Simulation of Low and Atmospheric-Pressure Water-Vapour Plasma

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ABSTRACT: Low and Atmospheric-pressure capacitive discharge driven by radio frequency (rf) source have been investigated using a one-dimensional fluid model. The simulation has been performed using the commercial software Comsol Multiphysics. The results show that pure water-vapour discharge can be created just at low pressure when using rf source. However for a mixture of (5%H_2O + 95%He), a stable plasma can be created at atmospheric pressure and room temperature. The mechanism for suppressing plasma ignition in the first case can be attributed to the high rate of electrons cooling due to vibrational and rotational excited states reactions. We have suggested two ways in order to overcome these difficulties. The first one is by adding just a few fraction of water to another main feed gas such as helium or Ar. The second one is by using a nanosecond pulsed generator instead of RF source. Input parameters for plasma ignition have been identified and plasma density profiles have been represented. The production of some important species such as OH, H and UV radiations have been also obtained.

KEYWORDS: Atmospheric water-vapour; RF and Nanosecond pulsed source; Electrons cooling by rotational and vibrational reactions; Production of some species potentially used in medical remediation and environmental applications.

1. *Introduction*

Atmospheric water vapour discharges are an effective source of hydroxyl OH* radicals, H and O atoms, charged particles, and UV radiation. As a result they have been receiving growing attention in recent years [1] and [2] due to their applications in environmental remediation, health and medicine [3]. Experimental RF 100% water vapour plasma at low pressure has been created and reported by [4] and [5]. But at atmospheric pressure, Sarani et Al [6] have developed an Ar+5% of water plasma torch. Results show higher intensity of OH radicals. Electron temperature has estimated as 0.97 eV in pure Ar and it decreases with an increase in water content in plasma.

The motivation for this work is to test the feasibility of producing water vapour discharge operating at atmospheric pressure and room temperature. The ignition of plasma in pure water vapour plasmas is difficult, especially due to large permanent electric dipole that the water molecule has got. Cross sections for electron collisions with water molecules [7] and [8] show that rotational and vibrational excitation are very dominant at low energy. Consequently electron cooling rates are very important and therefore plasma ignition will be very delicate. As a starting point a one-dimensional fluid model is presented. The discharge is generated between two electrodes separated by 1 mm gap.

Presently the model tracks the evolution of 26 important species through 62 reactions table n°01. The model was set up based on the well-known fluid approach. The governing equations include transport of charged and neutral species, drift-diffusion approximation, electron energy equation, and Poisson's equation for the electric potential and field.

Metastable and excited states	Ionic species	Ground state neutral species
H_2O^*(J0)	OH^-	H_2O
H_2O^*(J1)	H^-	H_2
H_2O^*(J2)	O^-	OH
H_2O^*(J3)	H_2O^+	H
H_2O^*(V010)	H^+	O
H_2O^*(V001)	OH^+	
OH^*(A)	H_2^+	
H^*(n3)	O^+	
H^*(n4)		
H^*(n2)		
O^*(1S)		
O^*(3S)		
O^*(3P)		
O^*(5P)		

Table n°01: Species included in the model

The species continuity equation:

$$\frac{\partial n_i}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma}_i = S_i(\varepsilon) \qquad (1)$$

The drift-diffusion approximation:

for electrons:

$$\vec{\Gamma}_e = +n_e \mu_e(\varepsilon)\vec{E} - D_e(\varepsilon)\vec{\nabla} n_e \qquad (2)$$

for charged ions:

$$\vec{\Gamma}_i = \pm n_i \mu_i \vec{E} - D_i \vec{\nabla} n_i \qquad (3)$$

for neutrals:

$$\vec{\Gamma}_n = -D_n \vec{\nabla} n_n \qquad (4)$$

Electron energy equation:

$$\frac{\partial (n_e \varepsilon)}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma}_\varepsilon = -e\vec{\Gamma}_e \cdot \vec{E} - Q_{e-N} \qquad (5)$$

where

$$\vec{\Gamma}_\varepsilon = \frac{5}{3} n_\varepsilon \mu_e \vec{E} - \frac{5}{3} D_e \vec{\nabla} n_\varepsilon \qquad (6)$$

and the Poisson's equation:

$$\Delta\Phi = -\vec{\nabla} \cdot \vec{E} = -\frac{1}{\varepsilon_0} \sum_i q_i z_i n_i \qquad (7)$$

1. *Results and discussion:*

First case: 100% water vapour; 12 species and 52 chemical reactions without including excited state species. The break-down parameters are: Driven frequency f = 13.56 MHz, initial voltage V (0) = 200 Volts and power density P_{set} = 23 W/m^2.

