3D MHD Modelling of a Hydrogen Three-Phase AC Plasma Torch

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Abstract: With the growing interest of methane pyrolysis via thermal plasma, and with the ability to use part of the produced hydrogen in the process, a numerical analysis is conducted on a three-phase plasma system running on hydrogen as plasma gas. A magnetohydrodynamic model is developed on Ansys FLUENT, simulating a three-phase AC electric arc in a 3d, time-dependent domain. The Joule-Heat, radiation losses, and Thompson effect are added in the energy equation of Fluent, and the Lorentz forces are added in the momentum equations. Results confirm experimental observations and previous analytical and numerical findings regarding arc temperature, discharge gas flow shape, arc formation, and the effect of Lorentz forces on the arc shape and on the Maecker jets. This work is novel in that it is the first MHD model of a hydrogen, three phase AC plasma system developed on Ansys FLUENT, paving way for future parametric studies on the different system parameters.

Keywords: MHD, Plasma, Three-Phase, Alternative Current, Hydrogen, Methane Pyrolysis

1. Introduction

With the release of the latest Intergovernmental Panel on Climate Change (IPCC)'s "World Energy Outlook" report [1], several strategies were proposed for reaching net-zero emissions by 2050. This can only be achieved through the electrification of the industry, where thermal plasma technologies may play an important role as they convert electric energy to thermal energy with very high efficiency.

On the other hand, hydrogen is gaining interest as an energy vector for a decarbonized world, notably for applications such as ammonia production, steel manufacturing, heavy duty transport such as trucks and trains, and in remote microgrids.

The environmental benefit of transitioning towards hydrogen is only achieved if the hydrogen produced has a low carbon intensity. Green hydrogen made by electrolysis using renewable energy is being promoted in policies. However, a high electrical energy input is required. An alternative hydrogen production method with a comparable carbon intensity is that of methane pyrolysis. From a thermodynamic perspective, hydrogen produced through methane pyrolysis uses 7-8 times less energy input than electrolysis (38 kJ/mol vs 285 kJ/mol). Several methods were developed for pyrolyzing methane, with each presenting several drawbacks hindering its industrial viability. Only methane pyrolysis via thermal plasma is industrially viable, as it can produce valuable grades of carbon-black using only electrical energy as an input.

In fact, methane pyrolysis via thermal plasma has been studied for over 30 years at Mines Paris' plasma laboratory with Prof. Fulcheri's team, with the first study published in 1995 [2]. A collaboration has also been established with Monolith Materials in the USA, leading to the first methane pyrolysis via thermal plasma industrial plant, Olive Creek 1. Hydrogen has been reported to be produced at this scale with an energy intensity of 25 kWh/kg (compared to ~60kWh/kg using electrolysis) [3], and is expected to be produced using 10-15 kWh/kg in the very near future due to process optimization.

In parallel, a recently published article reporting a life-cycle-analysis of the Monolith process calculates the carbon intensity of turquoise hydrogen via plasma as 0.91 kgCO2e/kg, comparable to that of green hydrogen, and using renewable natural gas, becomes carbon negative [4].

All of this makes methane pyrolysis via thermal plasma a potential key player for the energy transition, with the latest IEA report "Global Hydrogen 2022" citing Monolith or methane pyrolysis in several sections [5].

In light of the recent interest on methane pyrolysis via thermal plasma, developments of numerical models to simulate the plasma process have been carried out at Mines Paris. With the intrinsic nature of a plasma state having electromagnetic forces, standard CFD methods are insufficient by themselves to describe plasmas. Thus, a coupling of the Navier Stokes equations with the Maxwell equations is done, leading to what is known as MagnetoHydroDynamic (MHD) modelling.

The MHD model is developed and coded on Ansys FLUENT. Section 2 presents the methodology for the model development. Considering that in methane pyrolysis, part of the produced hydrogen can be used internally in the process, the chosen case for the simulation is that of hydrogen as plasma gas, running a three-phase AC plasma torch at 1 bar using 400A current. Section 3 presents the results for one complete cycle at 50 hz.

2. Methodology

2.1. Governing Equations:

The main four equations describing the electromagnetic part of the plasma domain are the Gauss' law, the Faraday's law, Ampere's generalized law, and the magnetic Gauss field law. The solution of these equations is needed to determine the current density inside the arc, and the induced magnetic field.

