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# Hydrogen production from methane via inductively coupled plasma reactor: 2D simulation of impact of input power

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**Keywords:** hydrogen production, methane conversion, low temperature plasma, inductively coupled plasma, ICP reactor

## Abstract

This study presents a numerical investigation of hydrogen production from methane using an Inductively Coupled Plasma (ICP) reactor, emphasizing the influence of the input power on plasma characteristics and methane conversion. A two dimensional fluid model was developed and solved using the finite element method, incorporating more than 300 plasma chemical reactions to capture detailed kinetics. Simulations were performed for power levels ranging from 100W to 700W. Results show that increasing the input power significantly enhances plasma temperature from approximately 4500K to 8200K and elevate electron density from  $1.2 \times 10^{16} \text{ m}^{-3}$  to  $8.9 \times 10^{16} \text{ m}^{-3}$ . Consequently, methane conversion efficiency rises from 35% to about 90%, with hydrogen yield increasing by nearly 70%. These findings confirm that higher input power strengthens electron energy and collision frequency, thereby improving energy transfer and methane dissociation. The proposed modeling approach provides valuable insights for optimizing plasma assisted methane reforming and supports the development of high efficiency hydrogen production technologies.

## 1. Introduction

Hydrogen has emerged as a crucial energy solution in the transition towards sustainability [1], offering a clean alternative to fossil fuels [2]. As a versatile energy carrier, it excels in generating electricity without polluting emissions, significantly contributing to greenhouse gas reduction [3]. However, challenges persist, including the urgent need to develop more sustainable production methods [4] and suitable distribution infrastructure [5]. Recent advancements in green hydrogen production technologies and decarbonization initiatives promise to strengthen its integration into the global energy landscape, paving the way for a cleaner and more sustainable energy future [6–10].

Concurrently, methane, the primary constituent of natural gas [11], plays a pivotal role as a precursor for hydrogen production owing to its high hydrogen content and established extraction and distribution infrastructure [12–15]. Within the framework of global efforts towards sustainable energy sources, methane is a versatile feedstock capable of generating hydrogen through various processes such as steam reforming [16], partial oxidation [17], and dry reforming [18]. These processes effectively exploit methane's hydrogen-rich composition and offer pathways to mitigate carbon emissions when coupled with carbon capture and utilization technologies [19, 20]. This paper investigates hydrogen production via methane dissociation in an inductively coupled plasma (ICP) reactor, with the aim of contributing to the advancement of clean energy technologies and mitigation of global environmental challenges.

Inductively Coupled Plasma (ICP) reactors represent an advanced and versatile technology in the field of chemical reactions [21–23]. In ICP reactors, a high-temperature plasma is generated by inductive electric fields produced from a time-varying electromagnetic field. These electric fields accelerate electrons, resulting in collisional heating and ionization of molecular species. [24, 25]. These devices offer several notable advantages,

including high energy efficiency, uniform heating, and the ability to operate at atmospheric or sub-atmospheric pressures [26, 27].

This study aims to explore the efficiency and feasibility of hydrogen production via plasma-assisted methane reforming, leveraging the capabilities of the reactor to enhance the reaction kinetics and yield. The main objective of this study is to predict the amount of hydrogen that could be produced.

Daghagheleh *et al* [28] investigated H<sub>2</sub> production from methane pyrolysis by refining process parameters and analyzing their qualitative impacts. For this they used design of experiment software for statistical analysis and utilized advanced characterization techniques such as Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), Raman spectroscopy, X-ray diffraction (XRD) analysis and Inductively Coupled Plasma Mass Spectroscopy (ICP-MS) analysis to study solid carbon properties and confirm product purity.

Dawkins *et al* [29] conducted experiments to optimize the catalytic activity through ball milling of iron ore, observing a significant increase in methane conversion to 5% after 270 min of milling, followed by a decrease to 4% due to particle agglomeration. Characterization techniques including Scanning Electron Microscopy (SEM), Raman spectroscopy, and Mössbauer spectra identified phase transitions in the catalyst from magnetite to maghemite and hematite with increased milling time. Analysis of the carbon byproduct highlighted its high purity, suggesting potential applications as an additive in steel production.

Abuseada *et al* [30] developed a novel solar-thermal methane pyrolysis process utilizing a fibrous carbon medium to simultaneously produce hydrogen fuel and high-value graphitic carbon. Parametric studies varied methane flow rate, solar power, peak flux, operating pressure, and medium thickness, achieving methane conversions from 22% to 96%, hydrogen yields from 21% to 94%, and high-purity graphitic carbon products collected within the medium.

McConnachie *et al* [31] evaluated the addition of metal sulfides to molten salt slurry systems for methane pyrolysis, conducting stability tests at 800 °C in eutectic sodium and potassium bromide for 6 h. Results show enhanced hydrogen production with metal sulfides (MoS<sub>2</sub>) particles achieving 2.75% methane conversion at 800 °C, demonstrating an apparent activation energy of 57 kJ mol<sup>-1</sup>. While MoS<sub>2</sub> exhibited good structural stability, it deactivated primarily due to coking in the melt, indicating potential to lower pyrolysis temperatures despite observed instability over extended operation.

Salakhi *et al* [32] focused on hydrogen and solid carbon co-generation via microwave-driven methane pyrolysis in a fluidized bed of carbon pellets. Numerical simulations employing a coupled gas-solid chemistry approach demonstrate enhanced methane conversion, H<sub>2</sub> selectivity, and carbon deposition rates due to microwave thermal effects. The dominant pathway for solid carbon production was found to be C<sub>2</sub>H<sub>2</sub> deposition onto carbon pellets, minimizing carbon black formation and enhancing H<sub>2</sub> selectivity, highlighting the effectiveness of carbon pellets in reducing the role of complex molecules like polycyclic aromatic hydrocarbons in the pyrolysis process.

Ibrahim *et al* [33] explored the enhancement of methane decomposition and hydrogen production with iron catalysts for using ultrasound-assisted preparation with La<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub> doping. Through comprehensive analyses including X-Ray Diffraction XRD, Hydrogen Temperature-Programmed oxidation Reduction (H<sub>2</sub>-TPR), H<sub>2</sub> chemisorption, Raman spectroscopy, Thermo-Gravimetric Analysis (TGA), and temperature-programmed oxidation (TPO), the research demonstrates that La<sub>2</sub>O<sub>3</sub> doping prevents FeAl<sub>2</sub>O<sub>4</sub> formation, enhances Fe reduction, and increases active sites on the catalyst surface. Compared to traditional methods, ultrasound-assisted catalysts show superior performance, achieving a remarkable methane conversion rate of 93% and hydrogen yield of 84% at 800 °C. This innovative approach not only enhances hydrogen production efficiency but also contributes significantly to advancing sustainable energy technologies.

Scheiblehner *et al* [34] explored various molten copper alloys for their effectiveness as catalytic agents in methane pyrolysis within an inductively heated bubble column reactor. Experimental results underscore the significant impact of the catalyst on methane conversion rates and the characteristics of the resulting carbon. Optimizing these factors is pivotal for enhancing the economic viability of the process.

Chen *et al* [35] compared hydrogen production from one-stage (autothermal reforming of methane) and two-stage processes (partial oxidation of methane followed by water gas shift reaction) using thermodynamic analyses. They found that while the autothermal reforming temperature crucially affects hydrogen yield in the one-stage process, the two-stage process shows higher efficiency, achieving a maximum hydrogen yield of 2.89 moles of hydrogen per mole of methane at 200 °C during the water gas shift reaction, indicating its superiority for hydrogen production.

Hydrogen yields of over 80% were achieved by Ahmed *et al* [36] who explored methane decomposition for hydrogen production using iron-based catalysts with 20% Fe was used as the active metal part of the catalyst.

While numerous studies have investigated methane pyrolysis and reforming through various thermal, catalytic, and solar-assisted methods, there is a relative lack of detailed investigation into plasma-assisted methane dissociation—particularly using low-temperature Inductively Coupled Plasma (ICP) reactors. Existing

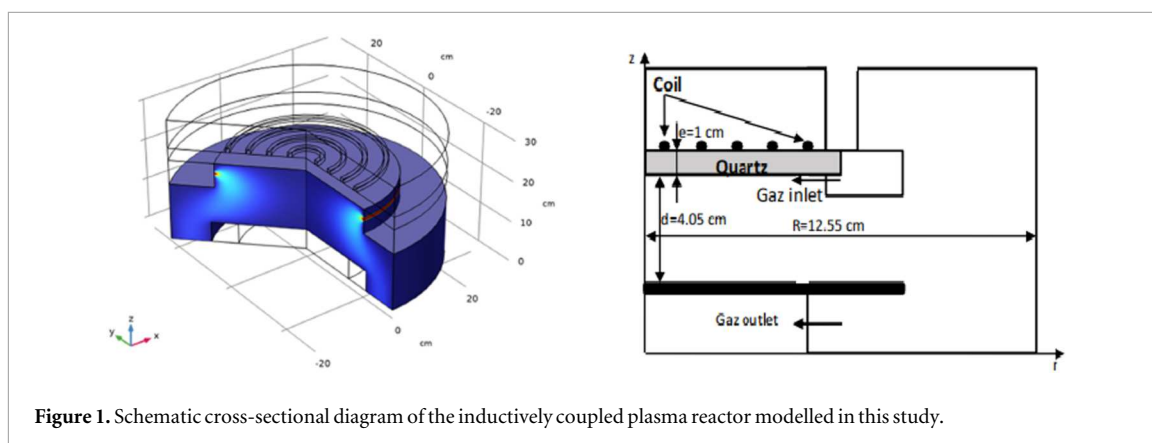


Figure 1. Schematic cross-sectional diagram of the inductively coupled plasma reactor modelled in this study.

research has largely focused on catalyst development or reactor optimization for high-temperature processes, often overlooking the complex plasma-chemical interactions and energy transfer mechanisms within ICP systems. Moreover, most studies have not systematically explored the full reaction pathways or provided predictive models of hydrogen yield based on plasma parameters.