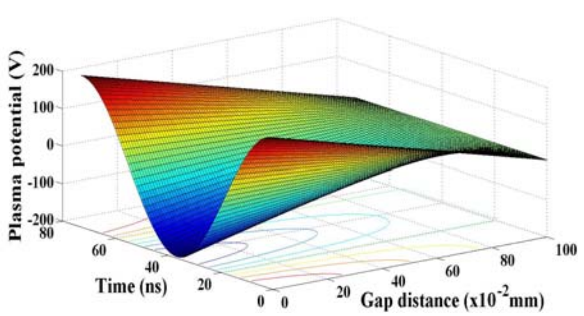

Fig01: Plasma potential profile perfectly sinusoidal. It follows the same variations as the driven frequency.

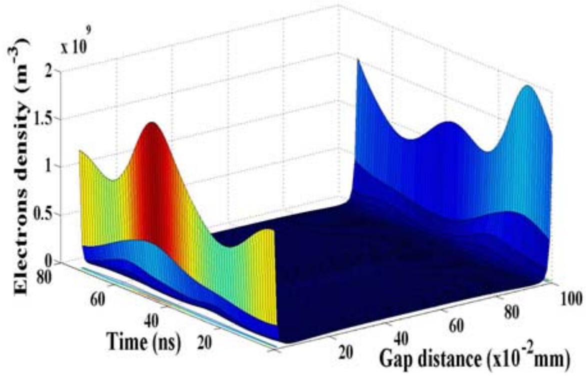

Fig02: Electron density profile, very important next to the electrodes but meager in the center between the electrodes.

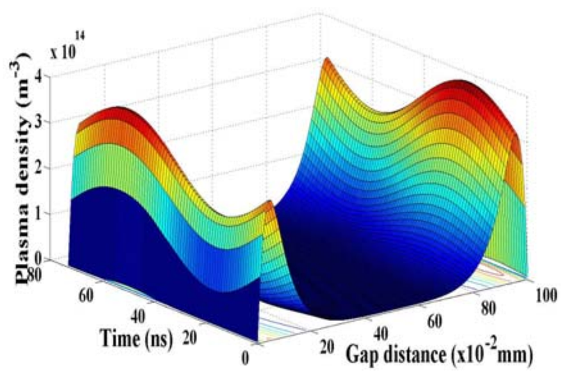

Fig03: Plasma density profile, very important next to the electrodes than smoothly flat and meager in the center between the electrodes.

Second case: All dominant reactions including excitations are taken account in this model, 26 species and 62 reactions. Driving frequency f = 13.56 MHz. Gas pressure P = 0, 01 Atm and Gap distance d = 1 mm. V(0) = 398.731 V

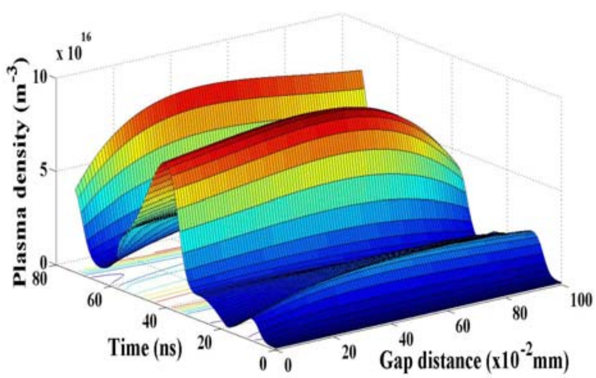

Fig04: Plasma density profile shows that is relatively sinusoidal; it is more important than in the first model.

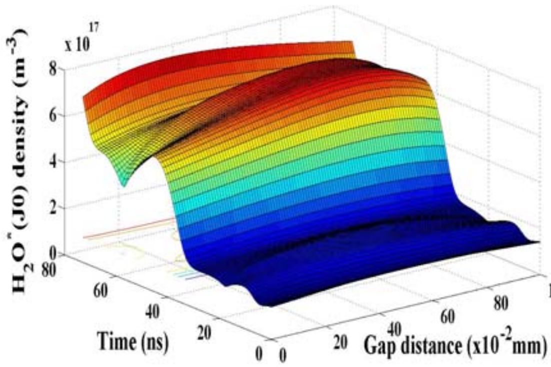

Fig05: H_2O*(rotJ0) density profile, production of excited species due to electron impact with H_2O molecule. It becomes very important with respect to the rf period between the electrodes.

