3D CFD MHD modeling of a very high pressure plasma reactor working at low current with helium

A. Lebouvier1, S.A Iwarere1, D. Ramjugernath1, L. Fulcheri2

1Thermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Howard College Campus, King George V Avenue, Durban 4041, South Africa
2MINES ParisTech – PERSEE, Rue Claude Daunesse, 06904 Sophia Antipolis, France

Abstract: A non-reactive 3D time-dependent magnetohydrodynamic (MHD) model of a non-transferred non-thermal arc discharge in peculiar conditions of very high pressure (from 2 MPa up to 10 MPa) and low current (< 1 A) in helium has been developed. The model simulates an experimental-based batch reactor used to experimentally study Fischer-Tropsch application, fluorocarbon production, and CO2 dissociation.

Keywords: MHD modeling, low current, very high pressure, batch reactor, plasma physics

1. Introduction

The field of below atmospheric pressure (up to atmospheric) plasma discharges has been widely explored and led to several applications in many fields. However, the field of above-atmospheric pressure discharges at low current (< 1 A) remains almost unexplored. Using plasma reactors at very high pressure (>> 1 MPa) could offer new development perspectives as it can promote new chemical routes and increase the efficiency of processes. Promising applications in many fields such as chemistry (new organic, or organometallic chemicals and/or synthesis pathways, chain growth, etc.), lightning, materials or nanomaterial synthesis (new materials, etc.) thanks to the combined effect of plasma reactivity and high pressure could see the light.

The lack of studies and knowledge are certainly in relation with technological and technical challenges to develop a reactor able to sustain a plasma at very high pressure (electrodes materials, power supply, high pressure mechanical strains, gas tightness,...). However, the authors have already proven the feasibility of fluorocarbons synthesis and synthetic fuel production by the Fisher-Tropsch process [1-4] at working pressures up to 20 MPa in a tip-tip configuration plasma batch reactor using a low current current and high voltage power supply.

Lebouvier et al. [8, 9] have previously model a low current flow plasma torch at atmospheric pressure. While most of the MHD arc models have focused on high current conditions plasma discharges at atmospheric or sub-atmospheric pressure [5, 6], a non-reactive computational fluid dynamics (CFD) model, working with very high pressure of helium and low current, has been developed to improve the understanding of this unusual technology [7]. Indeed, the low-current and very high pressure used imply numerical instabilities which makes the model challenging to converge.

2. Mathematical model

The 3D MHD model studied is time-dependent and based on the following main assumptions:
- The plasma is considered as a single continuous fluid (helium) and at local thermodynamic equilibrium (LTE).
- The gas is treated as incompressible and expandable. The thermo-physical properties depend only on the temperature and the working pressure.
- Gravity is taken into account in the –x-axis direction.

The model is defined by the set of Navier-Stokes fluid dynamics equations and Maxwell electromagnetic equations. The resistive MHD equations have been solved using Code_Saturne v. 2.1 [10], and its associated electric arc module.

The grid mesh, based on the experimental reactor which geometry is shown in fig. 1, contains 188 550 hexa-cells, is structured, and is refined in the interelectrode zone where the gradients are the highest. For the first 10000 time steps, the time step is set to 0.25 µs. This very small time step is needed to stabilize the arc and obtain convergence of the model in the early stage of calculation. Then, the time step is set to 1 µs for 47500 time steps (50 ms).

The thermo-physical coefficients, even for a common gas like helium, are rarely available for very high pressure (> 1 MPa) and high temperature (up to 20 – 30 K). These properties have been calculated using the T&TWinner software [11] up to 20 kK and for pressures up to 10 MPa.

Fig. 1 Schematic diagram of the plasma reactor.
3. Results and Discussion

3.1. Results for \( I = 0.35 \) A and \( P = 8 \) MPa.

The evolution of the arc temperature during the transient period for a reference case is shown in fig. 2. The cathodic arc root stays attached to the tip of the electrode while the anodic arc root slides along the anode between 2 ms and 32 ms, time for which it reaches its final position. The bending of the arc is a phenomenon observed experimentally. The arc core temperature ranges between 16200 K at the cathode tip and 12700 K at the anode. The value of every variable near the tip is higher than the rest of the arc due to the tip effect. The radius of the arc core can be estimated in the middle of the interelectrode gap to be 0.168 mm, which is in line with the observation of 0.16 mm arc radius of Rohani et al. [4].

