Modeling and Simulation of Dielectric Barrier Discharge Plasma Reactor for Nitrogen Fixation Reaction

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Abstract

Introduction

Chemical nitrogen fixation reactions have large industrial importance. Fixed nitrogen is used in many different forms ranging from nitric acid to hydrogen cyanide and used as such for large-scale industrial application (e.g. fertilizer, plastic manufacturing, etc.). The reactions to produce these products are highly endothermic and favored by high-temperature processing. The most simple and basic route of chemically fixing nitrogen is the direct reaction of nitrogen and oxygen. However, the major challenge to do so is to supply very high dissociation energy for nitrogen (7.4 eV).

Use of COMSOL Multiphysics®

The main objective of this project is to develop an energy efficient chemical nitrogen fixation process for nitric oxide synthesis by using catalyst in assistance with plasma, aiming to achieve a process on industrial scale. COMSOL Multiphysics® and Plasma Module will be used to simulate and to understand the plasma NO synthesis reaction and transport phenomena inside plasma reactor to obtain the temperature distribution, electron density and mean electron energy distribution. These results will be used to understand the optimal placement of the catalyst and to develop the holistic process design for plasma nitrogen fixation process [1,2].

Reference

[1] Hessel, V., Cravotto, G., Fitzpatrick, P., Patil, B., Lang, J. & Bonrath, W. Chemical Engineering and Processing: Process Intensification, doi:10.1016/j.cep.2013.02.002 (2013).

[2] Hessel, V., Anastasopoulou, A., Wang, Q., Kolb, G.A. & Lang, J. Catalysis Today, http://dx.doi.org/10.1016/j.cattod.2013.04.005, (2013).

Figures used in the abstract

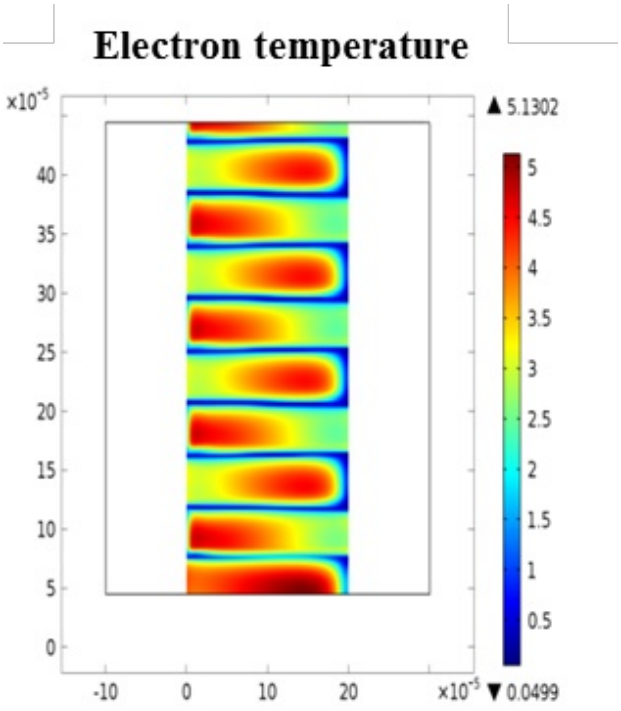

Figure 1: Electron temperature distribution

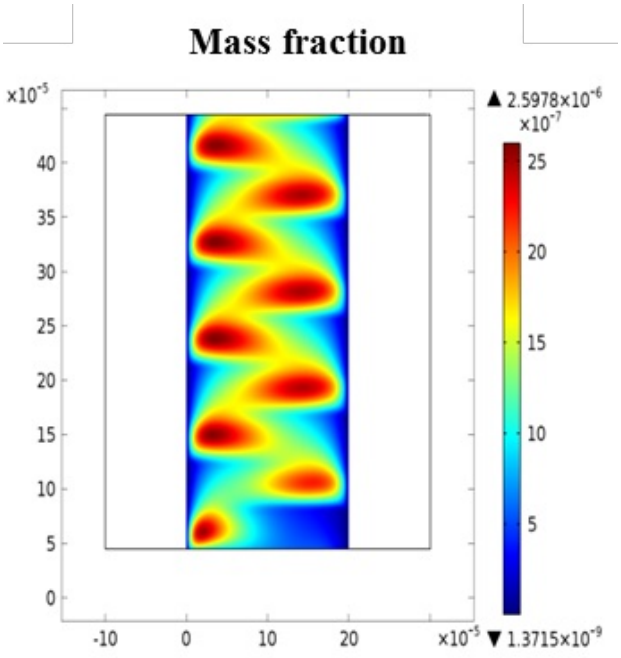

Figure 2: Mass fraction distribution