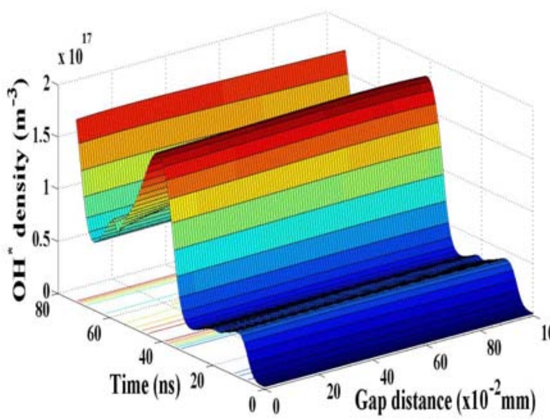

Fig06: OH* density profile, production of hydroxyl species very important for many applications. It increases with respect to rf period in the plasma bulk and next to the electrodes.

Third case: A comparison between cross sections set of electron impact with water molecule and helium [07] and [08] has let us to think about adding just a small fraction of water to another main gas such as Helium or Argon. This mixture can be helpful to enhance plasma breakdown excited by Rf source and produce the desired species.

Driving frequency f = 13,56 MHz. Gas pressure and P = 0,01 Atm. Gap distance d = 1 mm. Background gas is an admixture of 5 % water vapour and 95 % He. 29 species and 92 reactions channels are considered in this model. Power density 9992 W/m^2 and voltage 155 V. All main reactions (excitation, ionization, attachment and dissociations) for H_2O and He are included.

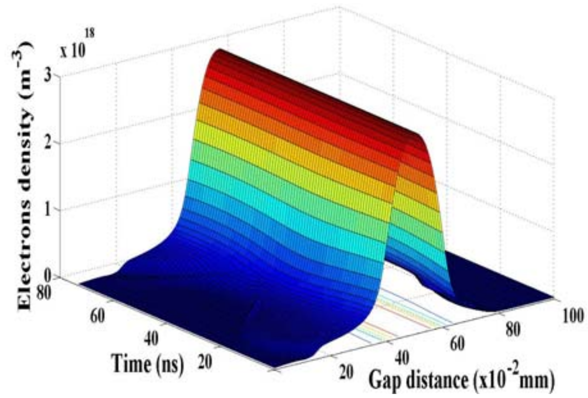

Fig07: Electron density profile, very important in the gap between the electrodes, then decreases smoothly towards the electrodes.

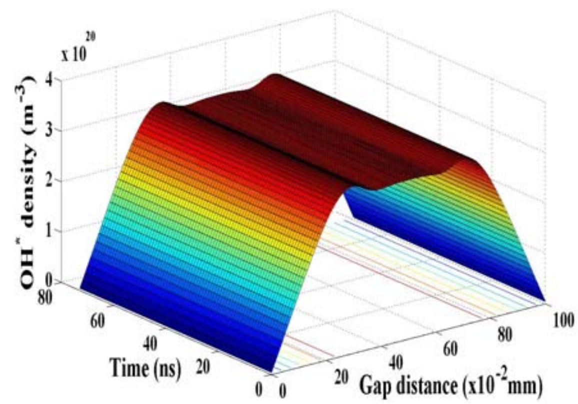

Fig08: OH* density profile. The production of hydroxyl species is very important in this case as compared to the previous case.

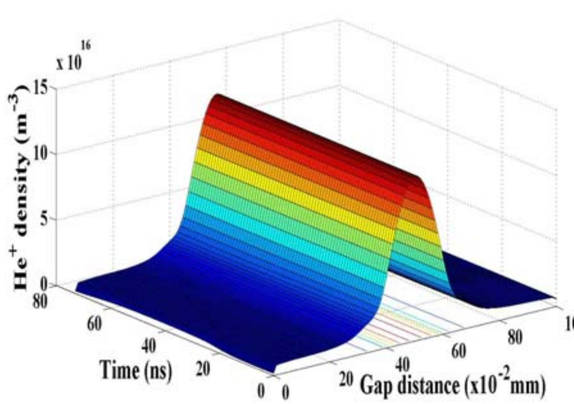

Fig09: He^+ density profile. The production of excited He^+ ion is very important in the plasma bulk which make plasma ignition easier.

The ongoing case: In this model, we are using a nanosecond pulsed generator [9] instead of Rf source. All the dominant reaction channels are included and the discharge is operating at atmospheric pressure using a pure water vapour. The results will be presented as soon as we will have finished with their interpretations.

Conclusion: The motivation behind this work is to test the feasibility of producing a water-vapour discharge operating at atmospheric pressure in order to produce some interesting species in biomedical and environment applications. The first model based on 52 chemical reactions (excitation were excluded) in 100 % H2O is tested. A complete model (26 species and 62 processes) including the dominant reactions failed to converge under the previous conditions, but did converge when the pressure was reduced to 0,01 Atm and the gap distance to 0.5 mm. In a third model, we have included all dominant reaction channels in water and Helium, but we have added just a 5% water to 95% to Helium. Another model based on the use of nanosecond pulse instead of RF generator has been achieved and we are getting the results in progress.

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