This study aims to numerically investigate hydrogen production from methane using an Inductively Coupled Plasma (ICP) reactor, with particular emphasis on the effect of input power on hydrogen yield. Building on the previous work of Gadoum *et al* [37], where methane dissociation reached approximately 90% under similar ICP conditions, this study further explores the role of power in enhancing plasma reactivity and methane decomposition efficiency. A 2D axisymmetric fluid plasma model was developed in COMSOL Multiphysics, incorporating over 300 plasma-chemical reactions to accurately represent the kinetics of methane decomposition. The model consists of four main components: a fluid model for plasma species, electromagnetic equations to determine the electric field via the magnetic vector potential, and neutral gas dynamics described by the Navier-Stokes and heat transfer equations. Together, these elements simulate weakly ionized plasma behavior under low-temperature conditions, providing deeper insight into the physical and chemical mechanisms of methane dissociation and contributing to the optimization of hydrogen production processes.

The Inductively Coupled Plasma (ICP) reactor was chosen for its stable, electrode-free plasma, ensuring minimal contamination and wide pressure operation. Its efficient energy transfer and precise power control enable effective methane dissociation and detailed analysis of plasma effects, making it ideal for optimizing methane-to-hydrogen conversion. This study explores methane dissociation and hydrogen production under varying plasma conditions.

## 2. Model description

In our simulation, we employed an inductively coupled plasma (ICP) reactor configuration based on the Gaseous Electronics Conference (GEC) RF Reference Cell originally developed by Miller *et al* [38]. Figure 1 illustrates the reactor geometry: a 10 mm thick quartz window separates the plasma from the five-turn copper coil (3 mm wire diameter, 102 mm outer diameter). The stainless-steel lower electrode has a diameter of 165 mm and is positioned 40.5 mm below the quartz window, while the inner diameter of the cylindrical chamber is 251 mm. The coil is powered at a frequency of 13.56 MHz, with the central connection energized and the outer winding grounded. To ensure efficient plasma coupling, the coil is pressed firmly against the quartz plate and supported by a slotted five-arm holder mounted on top of the cell.

The oscillating current in the RF coil produces a time-varying magnetic field that induces azimuthal electric fields in the plasma via Faraday's law. These fields accelerate electrons, leading to ohmic (collisional) heating. Since no external magnetic field is applied, plasma confinement arises primarily from ambipolar electric fields and sheath potentials rather than magnetic trapping. The model represents a self-sustained inductively coupled discharge, combining a fluid description of plasma species with Maxwell's equations to determine the induced electromagnetic fields, and the Navier-Stokes equations to account for gas flow between the inlet and outlet.

In the axisymmetric (2D) implementation, the flat five-turn spiral coil is represented by five coaxial circular loops (rings) arranged along the axial direction, each carrying the same time-harmonic current and spaced to preserve the original radial footprint of the planar spiral. This approach follows the validated methodology described in the COMSOL Application Gallery tutorial 'Model of an Argon/Chlorine Inductively Coupled Plasma Reactor with RF Bias' (Application ID 110171). To ensure accurate representation of near-field electromagnetic distributions and power-absorption characteristics, a mesh sensitivity study was conducted. Refining

the mesh in the coil–plasma interface region from approximately 40,000 to 120,000 elements resulted in less than 2% variation in both the total absorbed power and the azimuthal electric-field maxima. Consequently, the axisymmetric ring representation and adopted mesh resolution are considered sufficient to reproduce the relevant physical behavior of the actual five-turn spiral coil.

## 2.1. Equations of the plasma species

In fluid models, each species is modeled independently to ensure conservation of mass throughout the computational domain. Following Costin *et al* [39], the electrons were assumed to conform to a Maxwellian distribution, which is generally not valid when their energy is below 15eV at low pressures. However, deviations from this distribution, particularly in the form of a high-energy tail in the electronic energy distribution function (EEDF), can lead to discrepancies between model predictions and experimental observations [40]. References [39, 40] show that the Maxwellian assumption reasonably approximates reaction rates under similar conditions, with non-Maxwellian effects having minimal impact on overall chemistry within typical fluid modeling uncertainties.

The governing equations for electrons in these models encompass continuity, momentum, and energy equations. The model considers only continuity and momentum equations for ions. These equations are inter-linked and coupled by Poisson's equation, which establishes the relationship between the space charge and the electrostatic potential within the framework of inductively coupled discharges [39].

The detailed equations used in this work are fully described in references [41, 42].

In order to resolve the equations of this self-consistent fluid model, we used the following boundary conditions.

- **Electrical potential and magnetic potential:** The reactor walls are considered perfectly conductive and connected to the ground, this implies that the electric potential and the magnetic vector potential are zero at the metal walls, at the level of the dielectric wall, the electric potential can be obtained taking into account the following condition:

$$\frac{\partial \sigma_s}{\partial t} = nJ_i + nJ_e \quad (1)$$

$$-n(D_p - D_d) = \sigma_s \quad (2)$$

$\sigma_s$ ,  $n$ ,  $J_i$ ,  $J_e$ ,  $D_p$ , and  $D_d$  are, respectively, the charge accumulated on the surface of the dielectric, the surface norm, the ion current density, the electronic current density, and the electric displacement vectors in the plasma side and in the dielectric side.

- **Density, flux and energy species:** The electron flow at the walls and electrodes is obtained using the boundary condition of a Maxwellian flux where:

$$\Gamma_e = \frac{1}{4} v_{e,th} \cdot \exp\left(-\frac{\Delta\Phi}{k_B T}\right) \quad (3)$$

Where  $\Delta\Phi = \Phi_w - \Phi_p$  With:  $\Phi_w$  is the wall potential and  $\Phi_p$  is the plasma potential

$$v_{e,th} = \sqrt{\frac{8k_B T_e}{\pi m_e}} \quad (4)$$

where the signs  $\pm$  correspond to the direction of the electron flux,  $V$  is the potential of the wall,  $V_{e,th}$  is the electron thermal velocity.

Ignoring the thermal conduction of electrons, the energy flux to the electrodes and the walls is given by:

$$\Gamma_\varepsilon = \frac{5}{2} n_e T_e \Gamma_e \quad (5)$$

The ion density and velocity gradients are set to zero at the boundaries:

$$\nabla n_i = 0, \nabla v_i = 0 \quad (6)$$

- **Gas flow:** the Navier–Stokes equation is solved taking into account as boundary conditions, the gas velocity at the reactor inlet, zero velocity at the walls and electrodes, and a constant pressure at the reactor outlet.

Electron mobility is calculated from their cross section and the diffusion coefficient is calculated using the Einstein relation which relates the mobility to the diffusion coefficient. The mobility of the ions is calculated using the relation of Dalgarno [43], while taking a long-range polarization interaction potential and the diffusion coefficient by the Einstein relation, which are expressed as follows:

$$\mu_i = \frac{36}{\sqrt{\alpha_n m_r}} \frac{2.69 \times 10^{25}}{N} \quad (7)$$

$$\frac{D_i}{\mu_i} = \frac{k_B T_i}{q_i} \quad (8)$$

where  $N$  is the gas density,  $q_i$  is the charge of the ion,  $\mu_i$  is its mobility,  $m_r$  is the reduced ion-neutral mass,  $\alpha_n$  is the polarizability in  $a_0^3$  (where  $a_0$  is the Bohr radius),  $D_i$  is the ionic diffusion coefficient,  $k_B$  is the Boltzmann constant, and  $T_i$  is the ionic temperature.

