ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-TUPTS095

GLOBAL MODEL OF MULTI-CHAMBER NEGATIVE HYDROGEN ION SOURCES WITH UPDATED HYDROGEN PLASMA CHEMISTRY*

S. N. Averkin†, S. A. Veitzer, Tech-X Corporation, Boulder, Colorado, USA

Abstract

We present the extension of the Global Enhanced Vibrational Kinetic Model (GEVKM) [1] for the multi-chamber design with the updated hydrogen plasma chemistry [2]. The extended GEVKM consists of separate global models for macroscopic parameters of all species in each chamber coupled through interface boundary conditions. We compare our model with fluid simulation results for a plasma composition and species temperatures in the negative hydrogen ion source developed at IPP Garching.

INTRODUCTION

The range of numerical models of chemically reacting plasmas found in negative hydrogen ion sources (NHIS) span from detailed kinetic models (e.g. Particle-In-Cell method coupled with Direct Simulation Monte Carlo) to fluid models (e.g. Magnetohydrodynamics coupled with electromagnetic solvers), and then further to simple 0D or volume-averaged global models. Kinetic solvers provide detailed information about distribution functions of plasma components but have significant computational costs. In addition, inclusion of many chemical species and chemical reactions that could be found in real NHIS make a single simulation implausible due to very high computational costs. Fluid models coupled with electromagnetic solvers can still provide detailed information about space and time distribution of species number densities, velocities and temperatures with a reduced computational costs compared to kinetic solvers. In principle a single simulation of realistic chemically reacting plasma for one set of parameters is possible. However, the parametric investigation that can be used to model device optimization is still challenging task. For such reasons global models are widely used to perform quick simulations to extract most important chemical reactions and species information that can be further used in detailed fluid simulations. Our ultimate research goal is to provide the means to accurately model NHIS devices for long time scales, and to optimize NHIS designs over a wide range of parameters using commercial fluid code USim [2]. To achieve this goal we use Global Enhanced Vibrational Kinetic Model (GEVKM) [1] that allows to quickly estimate main plasma parameters (number densities and temperatures of different species) over a wide range of parameters (inlet flow rates, absorbed powers and geometrical configurations) and extract the most important chemical reactions and plasma species. Previously [3] we reported simulation results of a single chamber NHIS simulations with cesiated plasma grid. In this paper we present double chamber simulation results and describe interface boundary conditions and other modifications that were done in the GEVKM in order to perform such simulations.

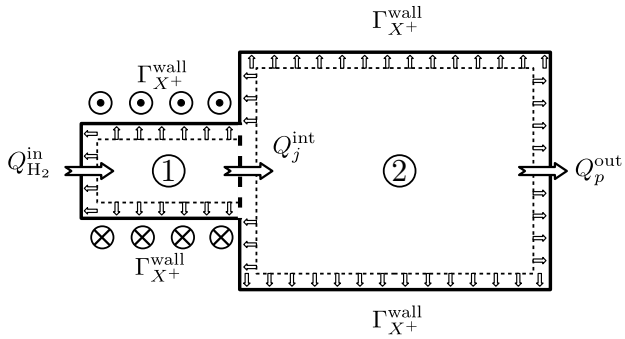

Figure 1: Double chamber negative hydrogen ion source.

GLOBAL ENHANCED VIBRATIONAL KINETIC MODEL

In the original GEVKM a set of steady-state species particle balance equations supplemented by quasineutrality condition is solved together with electron and total volume averaged energy equations in order to estimate number densities and electron and heavy species temperatures. This model included electrons, neutral hydrogen species such as $\text{H}(n), n = 0, ..., 3$, all vibrational states of molecular hydrogen $\text{H}_2(v), v = 0, ..., 14$, positive ions H^+, H_2^+, H_3^+ and negative ions H^-. This model included comprehensive list of chemical reactions with more than 1,000 of vibrationally resolved reactions whose numerical values are available in [4]. Recently the reaction rate coefficients in the GEVKM were updated based on the benchmarking with another global model (GMNHIS) [5].

For double-chamber designs shown in Fig. 1 for each chamber we consider separate steady-state global models based on the GEVKM. These global models are coupled through interface boundary conditions. Previously we have used isentropic and Fanno flow theory for deriving outflow boundary conditions for a nozzle and pipes [6]. In this work we assume that the flow rates of neutral and ion species from the first to the second chamber can be estimated based on the simple thermal fluxes as

$$Q_j^{\text{int}} = \frac{1}{4}\left(n_j^{(1)} v_{\text{th},j}^{(1)} - n_j^{(2)} v_{\text{th},j}^{(2)}\right) A_{\text{int}},$$

where j is the species number, $n_j^{(i)}$ is the number density of the j-th species in the i-th chamber, $v_{\text{th},j}^{(i)}$ is the thermal speed of the j-th species in the i-th chamber, A_{int} is the interface area. These boundary conditions are somewhat similar to

* Work supported by Department of Energy, Office of Basic Energy Sciences Award #DE-SC0009585
† averkintxcorp.com

ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-TUPTS095

so-called perfect open boundary conditions used in [5] for neutral species. For electrons the flow rates are estimated using the condition of zero net current. Even though these interface boundary conditions are not physical, they still allow to capture the most important aspects of physical processes in both chambers with the lower computational cost compared to full fluid simulation.

