposite directions, as shown in Fig. 4. In the scaled units for this problem where we have taken the ion mobilities as unity, the velocity is $v = \mu E \approx 0.08$. One can see that in scaled time units, the distance moved by $t = 1.0$ is roughly $\delta x = 0.08$, showing that the model does capture the multi-component drifts of the different ion species correctly.

CONCLUSION AND FUTURE WORK

In this paper we presented simulation results of plasma chemistry integration with a global model to determine the

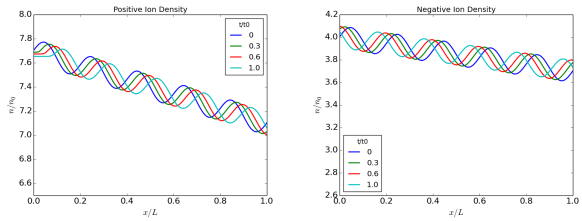

Figure 4: The positive (left) and negative (right) ion drift motion resulting from the electric field of the electrons. In the scaled time units we use, the distance moved by $t = 1.0$ is roughly $\delta x = 0.08$, as expected for the electric field value used.

effects of plasma properties such as electron temperature on overall volume negative hydrogen production. We also reported on progress developing a consistent fluid-based drift/diffusion model for negative hydrogen sources. We are actively integrating these two models to provide fully predictive simulation capabilities.

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REFERENCES

[1] J. Loverich and A. Hakim, "Two-dimensional modeling of ideal merging plasma jets," *Journal of Fusion Sciences*, vol. 29, no. 6, pp. 532–539, 2010.

[2] J. Loverich *et al.*, "Simulation of laboratory accretion disk and weakly ionized hypersonic flows using nautilus," in *42nd AIAA Plasmadynamics and Lasers Conference in conjunction with the 18th International Conference on MHD Energy Conversion (ICMHD)*, 2011, p. 4012.

[3] S. N. Averkin, N. A. Gatsonis, and L. Olson, "A Global Enhanced Vibrational Kinetic Model for high-pressure hydrogen rf discharges," *IEEE Transactions on Plasma Science*, vol. 43, no. 6, pp. 1926–1943, 2015.

[4] `https://www.d-pace.com/?p=about`

[5] S. N. Averkin, "A Global Enhanced Vibrational Kinetic Model for radio-frequency hydrogen discharges and application to the simulation of a High Current Negative Hydrogen Ion Source," PhD thesis, Worcester Polytechnic Institute, 2015.

[6] W. Yang *et al.*, "Benchmarking and validation of global model code for negative hydrogen ion sources," *Physics of Plasmas*, vol. 25, no. 11, p. 113 509, 2018.

[7] P. Deuflhard, "Order and stepsize control in extrapolation methods," *Numerische Mathematik*, vol. 41, no. 3, pp. 399–422, 1983.

[8] `https://www.boost.org/doc/libs/1_55_0/boost/numeric/odeint/stepper/bulirsch_stoer.hpp`

[9] I. Kaganovich, "Negative ion density fronts," *Physics of Plasmas*, vol. 8, no. 5, pp. 2540–2548, 2001.