Simulation of the Interaction Between Two Counterflowing Rarefied Jets

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Abstract.
A preliminary analysis of the flow between a jet of argon plasma and one containing argon excited states is conducted using the direct simulation Monte Carlo method (DSMC). As a prelude to the use of more advanced models and to help design the accompanying experiment, a simplified model is formulated that ignores electron kinetics and field effects. This model allows the capture of most of the gas dynamics phenomena present with a standard DSMC code. Two interaction criteria are then used and compared to analyze the flow pattern of the interaction. An increase in the mass flow rate of the neutral jet is found to increase the level of interaction between the jets.

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INTRODUCTION

Motivations

The accurate simulation of low temperature, weakly ionized rarefied plasmas is of paramount importance to optimize numerous industrial processes. Modern low-pressure plasma reactors used for etching or deposition [6] by the microelectronics industry frequently operate in the transition regime. Under these operating conditions, both electrons and heavy species (ions and neutrals) follow non-equilibrium distribution functions and require a kinetic modeling approach based on the Boltzmann equation. Any attempt at improving the behavior of most performance parameters of practical interest, such as the etching or deposition rates, can only be made by considering the distribution function (DF) of the various species of the flow. For certain species, desirable DF shapes that maximize the rate of given chemical reactions can further be identified. One should therefore ideally strive to selectively shape the DF of certain key species of the flow (usually that of the electrons) to optimize a particular process.
At the University of Michigan, over the course of the next several years, an extensive study, both experimental and numerical, will be conducted to investigate the possibility of controlling the electron energy distribution function (EEDF) in an argon plasma by the introduction of argon metastables. An experimental investigation of the flow presented in this paper will be conducted at the University of Michigan's Plasmadynamics and Electric Propulsion Laboratory (PEPL) while its numerical modeling will be conducted by the Nonequilibrium Gas and Plasma Dynamics Laboratory (NGPDL) of which both authors are members. Collaboration is also underway with the Computational Plasma Science and Engineering Group (CPSEG) to simulate the plasma source.

Test Case

Based on past work involving plasmas in the domain of electric propulsion and the layout of existing test facilities, the layout shown in Fig. 1 is chosen. A rarefied, weakly ionized, argon plasma (containing Ar, Ar^+ and e^-) produced by the helicon source described in [5] is subjected to a counterflowing jet of neutral argon containing metastables (primarily composed of Ar and Ar(4s), the first excited state, denoted Ar^* in the following). The aim is to take advantage of the following de-excitation reaction:

$$Ar^* + e^- \rightarrow Ar + e^- \tag{1}$$

to exchange energy between the excited states and the electrons so as to modify the shape of the EEDF. Although we have yet to fully characterize the composition of the two jets, the preliminary estimates shown in Table 1 was used in

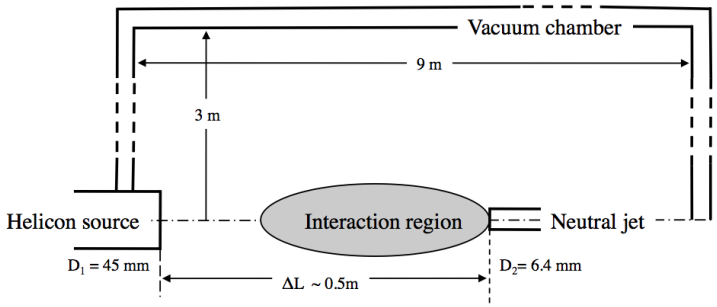

FIGURE 1. Sketch of the axisymmetric flow geometry

the simulations.

Objectives

The first goal of the study presented in this paper is to obtain, in short order, some insights into the rarefied gasdynamics phenomena that occur in the flow so as to be able to help design the experimental setup. To be able to fully take advantage of reaction (1), we want to design the experiment so as to maximize the extent of the region where this reaction can favorably take place and to know where its products are most highly concentrated. Our second aim is to establish, using an existing code that has been extensively validated, a credible baseline solution for the gas dynamics of the flow. Even when electrical field effects and electron kinetics are ignored, the flow is very challenging to simulate via DSMC due to the large disparity of scales (lengths, velocities and number densities) present. Furthermore, before using or devising more advanced models that specifically address electron kinetics, we want to be confident about the behavior of neutrals that we expect to only be weakly influenced by the former.