We consider a double chamber cylindrical ICP source with the radius $R_1 = 12$ cm and the length $L_1 = 14$ cm in the first chamber and the radius $R_2 = 21$ cm and the length $L_2 = 21$ cm in the second chamber. The parameters of this ion source were chosen to resemble negative hydrogen ion source developed at IPP Garching [7] that was previously used in plasma fluid simulations [8]. We also assumed that the total extraction grid area is 0.00566 m^2. The volumetric inlet flow rate of pure molecular hydrogen is assumed to be 402 sccm while absorbed power was taken in the range from 10 kW to 50 kW. The outlet flow rates of plasma components through the extraction grid are estimated based on the effusion. The ion source walls were assumed at fixed wall temperature 300 K due to possible water cooling. These inlet flow rate and the extraction grid parameters were chosen to result in the pressure 0.3 Pa in the negative hydrogen ion source without plasma turned on. The neutral gas temperature was set to 1000 K in the simulation for both chambers.

SIMULATION RESULTS

Positive hydrogen ions number densities are plotted on Fig. 2 as a function of absorbed power at fixed inlet flow rate 402 sccm for driver chamber (upper plot) and for expansion chamber (lower plot). The dominant positive ion in the driver chamber for all absorbed powers considered is H^+ while in the expansion chamber at low absorbed powers the dominant positive ion is H_3^+ and at high absorbed powers it is H^+. As absorbed power increases all positive ions number densities in both chambers increase except H_3^+ in the driver chamber. It first increases, reaches a maximum around 20 kW and then decreases.

Figure 3 presents atomic and molecular hydrogen number densities as a function of absorbed power in the driver (top) and expansion (bottom) chambers. In both chambers the atomic number density monotonically increases with increasing absorbed power while molecular hydrogen number density monotonically decreases. Above 20 kW the atomic hydrogen number density in the driver chamber exceeds the molecular hydrogen number. It contradicts 2D fluid simulations that predict that molecular hydrogen is dominant species [8]. The reason of such discrepancy is the usage of simple interface boundary conditions in this work. On the other hand, we correctly predict trends in the number densities behavior as well as their orders of magnitudes.

Electron number density and temperature in both chambers as a function of absorbed power are shown on Figs. 4 and 5 respectively. Electron number density in both chambers is monotonically increasing while temperatures are monotonically decreasing as absorbed power increases. The

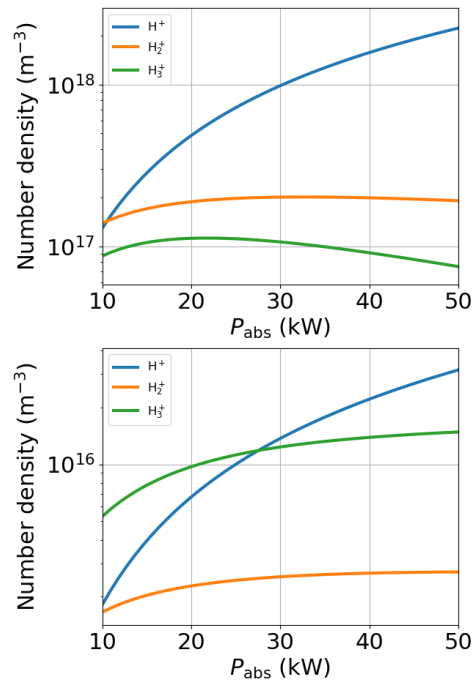

Figure 2: Positive hydrogen ions number densities in the driver (top) and in the expansion (bottom) chambers.