Once the current density and the magnetic field determined, they are used to calculate the joule-heat energy source, and the Lorentz forces.

In a finite-volume thinking, the idea is to reformulate these equations in what is known as the Patankar form [6]:

$$a\frac{\partial\rho\emptyset}{\partial t} + b\nabla.(\rho V\emptyset) = \nabla.(\Gamma_{\emptyset}V\emptyset) + S_{\emptyset} \qquad (1)$$

with "ρ" the density, "$\emptyset$" the scalar to be solved, "V" the velocity, and "$S_{\emptyset}$" the source term. Therefore, the Patankar form consists of a transient term, an advective/convective term, a diffusive term, and a reactive/source term. "a" and "b" are constants either 0 or 1 depending on whether there is a transient or advective term or not.

The strategy is to reformulate the electromagnetic equations according to this Patankar form. The optimal method is to develop a system of equations that are closed by the electric potential scalar.

First, several hypotheses can be made to simplify the equations:

1- The plasma domain is in local thermodynamic equilibrium (LTE)
2- Plasma fluid is taken as an incompressible gas
3- Flow is laminar
4- Gravity is neglected
5- Magneto-Quasi-Static (MQS) state is used

With these hypotheses, and using ampere's law and the conservation of charge $(\nabla.\vec{j} = 0)$, the electric potential can be deduced according to a Patankar form:

$$-\nabla.(\sigma\nabla V) = 0 \quad (2)$$

with "σ" the electrical conductivity, and "V" the electric potential

From the electric potential, the current densities can in turn be deduced:

$$j_x = -\sigma\frac{\partial V}{\partial x} \qquad (3)$$

$$j_y = -\sigma\frac{\partial V}{\partial y} \qquad (4)$$

$$j_z = -\sigma\frac{\partial V}{\partial z} \qquad (5)$$

As for the magnetic field, in order to get rid of its curl component in the magnetic field equation, a mathematical manipulation commonly performed is to create a "potential vector" "A" as:

$$\vec{B} = \nabla \times \vec{A} \qquad (6)$$

Therefore, the ampere's law can be rewritten in a Patankar form, with "μ_0" the permeability of free space:

$$\nabla \times \vec{B} = \mu_0\vec{j} \quad (7)$$

$$-\nabla^2\vec{A} = \mu_0\vec{j} \quad (8)$$

The induced magnetic field can then be calculated from the potential vector "A". This method of using the potential vector has already been implemented on Fluent in 2d and 3d by Gonzalez and Freton's team [7-8].

2.2. Model Implementation:

With the magnetohydrodynamic equations formulated in the Patankar form (eq. 1), four new user-defined-scalars need to be created on Fluent for the implementation of the developed module, one for the electric potential, and three for the potential vector in the x, y and z coordinates. As explained in the previous subsection, these scalars are used to find the current densities and the induced magnetic field. Subsequently, the joule-heat term is added in the Fluent energy equation as source term, and the Lorentz forces are added in the momentum equations.
Table 1 details all the modifications made on Fluent, i.e. the governing equations in the Patankar form used in the developed module.

Table 1. Governing Equations of The Developed Module

	$\boldsymbol{b}$	$\emptyset$	$\boldsymbol{\Gamma_{\emptyset}}$	$\boldsymbol{S_{\emptyset}}$
x momentum	1	v_x	μ	j_yB_z-j_zB_y
y momentum	1	v_y	μ	j_zB_x-j_xB_z
z momentum	1	v_z	μ	j_xB_y-j_yB_x
Energy	1	H	$\frac{k}{C_p}$	$\frac{{j_x}^2+{j_y}^2+{j_z}^2}{\sigma} + \frac{5}{2}\frac{k}{e}(\frac{j_x}{C_p}\frac{\partial h}{\partial x} + \frac{j_y}{C_p}\frac{\partial h}{\partial y} + \frac{j_z}{C_p}\frac{\partial h}{\partial z}) - 4\pi\epsilon_N$
x potential vector	0	A_x	1	$\mu_0 j_x$
y potential vector	0	A_y	1	$\mu_0 j_y$
z potential vector	0	A_z	1	$\mu_0 j_z$
Electric Potential	0	V	σ	0

In addition to the joule-heat term, the Thompson effect related to the electron drift is also added, along with the radiative term that is calculated according to the net emission coefficient [9].