PHYSICAL AND NUMERICAL MODELS

Physical Model

Motivation

In order to obtain the most accurate solution possible, one would ideally want to solve for the velocity distribution function (VDF) of all the heavy species and the EEDF (that we are anyway ultimately interested in studying). A full-fledged DSMC solution where electrons are included as particles is however computationally prohibitive. The most likely solution to that problem appears to be the use of advanced hybrid techniques [4] that solve kinetic equations for the electrons. The implementation of such models, as of now untested in the context of complex rarefied flows, will be the subject of upcoming work. This, coupled with the need to quickly design the experiment, in turn motivates us to study the flow using the 3 species models detailed in the next paragraph.

Reduced order model

Due to the low level of ionization, gas dynamics phenomena are not expected to be substantially influenced or modified when the effects of the electrons or electrical fields are accounted for. The gas dynamics are however conversely expected to substantially impact the EEDF. Hence, to first order, the influence of the electrons on the heavy species can be neglected by assuming ambipolar diffusion of the ions and electrons in the flow so that $n_{\mathrm{Ar}^+} = n_{\mathrm{e}^-}$; which allows us to further neglect the effect of the electrical field. We therefore choose to only simulate the heavy species of the flow: $\mathrm{Ar}, \mathrm{Ar}^*$ and Ar^+. Lacking data for the concentration of excited states in the neutral jet flow, we

TABLE 1. Composition of jets used in the simulations.

	Species	Number density $[\mathrm{m}^{-3}]$	x-Velocity [m/s]	Temperature [K]
Helicon source	Ar	1×10^{18}	322*	300
	Ar^+	1×10^{17}	10,760	300
Neutral jet	Ar*	$\Xi\times6.5\times10^{21}$ †	−322*	300

* Sonic velocity (choked flow)
† $\Xi \equiv \dot{m}_{\text{neutral jet}}/\dot{m}_{\text{helicon source}}$

assume it to be composed of pure Ar*. The concentrations of the two jets, under this simplified model, are detailed in Table 1.

Numerical Method

The simulations were conducted using MONACO [2], a parallel unstructured DSMC code that has been extensively used to simulate hypersonic rarefied flows and electric propulsion engines. The adaptive time step strategy described in [3] is used to ensure the accuracy of the simulations while keeping the computation time tractable. Elastic collisions between particles was modeled with the Variable Hard Sphere (VHS) model [1].

INTERACTION QUANTIFICATION

Our aim in the following is twofold. First, we would like to define a local criterion that, for a given flow, reveals where electrons that have reacted according to (1) are most likely to be found and where those reactions are taking place. This will give an indication as to the best region where to make measurements of the EEDF. Two such local criteria are presented; the first is based on an Eulerian description of the flow, and the other on a Lagrangian one. Based on these local criteria, we present several global measures, termed "global criteria" that allow us to compare the suitability of different flow configurations between one another based on a single parameter. The use of these global criteria is demonstrated within the context of a numerical parametric study where the mass flow rate of the second jet is varied.

Local Criteria

Equilibrium Reaction Rate

We can identify high reactivity regions as those where a comparatively large number of (1) reactions per unit volume and unit time occurs:

$$r_1 = k_1 n_{\mathrm{Ar}^*} n_{\mathrm{e}} \ , \tag{2}$$

where n is the species number density and k_1 is the reaction rate of (1) that we approximate as the equilibrium rate reported in [6]: $k_1 = 4.3\times10^{-16} T_{\mathrm{e}}^{0.74}\left[\mathrm{m}^3/\mathrm{s}\right]$ with a constant electron temperature of 1 eV †.

Streamline Integrated Reaction Rate

The interaction can also be described from a Lagrangian viewpoint by estimating the number of reactions that electrons emitted by the plasma source undergo with particles from the neutral source as they travel on their respective streamlines (that we assume to be identical to those of the ions by the ambipolar assumption). This mean number of reactions as a function of time along a streamline can be obtained from the following integral:

† The reverse excitation reaction with a rate $k_{1,r} = 5\times10^{-15} T_{\mathrm{e}} \exp(-11.56/T_{\mathrm{e}})$ can effectively be neglected.

$$N_{1,SL} = \int_{\mathrm{SL}} k_1 \, n^*_{\mathrm{Ar}} \, dt|_{\mathrm{SL}} \approx \int_{\mathrm{SL}} k_1 \frac{n_{\mathrm{Ar}^*}}{2} \left(\frac{dz}{u_z} + \frac{dr}{u_r} \right) . \tag{3}$$