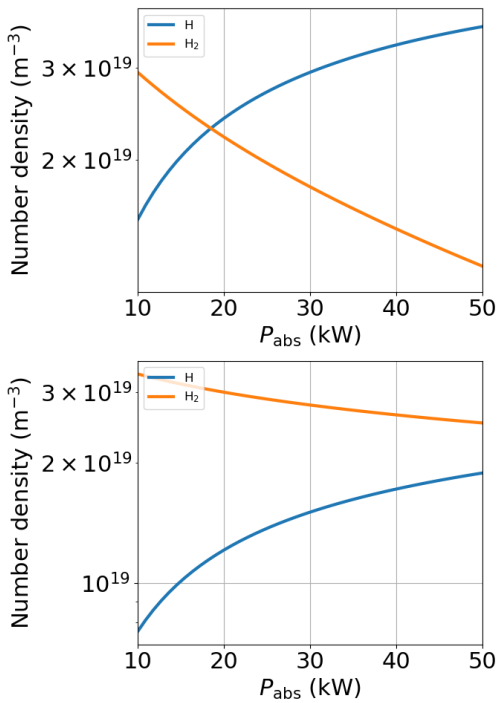

Figure 3: Molecular and atomic hydrogen number densities in the driver (top) and in the expansion (bottom) chambers.

latter is due to the discharge pressure increasing with absorbed power as can be seen from neutral species number densities shown in Fig. 3 (we assumed constant heavy species temperature 1000 K). Compared to fluid simulation from Ref. [8], our global model does not predict the same electron temperatures in both chambers while fluid simulations

ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-TUPTS095

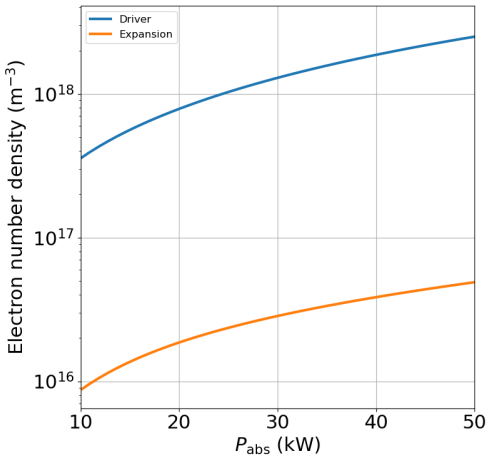

Figure 4: Electron number densities in the driver and in the expansion chambers.

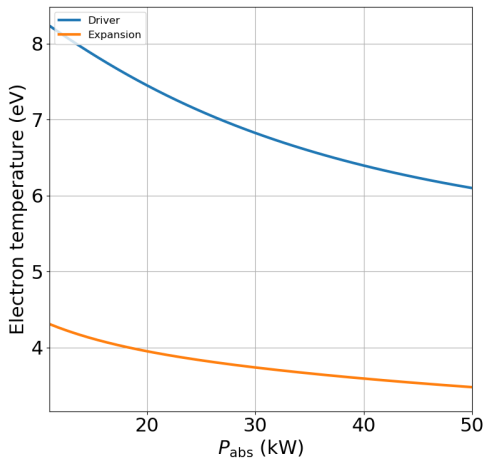

Figure 5: Electron temperatures in the driver and in the expansion chambers.

showed almost uniform electron temperature distribution. This is again due to very simple interface boundary condition used in this work.

CONCLUSION AND FUTURE WORK

In this paper we presented simulation results of the two-chamber global model that allows to make quick estimates of the number densities of all plasma components and electron temperatures. Our global model is based on the usage of two separate global models derived from the GEVKM model for each chamber of the source. The coupling between separate global models is achieved by using simple interface boundary conditions. We found good agreements between our global model predictions and previous fluid simulations in terms of trend in the predicted number densities and temperatures as well as orders of their magnitudes. On the other hand, there is some discrepancy associated with our usage of simple interface boundary conditions that we are going to improve in our future research.

Global model predictions are intended to be used in our fluid simulations using commercial fluid model USim. It will allow to speedup simulations by considering only a subset of most important species and chemical reactions for each set of simulation parameters.

ACKNOWLEDGMENTS

This work was performed under the auspices of the Department of Energy, Office of Basic Energy Sciences Award #DE-SC0009585.

REFERENCES

[1] 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.

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

[3] S. N. Averkin, S. A. Veitzer, and M. Kundrapu, "Global model of a negative hydrogen ion source with caesiated plasma grid," in *AIP Conference Proceedings*, AIP Publishing, vol. 2011, 2018, p. 050 026.

[4] 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.

[5] 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.

[6] S. N. Averkin, N. A. Gatsonis, and L. Olson, "Investigation of the radio-frequency discharge in a High Current Negative Hydrogen Ion Source with a Global Enhanced Vibrational Kinetic Model," *IEEE Transactions on Plasma Science*, vol. 45, no. 9, pp. 2460–2471, 2017.

[7] E. Speth *et al.*, "Overview of the rf source development programme at ipp garching," *Nuclear Fusion*, vol. 46, no. 6, S220, 2006.

[8] J. Boeuf, G. Hagelaar, P. Sarrailh, G. Fubiani, and N. Kohen, "Model of an inductively coupled negative ion source: II. Application to an ITER type source," *Plasma Sources Science and Technology*, vol. 20, no. 1, p. 015 002, 2011.