ID 1024

Chemical Kinetic Investigation for Methane Conversion Into Hydrogen Via Non-Thermal Plasma Process

Djouama Nadine* [1], Labsi Saliha Roumaissa[1], Khodja Khadidja [2], Bendjaballah-Lalaoui Nadia[1]

[1] Faculty of Mechanical Engineering and Process Engineering USTHB, BP32 El-Alia Bab-Ezzouar, 16111 Alger, Algeria

[2] Centre de Développement des Energies Renouvelables, (CDER), B.P. 62, Route de l'Observatoire, 16340, Bouzareah, Algiers, Algeria

*Corresponding author's email: nadinedjouama0612@gmail.com

ABSTRACT

Hydrogen (H_2) is considered as the future energy carrier. It can be used as an alternative solution of fossil fuels. H_2 can be produced by converting hydrocarbons, using non-thermal plasma (NTP) as an alternative to the traditional steam reforming process, which has minimal energy consumption and low CO_2 emission, NTP is considered a dry reforming process. In the present paper, we carried out a theoretical study of various transport parameters such as rate coefficients, cross-sections using electron Boltzmann equation (BE) solver. It provides steady-state solutions of the BE for electrons in a uniform electric field. The H_2 yield and methane (CH_4) conversion are also calculated using the transport parameters. This study involves an NTP reactor containing pure methane gas. The choice of the feed gas is based on it being a subject of interest for low-energy electron collision studies.

Keywords: plasma reactor, non-thermal plasma process, kinetic reactions, hydrogen production, methane conversion.

1. Introduction

Plasma, fourth state of matter, constitutes about 90% of the observable universe and manifests in both thermal and non-thermal forms. Its manipulation has become a key element in innovative technologies across various industries. The renewed interest in plasma research has led to the development of advanced reactors, such as Dielectric Barrier Discharge reactor demonstrated in an experimental setup in Figure 1, the process involves an electric discharge in methane gas, generating non-thermal plasma. pivotal for the conversion of methane to hydrogen. This process, addressing environmental crises, aligns with the vision of hydrogen as a future energy carrier.

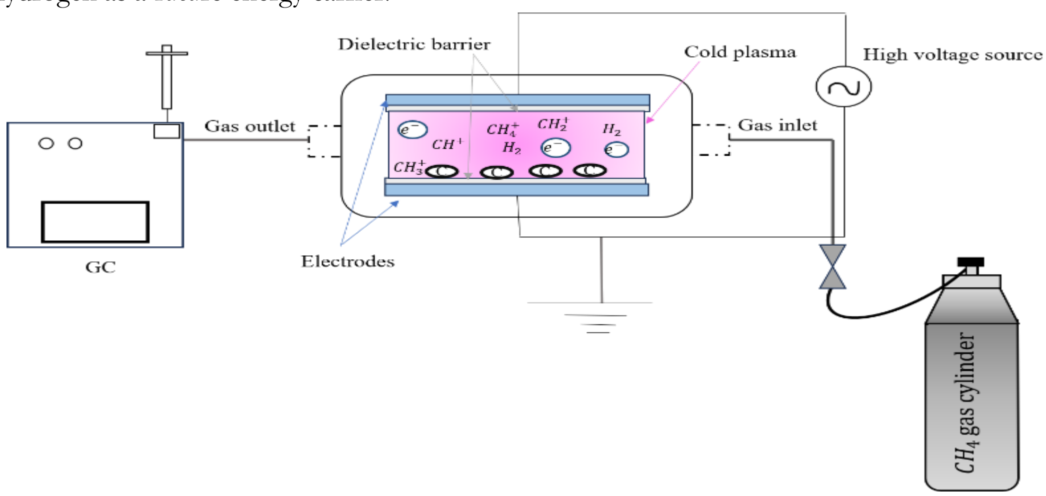

Figure 1: Schematic diagram of the plasma reactor setup

2. Methodology

The results presented in this paper were obtained through the utilization of BOLSIG+ solver, a computer software Developed by Hagelaar *et al.* [1] for the modeling of low-temperature plasmas and the simulation of the transport parameters for gases and plasmas. It serves as predictive tool by employing cross section data and various other input parameters which contributes to a comprehensive understanding for electron-driven kinetics including ionization, excitation and elastic collisions. The cross-section data of the ionized

DOI: 10.21467/abstracts.169 ISBN: 978-81-970666-4-1 (eBook)

reaction mechanisms employed in this software were taken from Janev *et al.* [2], enhancing the reliability of the simulations conducted.