Discussion

The isocontours of the two criteria plotted in Fig. 2 exhibit different patterns although both reach their respective maximum close to the second jet. The most natural quantification that comes to mind to gauge how strongly the two streams interact is, of course, the reaction rate r_1, that is often related to the bimolecular collision rate via the steric factor [7]. However in the present case, it is not appropriate to describe the system, as each Ar^* atom can only effectively react once with an electron. Far more than a quantity that only depends on the value of the product of the number densities at a given location of the flow, we are interested in one that depends on the history, i.e. the trajectories, followed by the particles to reach that point. This argues for the use of $N_{1,SL}$, which however does not incorporate any dependence on n_{Ar^+}. Its isocontours cannot directly indicate the best regions for the measurement of the EEDF. For instance, it reaches very high values where the electron number density is very low (which makes measurement difficult) such as very close to the neutral jet. A more useful plot in that sense is $n_{Ar^+}|_{N_{1,SL}>N^{min}_{1,SL}}$, i.e. a plot of the electron or ion number density in the region where $N_{1,SL}$ is greater than a threshold value $N^{min}_{1,SL}$, above which electrons are assumed to have reacted according to (1). Figure 3 shows such a plot and suggests that a region suitable for measurements exists around $r = 0.01$ m.

Global criteria

Formulation

To obtain a more quantitative comparison between flow configurations, a series of global criteria, based on r_1 or $N_{1,SL}$ can be defined. One is the integral of r_1 over the part of the domain where measurements can be made, such as for instance $\Omega_{\mathrm{exp}} = \{0 < z < 0.5 \text{ m} \; ; \; 0 < r < 1 \text{ m}\}$:

$$\langle N_1 \rangle \equiv \int_{\Omega_{\mathrm{exp}}} r_1 \, dV \tag{4}$$

that defines a total mean number of reactions that occurs per unit time. $N_{1,SL}$ can be used to judge the extent of the interaction region by for instance calculating the volume $V_{N^{min}_{1,SL}}$ of the region where $N_{1,SL}$ is greater than a threshold value $N^{min}_{1,SL}$:

$$V_{N^{min}_{1,SL}} = \int_{\Omega_{\mathrm{exp}} \cap \left(N_{1,SL} > N^{min}_{1,SL} \right)} dV \; . \tag{5}$$

One last global measure of the interaction can be the number of electrons (or ions in the present case), likely to already have reacted that are in the interrogation window:

$$N_{\mathrm{e}^-, N^{min}_{1,SL}} = \int_{\Omega_{\mathrm{exp}} \cap \left(N_{1,SL} > N^{min}_{1,SL} \right)} n_{\mathrm{Ar}^+} \, dV \; . \tag{6}$$

Discussion

Plots of the effect of Ξ on $\langle N_1 \rangle, V_{N^{min}_{1,SL}}$ and $N_{\mathrm{e}^-, N^{min}_{1,SL}}$ (for both $N^{min}_{1,SL} = 0.5$ or 1) are shown in Fig. 4. As expected, they all exhibit monotonic behavior with increasing Ξ. It is notable that $N_{\mathrm{e}^-, N^{min}_{1,SL}}$ increases less rapidly than $V_{N^{min}_{1,SL}}$ because the increase brought about when Ξ rises (through the greater size of $\Omega_{\mathrm{exp}} \cap N_{1,SL} > N^{min}_{1,SL}$) is balanced by a decrease in that same volume of the value of n_{Ar^+} because Ar^+ has more difficulty diffusing towards the second jet. Hence, we see that the global criterion defined by (6) better reflects the suitability of a given flow field for EEDF measurements compared to that defined by (5) inasmuch as the contour plots of Fig. 3 are more useful than those of Fig. 2 b) at determining where to take these measurements.

