1D Model Of Low-Pressure Plasma As A Platform To Study Gas Decomposition Reactions

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Abstract

Thermal decomposition of plastic waste results in gas products, mainly hydrocarbon molecules (C2-C6), which cannot be released to the atmosphere for environmental reasons. Here, we propose a secondary gas treatment to decompose the hydrocarbon gas products into smaller molecules by capacitively-coupled plasma (CCP) generated by a radio-frequency (13.56 MHz) power supply. Our experimental system includes a plasma chamber equipped with in situ spectroscopy tools that allow us to track and identify species (both radicals and ions) under different conditions (such as power and pressure). The study will allow us to understand the fundamental mechanisms of plastic waste decomposition towards improved treatment.
We are using COMSOL Multiphysics® Plasma Module (plasma-time-periodic [ptp]) to better understand the plasma-chemistry reactions occurring in the plasma chamber. We have constructed a 1D model to explore formation of excited and ionized species under our plasma conditions, while varying input power and pressure. The 1D model contains the RF electrode and the ground electrode as a representation of the plasma chamber, along with its area, and with scattering cross section information imported from the LXCat database (https://nl.lxcat.net). We are also using the time-dependent study of the Plasma Module, which allows us to simulate the plasma from ignition to steady-state.
The results from the model allow us to predict observed trends in the experimental setup for a range of gas mixtures and conditions. The model runs conveniently with the auxiliary sweep functionality for different power and pressure conditions. The main challenge in the model is to simulate the multiple species and multitudinous plasma chemistry reactions. Therefore, the set of reactions from the LXCat database was added one-by-one to carefully look for species or reactions that cause the model to fail.
The model allows us to calculate average or maximum values of the number density (1/m3) of the different species in the plasma regime. We have found good correlation between intensity trends from our experimental spectroscopy diagnostics and the 1D model predictions.

Figures used in the abstract

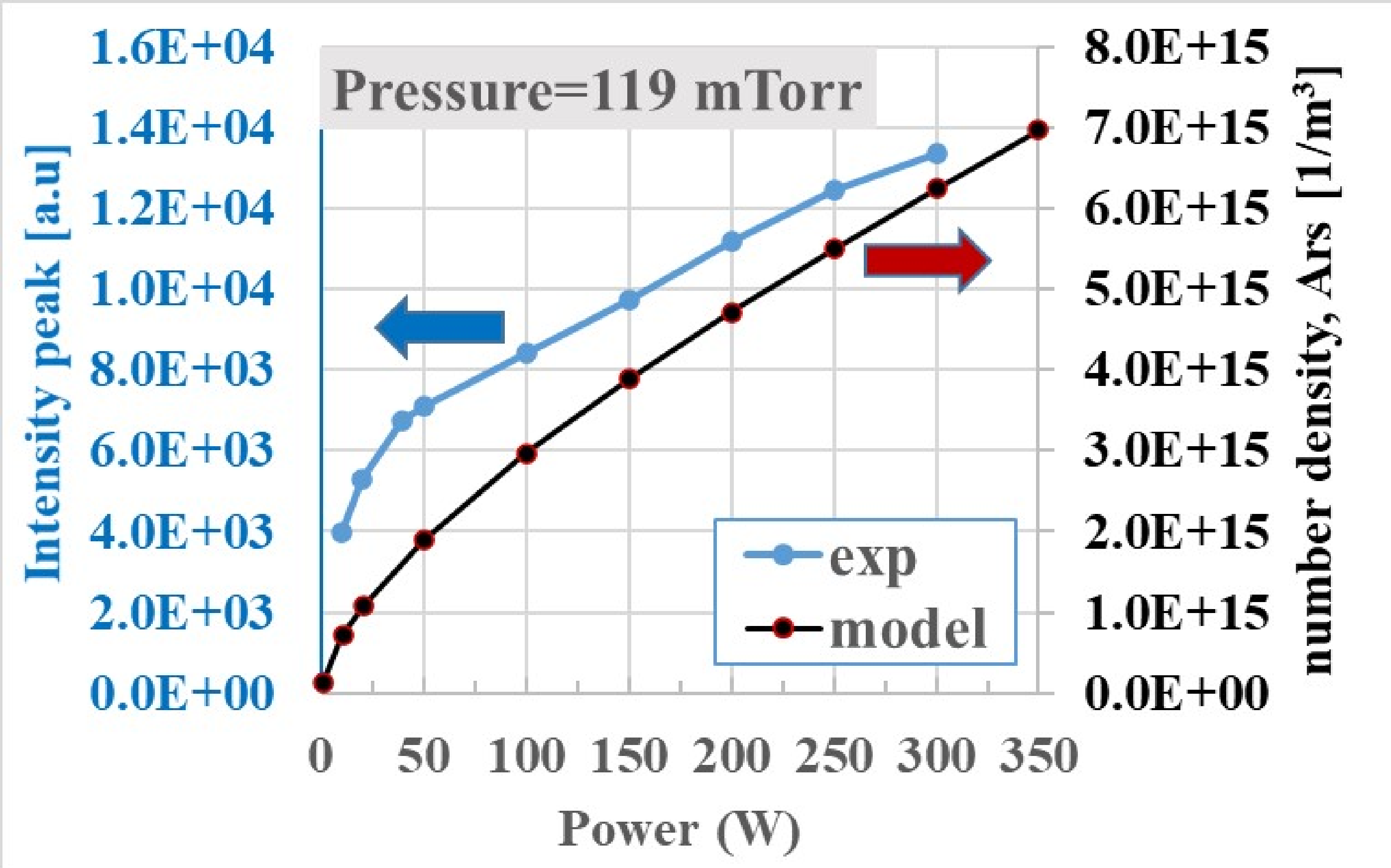

Figure 1 : Observed Ar emission intensity from a representative line, compared with the model's predicted number density of excited Argon