The diffusion coefficient of the excited particles is calculated taking into account a Lennard-Jones type interaction potential.

$$D_* = 0.0018583 \sqrt{\frac{T^3}{m_r p \sigma_{EN}^2 \Omega_D}} \quad (9)$$

$$\Omega_D = \frac{1.06036}{\psi^B} + \frac{0.193}{e^{D\psi}} + \frac{1.03587}{e^{F\psi}} + \frac{1.76464}{e^{H\psi}}$$

$$\sigma_{EN} = \frac{\sigma_E + \sigma_N}{2}, \quad \Psi = \frac{T}{\sigma_{EN}}, \quad \varepsilon_{EN} = \sqrt{\varepsilon_E \varepsilon_N}$$

where  $T$  and  $p$  are the gas temperature and the pressure,  $m_r$  is the reduced mass,  $(\sigma_E, \varepsilon_E)$  et  $(\sigma_N, \varepsilon_N)$  are respectively the parameters of Leonard-Jones potential of the excited particle  $E$  and the ground state particle  $N$ .  $B, D, F$  and  $H$  are constants given by:

$$B = 0.15610, D = 0.47635, F = 1.52996, \text{ and } H = 3.89411.$$

The reaction rate with the walls and the electrodes can be calculated as follows:

$$k_* = \frac{D_*}{A^2} \quad (10)$$

For a reactor of radius  $R$  and height  $L$ , the effective diffusion length  $\Lambda$  can be expressed from the following relation [44]:

$$\Lambda^2 = \left[ \left( \frac{\pi}{L} \right)^2 + \left( \frac{2.405}{R} \right)^2 \right]^{-1} \quad (11)$$

### 3. Chemical model

In this work we take into account 34 species shown as follow:

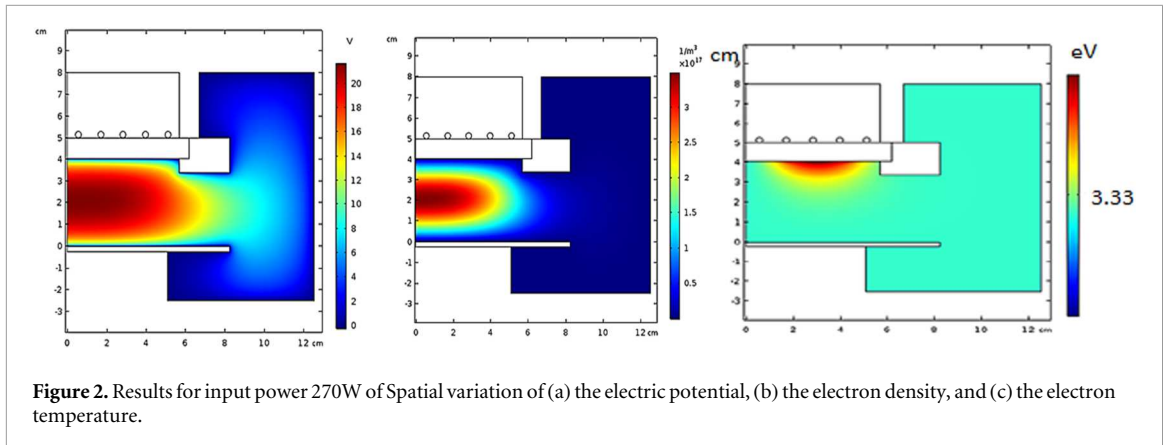
electrons (e), CH<sub>4</sub>, C, C<sub>2</sub>, C<sub>2</sub>H, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>3</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>10</sub>, H<sub>2</sub>, H, CH<sub>3</sub>, CH<sub>2</sub>, CH, C<sub>2</sub>H<sub>5</sub>, H, CH<sub>4</sub><sup>+</sup>, CH<sub>5</sub><sup>+</sup>, CH<sub>3</sub><sup>+</sup>, CH<sub>2</sub><sup>+</sup>, CH<sup>+</sup>, C<sup>+</sup>, C<sub>2</sub><sup>+</sup>, C<sub>2</sub>H<sup>+</sup>, C<sub>2</sub>H<sub>2</sub><sup>+</sup>, C<sub>2</sub>H<sub>3</sub><sup>+</sup>, C<sub>2</sub>H<sub>4</sub><sup>+</sup>, C<sub>2</sub>H<sub>5</sub><sup>+</sup>, C<sub>2</sub>H<sub>6</sub><sup>+</sup>, H<sub>3</sub><sup>+</sup>, H<sub>2</sub><sup>+</sup>, H<sup>+</sup>.

The model includes a total of 320 reactions, as documented in tables 1–3 in the appendix. Among these are 107 electron impact reactions categorized as follows: e+CH<sub>4</sub>, e+CH<sub>3</sub>, e+CH<sub>2</sub>, e+CH, e+C, e+H<sub>2</sub>, e+H, e+C<sub>2</sub>H<sub>6</sub>, e+C<sub>2</sub>H<sub>4</sub>, and e+C<sub>2</sub>H. A detailed descriptions of electron impact cross sections for methane used in this study are provided by our previous work [45]; we note that similar compilations are available elsewhere [46]. Electron-impact dissociation and the dissociative ionization cross sections for the other hydrocarbons species we consider are given in table 3 of the appendix.

Rate coefficients (see table 1) are calculated by:

$$k = A \cdot T_g^n \cdot \exp\left(\frac{-E_a}{RT_g}\right) \quad (12)$$

In this study, wall sticking coefficients were constant, and carbon deposition was not dynamically tracked due to the short simulation timescale. Long-term soot accumulation effects on wall properties and plasma parameters will be addressed in future extended modeling.



#### 4. Results and discussions

The simulation examines a GEC RF ICP reactor using pure methane, incorporating gas dynamics through the solution of the Navier–Stokes equation. The study maintains a consistent gas flow rate at the inlet (100 sccm) and operates at a constant gas pressure of 25 mTorr. The results presented in figures 2(a)–(c) are based on an input power deposition of 270 W in the gas phase.

The ‘input power’ used in this study represents the absorbed power in the plasma, obtained by integrating the ohmic power density ( $\text{Re}(\mathbf{J} \cdot \mathbf{E})$ ) over the discharge volume. The RF excitation is applied to a five-turn copper coil operating at 13.56 MHz, with the center turn powered and the outer turn grounded. The coil current is prescribed in COMSOL’s electromagnetic interface, and the resulting power deposition is computed self-consistently through inductive coupling. This configuration ensures accurate evaluation of the actual plasma heating rather than the nominal generator power.

Figure 2(a) shows the spatial distribution of electric potential within the inductively coupled plasma (ICP) discharge. The electric potential remains relatively low—approximately 20 V—primarily due to space charge accumulation in the plasma region. In ICPs, electrons gain energy predominantly from azimuthal electric fields induced by the time-varying magnetic field generated by the RF current in the coil. These induced fields drive electron heating through collisional (ohmic) mechanisms, especially near the coil, where the skin effect leads to localized energy deposition.

Figure 2(b) illustrates the resulting electron density distribution, which peaks around  $4 \times 10^{12} \text{ cm}^{-3}$  near the coil due to the efficient transfer of energy from the induced fields. Figure 2(c) shows the corresponding electron temperature distribution, with elevated temperatures in regions where the induced electric fields are strongest. This spatial correlation between electric potential and electron temperature reflects how the dynamics of the induced electromagnetic field govern energy absorption and heating within the plasma.

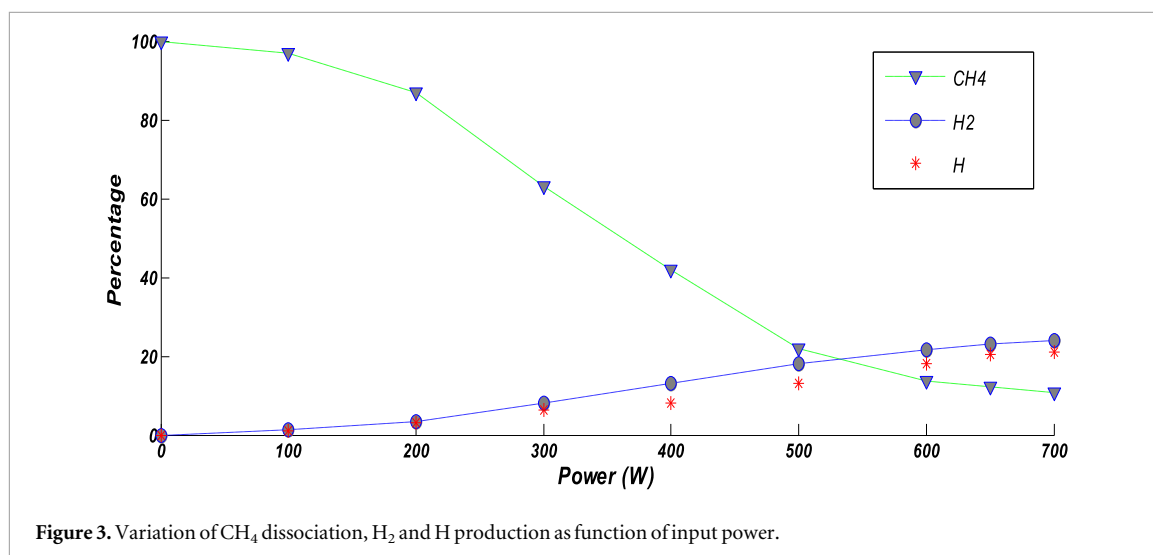
These behaviors are characteristic of inductively coupled plasmas, where electron heating and confinement are controlled by inductive electric fields, ambipolar potentials, and sheath effects, rather than magnetic trapping. It is important to note that no static magnetic field is applied in this setup; thus, charged particle confinement does not result from magnetic mirror or magnetron-like mechanisms. Increasing the input power amplifies the strength of the induced electric field, producing more energetic electrons that collide more frequently with  $\text{CH}_4$  molecules, thereby enhancing methane dissociation and hydrogen production.