Properties for hydrogen such as electrical conductivity, density, specific heat and viscosity are all calculated using T&T Winner [10].

2.3. Geometry:

The domain is reported in Figure 1. A small geometry is chosen, in the order of millimeters. Three electrodes are represented, each having a diameter of 18mms. Mesh quality is in the acceptable skewness range, with both equi-volume skew and equi-angle skew values <0.35.

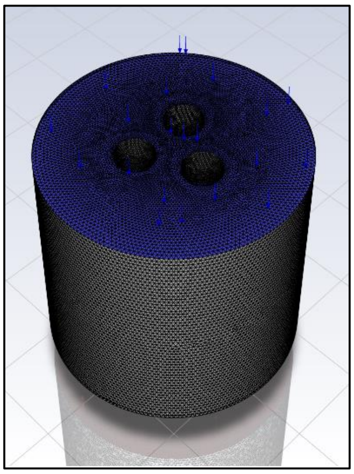

Fig. 1. Mesh of the Domain

2.4. Boundary Conditions:

Boundary conditions can be divided into those related to the fluid dynamics, and those related to the MHD model.

Globally, an inlet hydrogen gas at 300K and 0.1 m/s is used, with a 3500K imposed on the electrode walls, and a 6000K imposed on the electrode surface, as at this temperature range, hydrogen starts to become electrically conductive.

Additionally, a 400A current is implemented on the surface of the electrodes, imposed in a way such that the current density is concentrated on the center of the electrode and decreases the further away from the center. The signal is taken as sinusoidal for the current density, with a frequency of 50 hz.

The derivatives of the potential vector are taken as zero.

3. Results

The arc is simulated for one complete period, i.e. 20ms for this case. The main results are the following:

- From a dynamic perspective, after being in contact with the three-phase plasma arc, the flow of the discharge gas has a tripod shape, mainly due to the inter electrode gap shape and to the momentum forces created by the arc due to the Lorentz forces. This has also been shown in Rehmet's work on modelling a three-phase plasma system on Code Saturne [11].
- Additionally, another dynamic phenomenon that can be observed is that of the Maecker Effect. Jet velocities inside of the plasma arc are observed, reaching several hundreds of meters per second. This cannot be only due to thermal expansion; these maecker jet velocities are due to the constriction of the current conduction zone at the arc-electrode interface, which increases the current density in the near-electrode zone, creating an induced magnetic field more intense than around the arc column. In turn, this induced magnetic field produces Lorentz forces that are responsible for increasing the velocity to several hundreds of meters per second.
- Regarding arc dynamics, it has been proven that the Lorentz forces are what gives the arc an "arc" shape. In fact, removing the Lorentz forces from the model ultimately removes the Maecker Effect, and leads to an arc that keeps expanding in shape with time, therefore losing its "arc" shape
- From a thermodynamic perspective, due to the joule heat generated in the arc being an order of magnitude, and in some instances, two orders of magnitude higher than the thermal losses through radiation, the plasma arc reaches temperature in the range of 14,500-16,500K in its core (it is worthy to mention that the net emission coefficient values are taken for hydrogen from a database already available at Mines Paris)
- As for the electrical characteristics, an arc is formed between the two electrodes where the difference in voltage is the greatest. Therefore, in one complete cycle (20ms) for a three-phase plasma system, 6 arcs are observed, i.e. each electrode is successively an anode and a cathode

4. Conclusion

An MHD module has been developed on Fluent to simulate a three-phase plasma system. First simulations targeted hydrogen as plasma gas, mainly because it can be used as a recirculating plasma gas in a methane pyrolysis via plasma process. Results confirm on one hand experimental observations regarding arc dynamics and formation between the three electrodes and discharge gas flow shape, and on the other hand, results also confirm theoretical hypotheses previously made such as the effect of Lorentz forces on maecker jets and on giving the arc its shape. The arc temperature and the discharge gas flow shape also validate previous analytical and numerical studies. Future work will target parametric analysis on several simulation parameters, and on trying different plasma gases for comparison.

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