# Iodine as propellant for electric propulsion: updated global model and comparisons to experiments

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#### Abstract

Iodine is a promising replacement for xenon as propellant for electric propulsion devices. Cost-effective and dense, it also brings complexity in the modelling - as iodine comes as a molecule - and in the experiments, due to its low vapor pressure and slightly corrosive activity. We present an update of the global model from Grondein *et al.* [1], adding new reactions and electronegativity effects in the sheaths. The iodine density and temperature are measured in a real system by absorption at  $1.315 \,\mu$ m. A CRDS experiment allowing measurements at lower pressure, and spatially resolved Langmuir probe measurements for electron density and temperature are scheduled.

Keywords: Iodine, Global Model, CRDS, Absorption, Langmuir Probe

## 1 An updated global model

The simulation work presented here is a follow-up of the work done by Grondein *et al.* [1]. The model is a volume-averaged model solving two sets of equations corresponding to the power and particle balance. Eight equations summarize the temporal evolution of the density of I, I<sub>2</sub>, I<sup>+</sup>, I<sub>2</sub><sup>+</sup>, I<sup>-</sup> and the electrons, as well as the electron and neutral temperature. The ions and neutrals are considered to have the same temperature. The following reactions are taken into account:

$e^- + I$	$\longrightarrow$	$e^- + I$	Elastic collision on I
$e^- + I$	$\longrightarrow$	$e^{-} + I^{*}$	Excitation of I
$e^- + I$	$\longrightarrow$	$2 e^{-} + I^{+}$	Ionization of I
$e^{-} + I_{2}$	$\longrightarrow$	$e^{-} + I_{2}$	Elastic collision on I <sub>2</sub>
$e^{-} + I_{2}^{-}$	$\longrightarrow$	$2e^{-} + I_{2}^{+}$	Ionization of I <sub>2</sub>
$e^{-} + I_{2}^{-}$	$\longrightarrow$	$2 e^- + I^+ + I$	Diss. ionization
$e^{-} + I_{2}^{-}$	$\longrightarrow$	$I^- + I$	Diss. attachment
$e^{-} + I_{2}^{-}$	$\longrightarrow$	$e^- + 2I$	Dissociation
$I^{-} + I_{2}^{+}$	$\longrightarrow$	$I + I_2$	Charge exchange
$I^- + I^{\tilde{+}}$	$\longrightarrow$	2 I -	Ion recombination
2 I	$\longrightarrow$	$I_2$	Surface recombination

The new work comprises:

- verify and update when possible the reaction rates or cross sections of existing reactions;
- · add new reactions;

- characterize the uncertainty of existing reactions rates;
- implement uncertainty quantification methods to track the sensitivity of the code outputs to errors in the reaction rates or other parameters.

Since [1], the reaction rate for the ion recombination has been recalculated, considering only the fundamental state of I<sup>+</sup> and neglecting spin-orbit coupling. The new value is smaller than the one currently used, coherent with a higher I density in the code compared to what is actually measured, but not enough to explain the entire discrepancy. Two more reactions have also been added in the reaction scheme:

$$e^- + I_2^+ \longrightarrow e^- + I^+ + I$$
 Dissociation of  $I_2^+ e^- + I^- \longrightarrow 2e^- + I$  Detachment from  $I^-$ 

## 2 Experimental comparisons

In order to compare the model to data from actual experiments, an iodine injection line and a dedicated mass flow controller are installed to feed the 4 MHz radio-frequency inductively coupled ion source that is the base for the PE-GASES thruster [2]. Such a setup needs an extra care for operation, in particular in the heating of the injection line, any cold point resulting in a blockage that can deteriorate the setup if not dealt with quickly. Three experiments are or will be performed: absorption at 1.315 µm using a normal absorption setup, absorption at the same frequency using cavity ring-down spectroscopy (CRDS) and Langmuir probe diagnostics. The absorption probes a dipolar-magnetic and quadrupolar-electric transition in the fine structure of the fundamental state of atomic iodine [3] and gives the temperature and density of atomic I. The RF-compensated Langmuir probe will give the electron temperature and density.

A classical laser absorption experiment is only possible by artificially raising the pressure within the thruster: this is done by reducing the exit area of the thruster to 57 mm<sup>2</sup> (two holes of 3 mm of diameter), which represent a 0.6 % transparency of the exit plane. The laser does 7 passes in the plasma, which represents an effective absorption length of 84 cm. The pressure in the ionization chamber is varied from  $4 \times 10^{-2}$  mbar (4 Pa, 30 mTorr) to  $1.1 \times 10^{-1}$  mbar (11 Pa, 83 mTorr). The optical setup is shown Fig. 1.



Figure 1: Optical setup for the absorption experiment

The transmitted light acquired on an InGaAS photodiode are calibrated using a reference location of the peaks determined by Ha *et al.* [3] and a 10 cm piece of glass with perfectly parallel plans, whose interference pattern monitors the wavelength variation. Two absorption peaks from the hyperfine structure are fitted to extract temperature and density from the Doppler-broadened absorption bands, as shown Fig. 2. The wavelength is calibrated after analysing by analysis the output of the Fabry-Perot-like thick piece of glass. The peaks are then fitted with independent Gaussian curves. The temperature of the smaller peak is on average 18 K smaller than the one of the large peak, an effect that is currently unexplained.

The results show a strong increase of I density (absolute and ratio  $I/I_2$ ) (Fig. 3) and temperature (Fig. 4) with RF power, but the temperature dependence with the pressure is smaller than the current experimental noise, including on pressure measurements. The experiment will be repeated



Figure 2: Example of data and fit.

with a larger pressure range and a more precise pressure monitoring system to lower the experimental noise.



Figure 3: I density vs power for different pressure

#### 3 Comparisons code/experiment

Preliminary comparisons are encouraging: the code was successfully adapted to reproduce the exact conditions of the experiment and is able to predict correctly some factor that can be easily measured like the gas pressure. However, the discrepancies are significant and must be investigated: the modeled I density is for example a decade higher than was is effectively measured. Fig. 5 shows a simulation done at 7.5 sccm, corresponding to the 0.086 mbar (8.6 Pa) red curve on Fig. 3 and 4. This can come from a large underestimation of recombination reactions on surfaces. It should be kept in mind that the code shows here actual power absorbed by the plasma when the experimental curve include losses in the electrical system, and antenna. The losses in this system can and will be estimated using formula directly derived from the model by Chabert *et al.* [4].



Figure 4: I temperature vs power for different pressure



Figure 5: I and I2 densities predicted by the global model for 7.5 sccm of  $I_2$ . Power here is the power absorbed by the plasma, excluding losses, unlike RF power from the experimental curves.

## 4 Future work

Two further experiments will be presented: the absorption experiment will be improved by using Cavity Ring-Down spectroscopy technique, allowing to probe much lower pressures corresponding to realistic operating pressures for electric propulsion devices. A Langmuir probe diagnostic will be performed to measure the electron density and temperature, with spatial resolution within the ionization chamber.

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