These are common behaviors observed in this type of plasma reactor, as similarly reported in several previous studies [61–66], confirming the reliability and physical consistency of the present simulation results.

The dissociation of methane in plasma is governed by several interrelated factors, among which the input power plays a dominant role. Increasing the input power amplifies the electromagnetic field strength, producing a greater population of high-energy electrons. These electrons undergo more frequent and energetic collisions with methane molecules, leading to enhanced dissociation.

In figure 3, our results indicate a substantial increase in methane dissociation within the inductively coupled plasma reactor as input power increases from 100 W to 700 W. However, beyond 700 W, the dissociation process is anticipated to decelerate due to reduced availability of  $\text{CH}_4$  and diminished reactions involving methane. Conversely, the figure illustrates a significant rise in hydrogen molecules ( $\text{H}_2$ ) alongside free hydrogen atoms (H).

Figure 3 demonstrates a significant increase in methane dissociation as the input power rises from 100 W to 700 W. This enhancement is primarily driven by electron-impact reactions, where energetic electrons—heated by the azimuthal electric field induced by the RF coil—gain sufficient energy to overcome the C–H bond



dissociation threshold ( $\sim 4.5$  eV). As input power increases, the electron temperature also rises, reaching average electron energies in the range of 4–10 eV, which are well above the energy required for bond cleavage.

Key dissociation pathways included in the model are: ( $e + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H} + e$  and  $e + \text{CH}_4 \rightarrow \text{CH}_2 + \text{H}_2 + e$ ).

These reactions are part of a detailed plasma chemical mechanism incorporated into the simulation, ensuring a physically accurate representation of methane decomposition under varying plasma conditions.

The local plasma environment strongly influences dissociation rates. Space charge accumulation alters the electric field distribution, while ambipolar electric fields help confine charged species and maintain plasma quasi-neutrality. Although the time-varying magnetic field generated by the RF current is essential for inducing the heating electric field, it does not directly trap electrons or ions, as no static magnetic field is applied in this configuration.

Overall, the strong correlation observed between electron temperature, electric potential, and dissociation efficiency underscores the critical role of induced electric fields in governing energy transfer, reaction kinetics, and plasma chemistry in inductively coupled plasma discharges.

These findings highlight the importance of understanding the interplay between field strength, temperature, and particle dynamics for optimizing plasma-based methane conversion in Inductively Coupled Plasma (ICP) discharges.

Our simulation results are consistent with the findings reported in the most recent work by Ganjovi *et al* [67], who observed a clear dependence of methane conversion on the input RF power. As shown in their figure 6 of Ganjovi *et al* [67], (a), the methane conversion rate increases significantly with rising RF power due to enhanced energy available for ionization and dissociation processes. At higher power levels, the intensified electric field produces more energetic electrons, which collide with CH<sub>4</sub> molecules, leading to bond-breaking and the generation of reactive species such as CH<sub>3</sub>, CH<sub>2</sub>, CH, and H radicals through dissociation, vibrational excitation, and ionization. Their study reported methane conversion rates reaching 91% at 600 W, confirming the strong and rapid influence of RF power on methane cracking. This enhancement was directly attributed to the increase in plasma density and electron temperature at higher power levels, which collectively boost the overall reaction rates within the discharge region.

Thus, both our model and the experimental observations of Alireza G. *et al* demonstrate a consistent trend: higher input power leads to higher electron energy, stronger dissociation rates, and consequently, greater methane conversion efficiency.

In an inductively coupled plasma (ICP) discharge operating at 13.56 MHz, the relatively low electric potential ( $\sim 20$  V) observed in our simulation primarily results from space charge accumulation, which shapes the local electric field distribution. Importantly, no externally applied static magnetic field is present in this configuration. Electron heating and plasma sustainment are driven by inductive electric fields generated by the time-varying magnetic field associated with the RF coil current. These azimuthal electric fields accelerate electrons via the skin effect, leading to localized power deposition, particularly near the coil. The resulting increase in electron energy and density—reaching values around  $4 \times 10^{12} \text{ cm}^{-3}$ —supports efficient ionization and dissociation processes. Particle confinement in this system arises from ambipolar electric fields and sheath structures near boundaries, rather than magnetic trapping. Understanding the interplay between induced electric

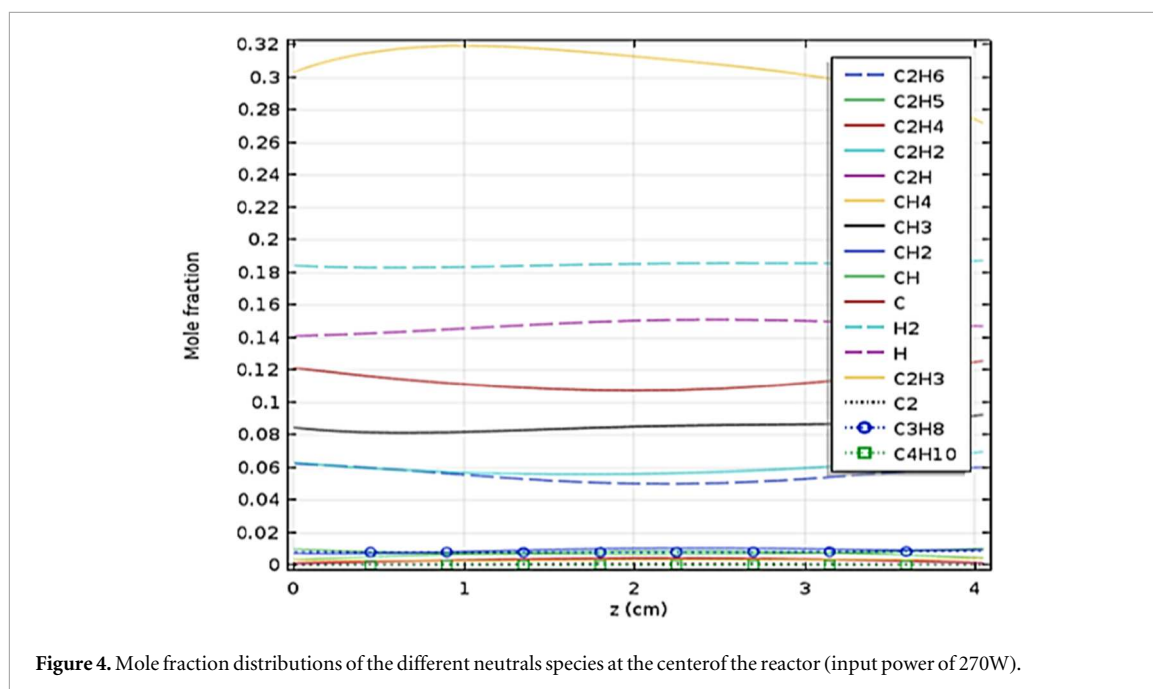


Figure 4. Mole fraction distributions of the different neutrals species at the center of the reactor (input power of 270W).

fields, electron heating, and ambipolar confinement is essential for optimizing plasma chemistry and process performance in ICP reactors.

Moreover, higher input power enhances energy transfer to electrons and ions, increasing plasma temperature and density—key parameters for accelerating dissociation processes. While the hydrodynamic residence time of methane molecules is mainly governed by flow rate, volume, and gas density, the effective reaction time within the plasma increases with power. Stronger electric fields accelerate charged particles and raise their collision frequency with methane molecules, leading to more frequent dissociation events and higher overall conversion efficiency.

Additionally, more power leads to a denser plasma with more reactive species, which further extends the interaction time of methane molecules with these species. Increased electron temperatures at higher power levels result in more effective energy transfer during collisions, breaking molecular bonds more efficiently. The higher energy input also raises the frequency of collisions among particles, giving methane molecules a longer time in the plasma before exiting. These combined effects—stronger electric fields, higher plasma density, increased energy transfer, and extended collision interactions result in a greater likelihood of methane dissociation, making the process more efficient.

The electromagnetic field's role in trapping electrons and ions is crucial in these reactors, particularly under the influence of coils, as shown in previous figures. This environment fosters multiple reactions, contributing significantly to the efficiency and effectiveness of methane dissociation processes within the plasma.