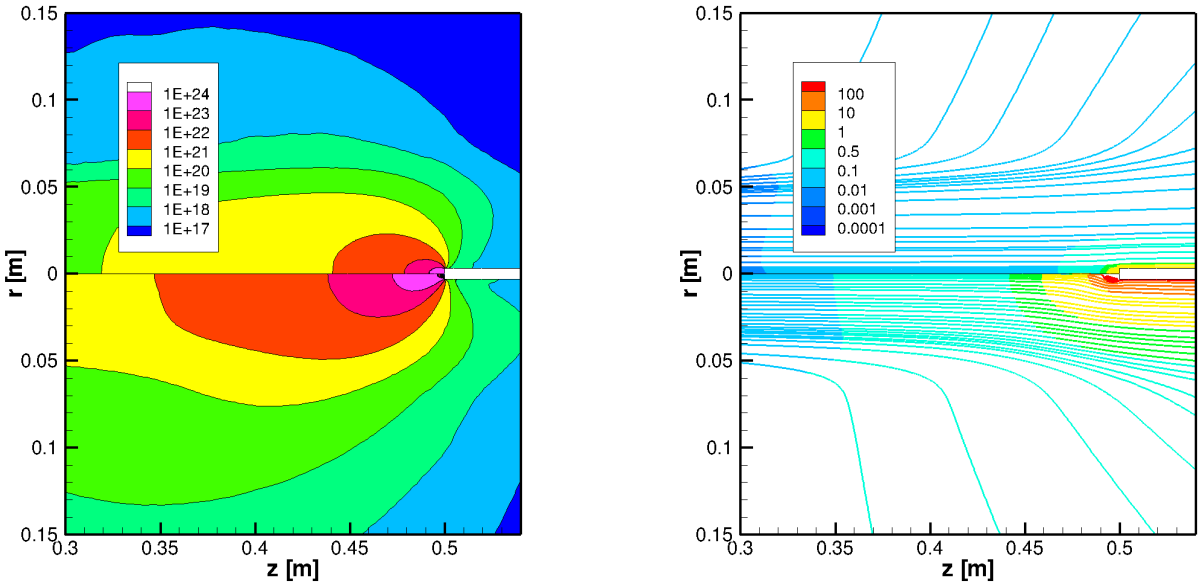

FIGURE 2. Closeup of the isocontours around jet 2 of r_1 $\left[\mathrm{m}^3/\mathrm{s}\right]$ (left) and of $N_{1,\mathrm{SL}}$ [# of Reac] (right) for $\Xi = 1$ (upper plot) and $\Xi = 8$ (lower plot).

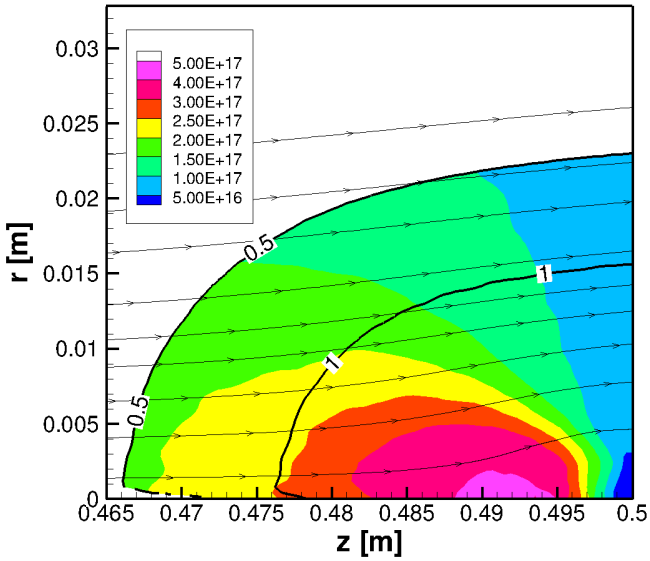

FIGURE 3. Contour plot of n_{Ar^+} $\left[\mathrm{m}^{-3}\right]$ in the region where $N_{1,SL} > 0.5$ with a few Ar^+ streamlines for $\Xi = 4$.

CONCLUDING REMARKS

In the framework of a preliminary study of two jets of rarefied argon crafted to measure the impact of metastables on the EEDF, we have formulated several criteria to assess the suitability of flows for that purpose. One criterion,

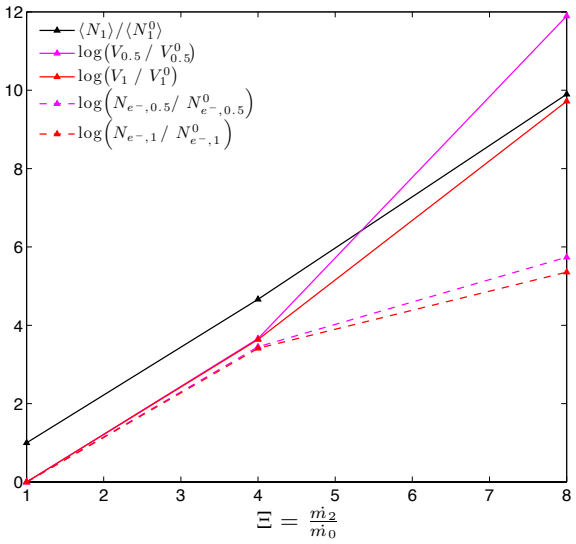

FIGURE 4. Influence of Ξ on the global criteria (normalized to their values for $\Xi = 1$).

$N_{1,SL}$ that can easily be obtained from mean velocities and number densities, was found particularly relevant to locally measure the degree of interactions between different species or streams within a DSMC simulation. A global figure of merit, based on the integration of that local criterion, was then formulated that can be used to gauge the overall degree of interaction that exists in a certain flow field.

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