3. Results and Discussion

The study of these electrons transport parameters showcased the following graphs:

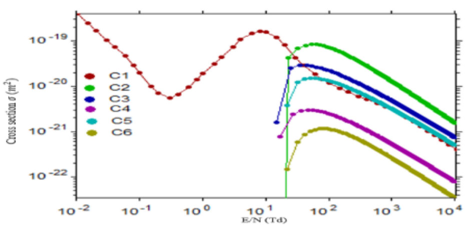

Figure 2: Cross section vs reduced electric current

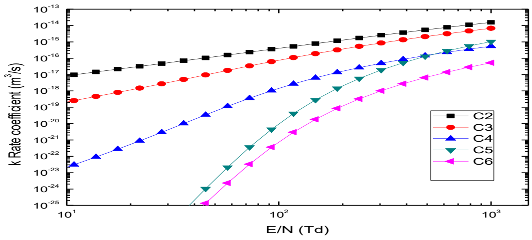

Figure 3: Variation of methane rate coefficients vs reduced electric field

Figure 2 represents: the graph showcases a distinct pattern for the elastic collisions (C_1) within the interval of [1-10 Td] which corresponds to an optimum of. However, it decreases as the reduced electric energy reaches the threshold for each of the five ionization mechanisms (C_2 to C_6), at this point inelastic collisions become predominant, each reaction peaks at approximately 10^2 Td, followed by a decline as the energy increases.

The variation of methane rate coefficients vs reduced electric field is plotted in figure 3. In the context of the five ionization reactions studied (C_2 to C_6), an increase in electric energy correlates with elevated rate coefficients. This relationship is attributed to the accelerated motion of electrons at higher electric energies, intensifying collisions and augmenting reaction rates, this insight facilitates predictive modeling of reaction pathways and efficiencies.

$$k_k = \gamma \int_0^{\infty} \varepsilon \sigma_k f_0 d\varepsilon \qquad (1)$$

Table 1: *Reactions used in the study*

N°	The reaction	Threshold (eV)
C1	$CH_4 + e \longrightarrow CH_4 + e$	Elastic
C2	$CH_4 + e \longrightarrow CH_4^+ + 2e$	12.63
C3	$CH_4 + e \longrightarrow CH_3^+ + H + 2e$	14.55
C4	$CH_4 + e \longrightarrow CH_2^+ + H_2 + 2e$	17.10
C5	$CH_4 + e \longrightarrow CH^+ + H_2 + H + 2e$	22.05
C6	$CH_4 + e \longrightarrow CH_3 + H^+ + 2e$	21.64

4. Conclusions

In this investigation, the examined electron transport parameters exhibited discernible variations, contributing to an enhanced understanding of non-thermal plasma kinetics for the purpose of optimizing methane conversion efficiency.

References

[1] Hagelaar GJM, Pitchford LC., Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models Plasma Sources Sci Technol. 2005;14(4):722.

[2] Janev RK, Reiter D., Collision processes of CH_y and CH_y^+ hydrocarbons with plasma electrons and protons Phys Plasmas. 2002;9(9):4071-81.

[3] Heijkers S, Aghaei M, Bogaerts A., Plasma-Based CH_4 Conversion into Higher Hydrocarbons and H2: Modeling to Reveal the Reaction Mechanisms of Different Plasma Sources J Phys Chem C. 22020;124(13):7016-30.

[4] Cheng L, Barleon N, Cuenot B, Vermorel O, Bourdon A., Plasma assisted combustion of methane-air mixtures: Validation and reduction Combust Flame. 2022; 240:111990.

ISBN: 978-81-970666-4-1

Series: AIJR Abstracts

DOI: 10.21467/abstracts.169