The profile density of different neutrals at the center axis of discharge ( $r = 0$ ) is shown in figure 4. This figure indicates that the most important species after  $\text{CH}_4$  in these conditions is the hydrogen molecule ( $\text{H}_2$ ), this molecule is created primarily by the first process in the plasma which is the electron impact collision, these reactions are the dissociation into:  $\text{CH}_2 + \text{H}_2$ ,  $\text{CH} + \text{H}_2 + \text{H}$ , and  $\text{C} + 2\text{H}_2$ , and also through dissociative ionization of methane molecule like:  $\text{CH}_2 + \text{H}_2$ ,  $\text{CH} + \text{H}_2 + \text{H}$ , and  $\text{C} + 2\text{H}_2$ . Other reactions also lead to increase the amount of the  $\text{H}_2$  produced, such as  $\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2$  and  $\text{CH}_3 + \text{H} \rightarrow \text{CH}_2 + \text{H}_2$ . Although  $\text{CH}_3$  and  $\text{CH}_2$  are the first molecule formed in this process ( $\text{e} + \text{CH}_4 \rightarrow \text{e} + \text{CH}_3 + \text{H}$  with threshold of 8.8 eV,  $\text{e} + \text{CH}_4 \rightarrow \text{e} + \text{CH}_2 + \text{H}_2$  with threshold of 9.4 eV) but their reactions especially ( $\text{CH}_3 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2$ ,  $\text{CH}_3 + \text{CH}_2 \rightarrow \text{C}_2\text{H}_4 + \text{H}$ ,  $\text{CH}_2 + \text{CH}_2 \rightarrow \text{C}_2\text{H}_4$ ) effectively reduces their quantities and increases mainly the amount of  $\text{C}_2\text{H}_4$  molecule, as shown in the figure 4.

## 5. Conclusion

This work presents a comprehensive numerical investigation of methane decomposition in an inductively coupled plasma (ICP) reactor using a self-consistent fluid model. The model incorporates over 300 plasma chemical reactions and couples species transport, electromagnetic field equations, and gas flow dynamics. Plasma behavior is governed by the conservation equations for electrons and ions, along with Poisson's

equation to compute the electric field distribution. Gas dynamics are accounted for via the Navier–Stokes equations, allowing for a realistic simulation of flow, pressure, and species transport within the reactor.

The results demonstrate that increasing the applied RF power significantly enhances key plasma parameters—including electron density, electron temperature, and overall energy transfer efficiency. These changes directly promote electron-impact dissociation of methane, leading to elevated production of reactive species and hydrogen. Notably, the model predicts a methane conversion rate approaching 90% at 700 W input power and a methane mole fraction of 10%, confirming the sensitivity of dissociation processes to plasma operating conditions.

Electron heating is achieved through inductive coupling, where time-varying currents in the RF coil generate azimuthal electric fields that accelerate electrons. This mechanism sustains the plasma through collisional heating, without the use of a static magnetic field. Particle confinement in this configuration arises primarily from ambipolar electric fields and sheath potentials near surfaces, not magnetic trapping.

The observed behavior is consistent with established physical principles of low-temperature ICPs. Higher power levels result in elevated electron energies and increased collision frequencies, both of which enhance the efficiency of energy transfer and methane dissociation. These processes are accompanied by a rise in the production of molecular and atomic hydrogen, highlighting the reactor's potential for hydrogen generation via plasma-assisted reforming.

Overall, the simulation confirms the strong capability of the developed fluid model to capture the key physical and chemical phenomena governing methane conversion in ICP discharges. However, experimental validation remains essential to verify these predictions and assess their applicability to real plasma systems.

Future work will aim to integrate diagnostic techniques—such as optical emission spectroscopy and mass spectrometry—to quantitatively validate species densities and conversion rates. Additional efforts will focus on extending the model to explore the effects of operating pressure, RF frequency, and reactor geometry on plasma uniformity and chemical selectivity. Incorporating surface reactions, vibrational kinetics, and more detailed chemical pathways will also be pursued to refine the model's accuracy. These improvements will support the optimization of plasma-based methane reforming for efficient hydrogen production and broader energy applications.

### Conflict of interest

The authors declare no conflicts of interest.

### Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

### Appendix

The kinetic mechanism used in this study incorporates gas-phase, wall, and electron-impact reactions essential for accurately modeling methane decomposition in the ICP reactor. Table 1 summarizes the bulk plasma reactions and their rate coefficients, which govern the formation and loss of major species and ions. Table 2 provides the sticking coefficients for wall reactions that account for radical quenching and surface recombination. Table 3 lists the electron-impact processes and threshold energies responsible for dissociation, ionization, and fragmentation of hydrocarbons under RF excitation. Together, these data ensure a consistent and comprehensive description of the plasma chemistry used in the simulations.

Table 1. Reactions with Rate coefficient.

N	Reactions	Rate coefficient			References
		A[m <sup>3</sup> /s.mol]	E[J/mol]	n	
01	$CH_4 + CH_2 \Rightarrow CH_3 + CH_3$	0.0713E-16	41988	0	[47]
02	$CH_4 + CH \Rightarrow C_2H_4 + H$	153E-16		-0.9	[46]
03	$CH_4 + H \Rightarrow CH_3 + H_2$	2.2E-26	33632	3	[45]
04	$CH_3 + CH_3 \Rightarrow C_2H_6$	4.66E-16		-0.37	[47]
05	$CH_3 + CH_3 \Rightarrow C_2H_4 + H_2$	170E-16	133030		[46]
06	$CH_3 + CH_3 \Rightarrow C_2H_5 + H$	0.5E-16	56540		[47]
07	$CH_3 + CH_2 \Rightarrow C_2H_4 + H$	0.7E-16			[47]
08	$CH_3 + CH \Rightarrow C_2H_3 + H$	0.5E-16			[46]
09	$CH_3 + C \Rightarrow C_2H_2 + H$	0.83E-16			[46]
10	$CH_3 + H_2 \Rightarrow CH_4 + H$	1.1E-26	39410	2.74	[46]
11	$CH_3 + H \Rightarrow CH_2 + H_2$	1E-16	63190		[47]
12	$CH_2 + CH_2 \Rightarrow C_2H_4$	0.017E-16			[48]
13	$CH_2 + CH_2 \Rightarrow C_2H_2 + 2H$	1.8E-16	3326		[46]
14	$CH_2 + CH_2 \Rightarrow C_2H_2 + H_2$	26.3E-16	50000		[46]
15	$CH_2 + CH_2 \Rightarrow CH_3 + CH$	4E-16	41572		[46]
16	$CH_2 + CH \Rightarrow C_2H_2 + H$	0.66E-16			[48]
17	$CH_2 + C \Rightarrow C_2H + H$	0.83E-16			[48]
18	$CH_2 + H_2 \Rightarrow CH_3 + H$	0.19E-16	53212	0.17	[46]
19	$CH_2 + H \Rightarrow CH + H_2$	2.2E-16			[46]
20	$CH + CH \Rightarrow C_2H_2$	2E-16			[47]
21	$CH + C \Rightarrow C_2 + H$	0.66E-16			[46]
22	$CH + H_2 \Rightarrow CH_2 + H$	5.46E-16	16055		[46]
23	$CH + H \Rightarrow C + H_2$	1.31E-16	665		[47]
24	$C + H_2 \Rightarrow CH + H$	6.64E-16	97278		[47]
25	$CH_4 + CH_4 \Rightarrow CH_5^+ + CH_3$	11.5E-16			[49]
26	$CH_4^+ + H_2 \Rightarrow CH_5^+ + H$	1.086E-16	-300	-0.14	[46]
27	$CH_4^+ + H \Rightarrow CH_3^+ + H_2$	0.1E-16			[46]
28	$CH_5^+ + CH_2 \Rightarrow CH_3^+ + CH_4$	9.6E-16			[46]
29	$CH_5^+ + CH \Rightarrow CH_2^+ + CH_4$	120E-16		-0.5	[46]
30	$CH_5^+ + C \Rightarrow CH^+ + CH_4$	12E-16			[46]
31	$CH_5^+ + H \Rightarrow CH_4^+ + H_2$	1.5E-16			[46]
32	$CH_3^+ + CH_4 \Rightarrow C_2H_5^+ + H_2$	9.6E-16			[49]
33	$CH_3^+ + CH_2 \Rightarrow C_2H_3^+ + H_2$	9.9E-16			[46]

Table 1. (Continued.)

