Plasma chemical reactor on a base of dielectric barrier discharge for molecules dissociation

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Abstract: Plasma chemical reactor (PCR) was designed to study chemical reactions in the dielectric barrier discharge (DBD) plasma. Electron energy distribution functions (EEDFs) were calculated to determine the number of electrons with required energy for dissociation of water molecules by electron strike in the DBD plasma.

Keywords: Dielectric Barrier Discharge, water, Boltzmann equation

1. Introduction
PCR was designed to study chemical reactions in the DBD plasma [1]. The method of estimating the parameters of PCR to implement the selected reaction is considered by the example of a water molecule. We considered EEDFs assuming one electron strike for dissociation of water molecules. Numerical calculations were carried out by website lxcat.net.

2. Experimental setup
PCR operates at atmospheric pressure. Reduced electric field in discharge gap was between 160 and 260 Td. More detailed information of the geometrical configuration of PCR, power supply and diagnosis system are given in previous articles [1-5].

3. Theoretical calculation
Calculation of reaction rates for the dissociation of water molecules by electron strike is introduced in Fig. 1 [6]. The calculation was carried out for the operation range of reduced electric field between 160 and 260 Td. Considered processes are listed in Table 1.

![Fig. 1](image1.png)

**Fig. 1.** Variation of reaction rates as a function of E/N; x – process 1; o – process 2; * – process 3; + – process 4; triangle – process 5.

**Table 1.** Dissociation processes

<table>
<thead>
<tr>
<th>Process number</th>
<th>Process expression</th>
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<tbody>
<tr>
<td>1</td>
<td>$e + \text{H}_2\text{O} \rightarrow e + \text{H} + \text{OH}$ (7 eV), excitation</td>
</tr>
<tr>
<td>2</td>
<td>$e + \text{H}_2\text{O} \rightarrow e + \text{O} + \text{H}_2$ (13 eV), excitation</td>
</tr>
<tr>
<td>3</td>
<td>$e + \text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$, attachment</td>
</tr>
<tr>
<td>4</td>
<td>$e + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{O}^*$, attachment</td>
</tr>
<tr>
<td>5</td>
<td>$e + \text{H}_2\text{O} \rightarrow \text{OH}^* + \text{H}$, attachment</td>
</tr>
</tbody>
</table>

Process 1 has highest reaction rate value. The probability of this process will have a higher value than others if electron energy range is between 13 and 23 eV (except elastic collisions) (Fig. 2) [7].

![Fig. 2](image2.png)

**Fig. 2.** $e/\text{H}_2\text{O}$ collision cross sections; + – elastic collisions; o – process 1; * – excitation without dissociation; x – ionization; triangle – process 2;

EEDFs were calculated to determine the number of electrons with required energy. EEDFs were calculated for reduced electric field between 160 and 260 Td. EEDFs for two boundary cases are presented in Fig. 3 [6]. The range from 13 to 23 eV was marked by two vertical lines. As can be seen from the graphs, this range lies in the beginning of the downturn EEDFs. Further sharp decrease...
in the value EEDFs can be explained by the fact that the electrons actively lose energy in the process of ionization and dissociation of water molecules.

4. Conclusion
According to theoretical estimations of collision cross sections we can conclude that the dissociation of water molecules in the plasma by electron strike will be the most effective if the energy of electrons is from 13 to 23 eV. EEDFs were calculated to determine the number of electrons in this range under the conditions realized in the developed PCR. Thus the applied voltage to the PCR electrodes from 10 to 16 kV corresponds to optimum theoretically calculated regime of operation for dissociation of water molecule by one electron strike.

5. References