CAE-Based Design and Optimization of a Plasma Reactor for Hydrocarbon Processing

F. A. Cassini¹, N. Padoin², C. Soares²

¹Federal University of Santa Catarina (UFSC), Department of Chemistry, Florianópolis-SC, Brazil
²Federal University of Santa Catarina (UFSC), Department of Chemical and Food Engineering, Florianópolis-SC, Brazil

Curitiba, 06th November 2015
Introduction

Research Overview

Macroscopically neutral substances with strong interaction of free electrons, atoms and charged molecules, or neutral excited, exhibiting a collective behavior due to the Coulomb forces

(Bittencourt, 2004)
Introduction

Research Overview

Plasma reactors can be applied to the conversion of waste, biomass and fuel to synthesis gas ($H_2 + CO$) with efficiencies as high as 90-95% and low energy demand.

- Design optimization
- Fluid flow
- Chemical reactions
- Electromagnetic field
Introduction

Research Overview

Objective

Apply a multi-step approach for the investigation of the main physics involved in a rotating gliding arc (RGA) discharge reactor used for hydrocarbon processing
Method

- 3D domain
- N₂ feed
- Velocity inlet
- Pressure outlet (P = 0 Pa)

Flow field

\[ \rho (u \cdot \nabla) u = \nabla \left[ -\rho I + \mu (\nabla u + (\nabla u)^T) - \frac{2}{3} \mu (\nabla \cdot u) I \right] + F \]

\[ \nabla \cdot (\rho u) = 0 \]

Compressible Navier-Stokes equations

Steady-state
Method

- **Electrostatics**

\[ E = -\nabla V \]

\[ \nabla \cdot (\varepsilon_0 \varepsilon_r \mathbf{E}) = \rho_v \]

- 2D axisymmetric domain
- Known voltage imposed at the electrode
- ddp applied according to the experimental setup
- Insulation and ground conditions at the remaining boundaries
- Different electrode geometries were evaluated
- Mesh dependence study was performed
Method

- **Chemical Equilibrium with Applications**
- **Home-made code (Pashen’s and Peek’s law)**
- **COMSOL**
- **Chemical composition of N₂ at the electrode region**
- **Breakdown voltage at the electrode as a function of pressure and gap length**
**Results**

**Fluid Flow Simulations**

- Vacuum at the electrode tip
- Gas flows mainly around the electrode surface

**Profiles at a plane positioned at the electrode tip**

- **Pressure (Pa)**
  - Range: -0.26 to 0 Pa

- **Velocity (m/s)**
  - Range: 0 to 2 m/s

**Region of Analysis**

- Inlet $\text{N}_2$ velocity of 1 m/s
- Velocity contour (m/s) at a central slice
Results

Electrostatics Simulations

(a) Electric field norm (V/m) contours at the electrode

(b) High electron density points: corona discharge is likely to occur

(c) Different electrode geometries: boosting performance through tip optimization
Results

NASA’s CEA Simulations

N₂ composition as a function of temperature at the electrode

Hydrocarbon composition can be assessed too
Results

Pashen’s Law (MATLAB)

Prediction of the breakdown voltage as a function of the gas pressure and the gap length.
Results

Peek’s Law (MATLAB)

An enhanced electric field develops at the electrode tip depending on the geometry.

Peek’s law allow the prediction of Corona discharge.
Analysis

Discharge Regimes

![Diagram showing discharge regimes with voltage and current axes.](image)
Conclusions

Rotating gliding arc (RGA) reactors can be efficiently used for chemical reactions, aiming at hydrocarbon reforming for syngas production.

A complex interaction of different physics dictates the performance of the equipment.

CAE tools can be used for design and optimization.

We have used a workflow, with COMSOL Multiphysics at the core, for phenomenological understanding and application design of RGA reactors.

This procedure will help us to translate the technology developed at laboratory bench scale to real field applications.


Acknowledgements

CAE-Based Design and Optimization of a Plasma Reactor Applied to Hydrocarbon Processing
Thank You!

Contact
Prof. Dr. Cíntia Soares
cintia.soares@ufsc.br
+55 (48) 3721 6409