N	Reactions	Rate coefficient			References
		A[m <sup>3</sup> /s.mol]	E[J/mol]	n	
34	$CH_3^+ + CH \Rightarrow C_2H_2^+ + H_2$	123E-16		-0.5	[46]
35	$CH_3^+ + C \Rightarrow C_2H^+ + H_2$	12E-16			[46]
36	$CH_3^+ + H \Rightarrow CH_2^+ + H_2$	7E-16	87800		[46]
37	$CH_2^+ + CH_4 \Rightarrow C_2H_5^+ + H$	2.88E-16			[46]
38	$CH_2^+ + CH_4 \Rightarrow C_2H_4^+ + H_2$	5E-16			[46]
39	$CH_2^+ + CH_4 \Rightarrow C_2H_3^+ + H_2 + H$	2.64E-16			[46]
40	$CH_2^+ + CH_4 \Rightarrow C_2H_2^+ + 2 H_2$	1.44E-16			[46]
41	$CH_2^+ + C \Rightarrow C_2H^+ + H$	12E-16			[46]
42	$CH_2^+ + H_2 \Rightarrow CH_3^+ + H$	7.2E-16			[49]
43	$CH_2^+ + H \Rightarrow CH^+ + H_2$	10E-16	58866		[46]
44	$CH^+ + CH_4 \Rightarrow C_2H_4^+ + H$	0.77E-16			[46]
45	$CH^+ + CH_4 \Rightarrow C_2H_3^+ + H_2$	10.57E-16			[46]
46	$CH^+ + CH_4 \Rightarrow C_2H_2^+ + H_2 + H$	1.55E-16			[46]
47	$CH^+ + CH_2 \Rightarrow C_2H^+ + H_2$	10E-16			[46]
48	$CH^+ + CH \Rightarrow C_2^+ + H_2$	128E-16		-0.5	[46]
49	$CH^+ + C \Rightarrow C_2^+ + H$	12E-16			[46]
50	$CH^+ + H_2 \Rightarrow CH_2^+ + H$	10.1E-16			[46]
51	$CH^+ + H \Rightarrow C^+ + H_2$	74.75E-16	241	-0.37	[46]
52	$C^+ + CH_4 \Rightarrow C_2H_3^+ + H$	10.3E-16			[46]
53	$C^+ + CH_4 \Rightarrow C_2H_2^+ + H_2$	4.2E-16			[46]
54	$C^+ + CH_3 \Rightarrow C_2H_2^+ + H$	13E-16			[46]
55	$C^+ + CH_3 \Rightarrow C_2H^+ + H_2$	10E-16			[46]
56	$C^+ + CH_2 \Rightarrow C_2H^+ + H$	5.2E-16			[46]
57	$C^+ + CH_2 \Rightarrow CH_2^+ + C$	5.2E-16			[46]
58	$C^+ + CH \Rightarrow C_2^+ + H$	65.8E-16		-0.5	[46]
59	$C^+ + CH \Rightarrow CH^+ + C$	65.8E-16		-0.5	[46]
60	$C^+ + H_2 \Rightarrow CH^+ + H$	1E-16	38579		[46]
61	$H_3^+ + CH_4 \Rightarrow CH_5^+ + H_2$	10.3E-16			[46]
62	$H_3^+ + CH_4 \Rightarrow CH_3^+ + 2 H_2$	10.3E-16			[46]
63	$H_3^+ + CH_3 \Rightarrow CH_4^+ + H_2$	21E-16			[46]
64	$H_3^+ + CH_2 \Rightarrow CH_3^+ + H_2$	17E-16			[46]
65	$H_3^+ + CH \Rightarrow CH_2^+ + H_2$	207E-16		-0.5	[46]
66	$H_3^+ + C \Rightarrow CH^+ + H$	20E-16			[46]

Table 1. (Continued.)

N	Reactions	Rate coefficient			References
		A[m <sup>3</sup> /s.mol]	E[J/mol]	n	
67	$H_2^+ + CH_4 \Rightarrow CH_4^+ + H_2$	14E-16			[46]
68	$H_2^+ + CH_4 \Rightarrow CH_5^+ + H$	1.1E-16			[46]
69	$H_2^+ + CH_4 \Rightarrow CH_3^+ + H_2 + H$	22.8E-16			[46]
70	$H_2^+ + CH_2 \Rightarrow CH_2^+ + H_2$	10E-16			[46]
71	$H_2^+ + CH_2 \Rightarrow CH_3^+ + H$	10E-16			[46]
72	$H_2^+ + CH \Rightarrow CH^+ + CH_2$	123E-16		-0.5	[46]
73	$H_2^+ + CH \Rightarrow CH_2^+ + H$	123E-16		-0.5	[46]
74	$H_2^+ + C \Rightarrow CH^+ + H$	24E-16			[46]
75	$H_2^+ + H_2 \Rightarrow H_3^+ + H$	21E-16			[46]
76	$H_2^+ + H \Rightarrow H^+ + H_2$	6.4E-16			[46]
77	$H^+ + CH_4 \Rightarrow CH_4^+ + H$	15.2E-16			[46]
78	$H^+ + CH_4 \Rightarrow CH_3^+ + H_2$	22.8E-16			[46]
79	$H^+ + CH_3 \Rightarrow CH_3^+ + H$	34E-16			[46]
80	$H^+ + CH_2 \Rightarrow CH_2^+ + H$	14E-16			[46]
81	$H^+ + CH_2 \Rightarrow CH^+ + H_2$	14E-16			[46]
82	$H^+ + CH \Rightarrow CH^+ + H$	329E-16		-0.5	[46]
83	$C_2H_4^+ + H \Rightarrow C_2H_3^+ + H_2$	3E-16			[46]
84	$CH_4 + C_2H_3 \Rightarrow C_2H_4 + CH_3$	2.41E-30	22860	4.02	[47]
85	$CH_4 + C_2H \Rightarrow C_2H_2 + CH_3$	0.03E-16	2079	0	[47]
86	$CH_3 + C_2H_6 \Rightarrow C_2H_5 + CH_4$	0.9E-30	34670	4	[47]
87	$CH_3 + C_2H_5 \Rightarrow C_3H_8$	8.11E-16		-0.5	[47]
88	$CH_3 + C_2H_5 \Rightarrow C_2H_4 + CH_4$	0.019E-16			[47]
89	$CH_3 + C_2H_3 \Rightarrow C_2H_2 + CH_4$	8833E-16	2494	-1.5	[46]
90	$CH_2 + C_2H_3 \Rightarrow C_2H_2 + CH_3$	0.3E-16			[45]
91	$CH_2 + C_2H \Rightarrow C_2H_2 + CH$	0.3E-16			[45]
92	$CH + C_2H_6 \Rightarrow C_2H_4 + CH_3$	4.8E-16	242.7	-0.52	[46]
93	$H_2 + C_2H \Rightarrow C_2H_2 + H$	3.9203e-25	1081	2.57	[46]
94	$H + C_2H_5 \Rightarrow C_2H_6$	0.6E-16			[48]
95	$H + C_2H_5 \Rightarrow CH_3 + CH_3$	0.6E-16			[50]
96	$H + C_2H_5 \Rightarrow C_2H_4 + H_2$	0.03E-16			[50]
97	$H + C_2H_4 \Rightarrow C_2H_5$	0.14E-20	4150	1.49	[47]
98	$H + C_2H_4 \Rightarrow C_2H_3 + H_2$	2.2E-24	51220	2.53	[46]
99	$H + C_2H_3 \Rightarrow C_2H_2 + H_2$	0.332E-16			[46]
100	$H + C_2H_2 \Rightarrow C_2H + H_2$	3.8E-16	113359		[46]

Table 1. (Continued.)