The recirculation of the gas in the reactor is shown in fig. 4. Thanks to the convection effect, the hot gas going up mixes with the cold surrounding gas of the reactor and cools down leading it to go towards the bottom and the sides of the reactor. Gravity and high temperatures lead to a natural convective motion of the gas to the top of the reactor contributing to the bending of the arc. The arc shape is a balance of the combined effects of convection, gravity, and electromagnetic forces. The main influence is given by the convective effects.

In a very high pressure batch reactor, the convective motion of the gas is only submitted to the natural convection which involves a very slow motion of the gas. In order to estimate the quantity of gas treated by the discharge, the average velocity of the gas in the arc (0.4 m/s) going through the arc section \( (3.2 \times 10^{-4} \text{ mm}^2) \), has been considered. Thus, the volumetric flow rate can be estimated to 0.128 cm\(^3\)/s. The volume of the reactor being 2.56 cm\(^3\), 3 times of the volume of the reactor can be treated in 1 min.
3.2. Influence of pressure for $I = 0.35$ A

Fig. 5 shows that the higher the pressure, the higher the voltage. It can also be observed that the higher the pressure, the higher the under-estimation of the voltage by the model. However, it is commonly known that the higher the pressure, the lower the discrepancy to the local thermodynamic equilibrium. The discrepancy between the experimental and simulated voltage may probably be attributed to the LTE assumption and electrode phenomena. Indeed, using a similar technology for argon, Izquierdo et al. [12] proved that the effect of the cathodic sheath-space on the voltage drop increases with pressure.

Under the gravity effect, the density gradients are the driving force of the natural convection in the reactor. Indeed, the Rayleigh number, which governs the onset of natural convection, depends mainly on the density, viscosity and the temperature differential. As the temperature differential and the viscosity are similar at high pressure, the density differential plays the most important role.

It can be seen in fig. 8 that the higher the pressure, the higher the convective motion of the gas, and thus the higher the displacement of the arc core and the anodic arc root towards the top of the reactor. The arc radius remains comprised between 0.153 mm and 0.168 mm. No constraint of the arc core by the surrounding pressure is observed.

3.3. Influence of current for $P = 8$ MPa

Fig. 9 shows a negative U-I characteristics commonly observed for a non-thermal plasma arc. The simulated characteristic presents a similar trend with a constant
underestimation of 65 V compared to the experimental characteristic most likely due to the omitted sheath model. The LTE assumption should lead to a lower discrepancy at higher current. Contrary to the pressure, the current has a very slight influence on other main parameters such as velocity, temperature, arc core radius or pressure.

The volume flow rate of gas treated by 0.168 mm and is close to the value observed experimentally. The developed model is a first approach for the simulation of low-current high-pressure plasma arc. The unusual conditions of very high pressure and low current cause instabilities in the ignition of the arc which leads to the use of a very small time step; drastically increasing the computational time. The discrepancies in voltage drop between the experiments and the model are mainly explained by the LTE assumption and the lack of a detailed electrode model to simulate the space-charge sheath. Further developments of the model will focus on the improvement of the cathodic space sheath which is assumed to have the major role in the voltage discrepancies.

4. Conclusions and Perspectives

The MHD modeling of a batch reactor, based on an experimental reactor, working at very high pressure with helium and in low current – high voltage conditions has been successfully implemented, assuming the LTE. The use of a very small time step has allowed the convergence of the model in these unusual conditions.

A reference case, for a pressure of 8 MPa and a current of 0.35 A, shows a bending of the arc shape and a motion of the anodic arc root towards the top of the reactor, as observed experimentally. This phenomenon is due to the combined effects of electromagnetic forces, gravity, and convection effects; convection having the main influence. Gas recirculation takes place in the reactor. The hot gas moves towards the top of the reactor; cools down mixing with the cold surrounding gas and is then driven to the sides and the bottom of the reactor. The temperature of the arc column ranges between 12700 K, at the anode, to 16200 K at the cathode. The cathode is indeed subjected to the tip effect which increases the value of all the variables. The arc core radius has been estimated to be 0.168 mm and is close to the value observed experimentally. The volume flow rate of gas treated by the arc is estimated to be 0.128 cm$^3$/s.

Pressure and current ranges have been investigated. While a pressure increase has almost no effect on the arc radius, it leads to an increase of the convective forces and so to a higher displacement of the arc root towards the top of the reactor. The density gradients between the hot and cold gas is the driving force for the arc motion at very high pressure. The U-I characteristic is typical of a non-thermal arc discharge. Even if the predicted voltage is

![Simulated voltage in function of current and comparison with experimental data.](image)

Fig. 9 Simulated voltage in function of current and comparison with experimental data.

References