N	Reactions	Rate coefficient			References
		A[m <sup>3</sup> /s.mol]	E[J/mol]	n	
101	$C_2H_6 + C_2H \Rightarrow C_2H_5 + C_2H_2$	0.067E-16	-515	0.28	[45]
102	$C_2H_5 + C_2H_3 \Rightarrow C_2H_6 + C_2H_4$	0.024E-16			[47]
103	$C_2H_5 + C_2H_5 \Rightarrow C_4H_{10}$	0.19E-16			[47]
104	$C_2H_5 + C_2H \Rightarrow C_2H_4 + C_2H_2$	0.03E-16			[47]
105	$CH_4^+ + C_2H_6 \Rightarrow C_2H_4^+ + CH_4 + H_2$	19.1E-16			[49]
106	$CH_4^+ + C_2H_4 \Rightarrow C_2H_4^+ + CH_4$	13.8E-16			[46]
107	$CH_4^+ + C_2H_4 \Rightarrow C_2H_5^+ + CH_3$	4.23E-16			[46]
108	$CH_4^+ + C_2H_2 \Rightarrow C_2H_2^+ + CH_4$	11.3E-16			[46]
109	$CH_4^+ + C_2H_2 \Rightarrow C_2H_3^+ + CH_3$	12.3E-16			[46]
110	$CH_5^+ + C_2H_4 \Rightarrow C_2H_5^+ + CH_4$	15E-16			[46]
111	$CH_5^+ + C_2H_2 \Rightarrow C_2H_3^+ + CH_4$	16E-16			[46]
112	$CH_5^+ + C_2H \Rightarrow C_2H_2^+ + CH_4$	9E-16			[46]
113	$CH_5^+ + C_2 \Rightarrow C_2H^+ + CH_4$	9.5E-16			[46]
114	$CH_3^+ + C_2H_6 \Rightarrow C_2H_5^+ + CH_4$	14.8E-16			[46]
115	$CH_3^+ + C_2H_4 \Rightarrow C_2H_3^+ + CH_4$	3.5E-16			[46]
116	$CH_3^+ + C_2H_3 \Rightarrow C_2H_3^+ + CH_3$	51.9E-16		-0.5	[46]
117	$C^+ + C_2H_6 \Rightarrow C_2H_5^+ + CH$	2.31E-16			[46]
118	$C^+ + C_2H_6 \Rightarrow C_2H_4^+ + CH_2$	1.16E-16			[46]
119	$C^+ + C_2H_6 \Rightarrow C_2H_3^+ + CH_3$	4.95E-16			[46]
120	$C^+ + C_2H_6 \Rightarrow C_2H_2^+ + CH_4$	0.825E-16			[46]
121	$C^+ + C_2H_5 \Rightarrow C_2H_5^+ + C$	5E-16			[46]
122	$C^+ + C_2H_4 \Rightarrow C_2H_4^+ + C$	0.17E-16			[46]
123	$C^+ + C_2H_4 \Rightarrow C_2H_3^+ + CH$	0.85E-16			[46]
124	$H_3^+ + C_2H_6 \Rightarrow C_2H_5^+ + 2 H_2$	34E-16			[49]
125	$H_3^{++} + C_2H_5 \Rightarrow C_2H_6^+ + H_2$	14E-16			[46]
126	$H_3^+ + C_2H_4 \Rightarrow C_2H_5^+ + H_2$	14.4E-16			[46]
127	$H_3^+ + C_2H_4 \Rightarrow C_2H_3^+ + 2 H_2$	21.6E-16			[46]
128	$H_3^+ + C_2H_3 \Rightarrow C_2H_4^+ + H_2$	346E-16		-0.5	[46]
129	$H_3^+ + C_2H_2 \Rightarrow C_2H_3^+ + H_2$	35E-16			[46]
130	$H_3^+ + C_2H \Rightarrow C_2H_2^+ + H_2$	17E-16			[46]
131	$H_3^+ + C_2 \Rightarrow C_2H^+ + H_2$	18E-16			[46]
132	$H_2^+ + C_2H_6 \Rightarrow C_2H_6^+ + H_2$	2.94E-16			[46]
133	$H_2^+ + C_2H_6 \Rightarrow C_2H_5^+ + H_2 + H$	13.7E-16			[46]

Table 1. (Continued.)

N	Reactions	Rate coefficient			References
		A[m <sup>3</sup> /s.mol]	E[J/mol]	n	
134	$H_2^+ + C_2H_6 \Rightarrow C_2H_4^+ + 2 H_2$	23.5E-16			[46]
135	$H_2^+ + C_2H_6 \Rightarrow C_2H_3^+ + 2 H_2 + H$	6.86E-16			[45]
136	$H_2^+ + C_2H_6 \Rightarrow C_2H_2^+ + 3 H_2$	1.96E-16			[45]
137	$H_2^+ + C_2H_4 \Rightarrow C_2H_4^+ + H_2$	22.1E-16			[46]
138	$H_2^+ + C_2H_4 \Rightarrow C_2H_3^+ + H_2 + H$	18.1E-16			[46]
139	$H_2^+ + C_2H_4 \Rightarrow C_2H_2^+ + 2 H_2$	8.8E-16			[46]
140	$H_2^+ + C_2H_2 \Rightarrow C_2H_2^+ + H_2$	48.2E-16			[46]
141	$H_2^+ + C_2H_2 \Rightarrow C_2H_3^+ + H$	4.8E-16			[46]
142	$H_2^+ + C_2H \Rightarrow C_2H^+ + H_2$	10E-16			[46]
143	$H_2^+ + C_2H \Rightarrow C_2H_2^+ + H$	10E-16			[46]
144	$H_2^+ + C_2 \Rightarrow C_2^+ + H_2$	11E-16			[46]
145	$H_2^+ + C_2 \Rightarrow C_2H^+ + H$	11E-16			[46]
146	$H^+ + C_2H_6 \Rightarrow C_2H_4^+ + H_2 + H$	14E-16			[46]
147	$H^+ + C_2H_6 \Rightarrow C_2H_3^+ + 2 H_2$	28E-16			[46]
148	$H^+ + C_2H_5 \Rightarrow C_2H_4^+ + H_2$	16.5E-16			[46]
149	$H^+ + C_2H_5 \Rightarrow C_2H_3^+ + H_2 + H$	30.6E-16			[46]
150	$H^+ + C_2H_4 \Rightarrow C_2H_3^+ + H_2$	30E-16			[46]
151	$H^+ + C_2H_4 \Rightarrow C_2H_2^+ + H_2 + H$	10E-16			[46]
152	$H^+ + C_2H_4 \Rightarrow C_2H_4^+ + H$	10E-16			[46]
153	$H^+ + C_2H_3 \Rightarrow C_2H_3^+ + H$	346E-16		-0.5	[46]
154	$H^+ + C_2H_3 \Rightarrow C_2H_2^+ + H_2$	346E-16		-0.5	[46]
155	$H^+ + C_2H_2 \Rightarrow C_2H_2^+ + H$	5.4E-16			[46]
156	$H^+ + C_2H \Rightarrow C_2H^+ + H$	15E-16			[46]
157	$H^+ + C_2H \Rightarrow C_2^+ + H_2$	15E-16			[46]
158	$H^+ + C_2 \Rightarrow C_2^+ + H$	31E-16			[46]
159	$C_2H_5^+ + H \Rightarrow C_2H_4^+ + H_2$	0.1E-16			[46]
160	$C_2H_4^+ + C_2H_3 \Rightarrow C_2H_5^+ + C_2H_2$	86.6E-16		-0.5	[46]
161	$C_2H_4^+ + C_2H_3 \Rightarrow C_2H_3^+ + C_2H_4$	86.6E-16		-0.5	[46]
162	$C_2H_3^+ + C_2H_6 \Rightarrow C_2H_5^+ + C_2H_4$	2.91E-16			[46]
163	$C_2H_3^+ + C_2H_4 \Rightarrow C_2H_5^+ + C_2H_2$	9.3E-16			[49]
164	$C_2H_3^+ + C_2H_3 \Rightarrow C_2H_5^+ + C_2H$	86.6E-16		-0.5	[46]
165	$C_2H_3^+ + C_2H \Rightarrow C_2H_2^+ + C_2H_2$	86.6E-16		-0.5	[46]
166	$C_2H_3^+ + H \Rightarrow C_2H_2^+ + H_2$	0.68E-16			[46]

Table 1. (Continued.)

N	Reactions	Rate coefficient			References
		A[m <sup>3</sup> /s.mol]	E[J/mol]	n	
167	$C_2H_2^+ + C_2H_6 \Rightarrow C_2H_4^+ + C_2H_4$	2.62E-16			[46]
168	$C_2H_2^+ + C_2H_6 \Rightarrow C_2H_5^+ + C_2H_3$	1.31E-16			[46]
169	$C_2H_2^+ + C_2H_4 \Rightarrow C_2H_4^+ + C_2H_2$	4.0E-16			[46]
170	$C_2H_2^+ + C_2H_3 \Rightarrow C_2H_3^+ + C_2H_2$	57E-16		-0.5	[46]
171	$C_2H_2^+ + H_2 \Rightarrow C_2H_3^+ + H$	10E-16			[46]
172	$C_2H^+ + CH_4 \Rightarrow C_2H_2^+ + CH_3$	3.74E-16			[46]
173	$C_2H^+ + CH_2 \Rightarrow CH_3^+ + C_2$	4.4E-16			[46]
174	$C_2H^+ + H_2 \Rightarrow C_2H_2^+ + H$	7.8E-16			[49]
175	$C_2^+ + CH \Rightarrow CH^+ + C_2$	55.4E-16		-0.5	[46]
176	$C_2^+ + CH_4 \Rightarrow C_2H_2^+ + CH_2$	1.82E-16			[46]
177	$C_2^+ + CH_4 \Rightarrow C_2H^+ + CH_3$	2.38E-16			[46]
178	$C_2^+ + CH_2 \Rightarrow CH_2^+ + C_2$	4.5E-16			[46]
179	$C_2^+ + C \Rightarrow C^+ + C_2$	1.1E-16			[46]
180	$C_2^+ + H_2 \Rightarrow C_2H^+ + H$	11E-16			[46]
181	$C_2H_6^+ + C_2H_6 \Rightarrow C_3H_8^+ + CH_4$	0.08E-16			[45]
182	$C_2H_6^+ + C_2H_4 \Rightarrow C_2H_4^+ + C_2H_6$	11.5E-16			[46]
183	$C_2H_6^+ + C_2H_2 \Rightarrow C_2H_5^+ + C_2H_3$	2.22E-16			[51]
184	$C_2H_6^+ + H \Rightarrow C_2H_5^+ + H_2$	1E-16			[46]

**Table 2.** Wall reactions with sticking coefficient [52].

N	Wall reaction	Sticking coefficient
01	CH <sub>2</sub>	0.026
02	CH <sub>3</sub>	0.001
03	CH <sub>4</sub>	0.01
04	C <sub>2</sub> H	0.8
05	C <sub>2</sub> H <sub>3</sub>	0.3
06	C <sub>2</sub> H <sub>5</sub>	0.01
07	H	0.07
08	C	1
09	C <sub>2</sub>	1

**Table 3.** Electronic impact reactions with threshold energy (CH<sub>4</sub>, CH<sub>3</sub>, CH<sub>2</sub>, CH, C, H, H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub>) [53–60].

N	Reactions	Threshold (eV)
01	e+CH <sub>4</sub> =>e+CH <sub>3</sub> +H	8.8
02	e+CH <sub>4</sub> =>e+CH <sub>2</sub> +H <sub>2</sub>	9.4
03	e+CH <sub>4</sub> =>e+CH+H <sub>2</sub> +H	12.5
04	e+CH <sub>4</sub> =>e+C+2H <sub>2</sub>	14
05	e+CH <sub>4</sub> =>2e+CH <sub>4</sub> <sup>+</sup>	12.63
06	e+CH <sub>4</sub> =>2e+H+CH <sub>3</sub> <sup>+</sup>	14.25
07	e+CH <sub>4</sub> =>2e+H <sub>2</sub> +CH <sub>2</sub> <sup>+</sup>	15.1
08	e+CH <sub>4</sub> =>2e+H+H <sub>2</sub> +CH <sup>+</sup>	19.9
09	e+CH <sub>4</sub> =>2e+2H <sub>2</sub> +C <sup>+</sup>	19.6
10	e+CH <sub>4</sub> =>2e+CH <sub>2</sub> +H <sub>2</sub> <sup>+</sup>	20.1
11	e+CH <sub>4</sub> =>2e+CH <sub>3</sub> +H <sup>+</sup>	18
12	e+CH <sub>3</sub> =>e+CH <sub>2</sub> +H	6.9
13	e+CH <sub>3</sub> =>e+CH+H <sub>2</sub>	7.2
14	e+CH <sub>3</sub> =>e+CH+2H	12.4
15	e+CH <sub>3</sub> =>e+C+H <sub>2</sub> +H	10.6
16	e+CH <sub>3</sub> =>2e+CH <sub>3</sub> <sup>+</sup>	9.84
17	e+CH <sub>3</sub> =>2e+CH <sub>2</sub> <sup>+</sup> +H	15.12
18	e+CH <sub>3</sub> =>2e+CH <sup>+</sup> +H <sub>2</sub>	15.74
19	e+CH <sub>3</sub> =>2e+H <sup>+</sup> +CH <sub>2</sub>	18.42
20	e+CH <sub>3</sub> =>2e+C++H+H <sub>2</sub>	19.50
21	e+CH <sub>3</sub> =>2e+H <sub>2</sub> ++CH	20.18
22	e+CH <sub>2</sub> =>e+CH+H	6.4
23	e+CH <sub>2</sub> =>e+C+H <sub>2</sub>	6.6
24	e+CH <sub>2</sub> =>e+C+2H	10.4
25	e+CH <sub>2</sub> =>2e+CH <sub>2</sub> <sup>+</sup>	10.4
26	e+CH <sub>2</sub> =>2e+CH <sup>+</sup> +H	15.53
27	e+CH <sub>2</sub> =>2e+C <sup>+</sup> +H <sub>2</sub>	14.67
28	e+CH <sub>2</sub> =>2e+H <sup>+</sup> +CH	18.01
29	e+CH <sub>2</sub> =>2e+H <sub>2</sub> <sup>+</sup> +C	18.83
30	e+CH= >e+C+H	5.3
31	e+CH= >2e+CH+	10.64
32	e+CH= >2e+C <sup>+</sup> +H	14.74
33	e+CH= >2e+H <sup>+</sup> +C	17.07
34	e+C= >2e+C <sup>+</sup>	11.26
35	e+H= >2e+H <sup>+</sup>	13.6
36	e+H <sub>2</sub> = >e+H+H	15.0
37	e+H <sub>2</sub> = >e+H+H	16.6
38	e+H <sub>2</sub> = >2e+H <sub>2</sub> <sup>+</sup>	15.4
39	e+H <sub>2</sub> = >2e+H+H <sup>+</sup>	18.1
40	e+C <sub>2</sub> H <sub>2</sub> = >e+C <sub>2</sub> H+H	7.5
41	e+C <sub>2</sub> H <sub>2</sub> = >e+C <sub>2</sub> +H <sub>2</sub>	8.7
42	e+C <sub>2</sub> H <sub>2</sub> = >e+C <sub>2</sub> +2H	11.38
43	e+C <sub>2</sub> H <sub>2</sub> = >e+CH+CH	10.6
44	e+C <sub>2</sub> H <sub>2</sub> = >e+CH <sub>2</sub> +C	9.8
45	e+C <sub>2</sub> H <sub>2</sub> = >2e+C <sub>2</sub> H <sub>2</sub> <sup>+</sup>	11.4
46	e+C <sub>2</sub> H <sub>2</sub> = >2e+C <sub>2</sub> H <sup>+</sup> +H	16.48

Table 3. (Continued.)

N	Reactions	Threshold (eV)
47	$e + C_2H_2 \Rightarrow 2e + C_2^+ + H_2$	16.76
48	$e + C_2H_2 \Rightarrow 2e + CH^+ + CH$	20.61
49	$e + C_2H_2 \Rightarrow 2e + C^+ + CH_2$	20.35
50	$e + C_2H_2 \Rightarrow 2e + H^+ + C_2H$	18.46
51	$e + C_2H_4 \Rightarrow e + C_2H_3 + H$	6.9
52	$e + C_2H_4 \Rightarrow e + C_2H_2 + H_2$	5.8
53	$e + C_2H_4 \Rightarrow e + C_2H_2 + 2H$	6.5
54	$e + C_2H_4 \Rightarrow e + C_2H + H_2 + H$	8.4
55	$e + C_2H_4 \Rightarrow e + CH_3 + CH$	8.7
56	$e + C_2H_4 \Rightarrow e + CH_2 + CH_2$	8.9
57	$e + C_2H_4 \Rightarrow e + C + CH_4$	8.1
58	$e + C_2H_4 \Rightarrow 2e + C_2H_4^+$	11.51
59	$e + C_2H_4 \Rightarrow 2e + C_2H_3^+ + H$	13.09
60	$e + C_2H_4 \Rightarrow 2e + C_2H_2^+ + H_2$	13.23
61	$e + C_2H_4 \Rightarrow 2e + C_2H^+ + H_2 + H$	19.06
62	$e + C_2H_4 \Rightarrow 2e + C_2^+ + 2H_2$	20.09
63	$e + C_2H_4 \Rightarrow 2e + CH_3^+ + CH$	16.91
64	$e + C_2H_4 \Rightarrow 2e + CH_2^+ + CH_2$	17.94
65	$e + C_2H_4 \Rightarrow 2e + CH^+ + CH_3$	18.2
66	$e + C_2H_4 \Rightarrow 2e + C^+ + CH_4$	18.94
67	$e + C_2H_6 \Rightarrow e + C_2H_5 + H$	7.45
68	$e + C_2H_6 \Rightarrow e + C_2H_4 + H_2$	4.0
69	$e + C_2H_6 \Rightarrow e + C_2H_3 + H_2 + H$	9.4
70	$e + C_2H_6 \Rightarrow e + C_2H_2 + 2H_2$	6.2
71	$e + C_2H_6 \Rightarrow e + CH_4 + CH_2$	6.95
72	$e + C_2H_6 \Rightarrow e + CH_3 + CH_3$	6.38
73	$e + C_2H_6 \Rightarrow 2e + C_2H_6^+$	11.52
74	$e + C_2H_6 \Rightarrow 2e + C_2H_5^+ + H$	12.50
75	$e + C_2H_6 \Rightarrow 2e + C_2H_4^+ + H_2$	11.43
76	$e + C_2H_6 \Rightarrow 2e + C_2H_3^+ + H_2 + H$	14.51
77	$e + C_2H_6 \Rightarrow 2e + C_2H_2^+ + 2H_2$	14.65
78	$e + C_2H_6 \Rightarrow 2e + C_2H^+ + 2H_2 + H$	17.73
79	$e + C_2H_6 \Rightarrow 2e + C_2^+ + 3H_2$	21.01
80	$e + C_2H_6 \Rightarrow 2e + CH_3^+ + CH_3$	13.51
81	$e + C_2H_6 \Rightarrow 2e + CH_2^+ + CH_4$	16.05
82	$e + C_2H_6 \Rightarrow 2e + CH^+ + CH_4 + H$	19.1
83	$e + C_2H_6 \Rightarrow 2e + C^+ + CH_4 + H_2$	18.77

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