The Energy Barrier and Collision Number of O++H2(v=0,j=0)Reaction in the Earth Ionosphere

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INTRODUCTION

The Earth’s ionosphere is located at the height of 60-1000 km containing free electrons and ions (Brasseur and Solomon, 2005). Changes in the ionospheric system are crucial importance on communications, navigation and the exploration of the near earth space. Thus the study of the ionospheric phenomena has become an important field of present day’s research (Itikawa, 2007; Mangla and Yadav, 2011).

The ionosphere has a very complex structure due to its physical and chemical composition. The description of the photochemical processes and the ionosphere chemical kinetics in the theoretical model, with the account of chemical composition of the neutral particles and ions considered, includes the processes of photoionization, photodissociation, dissociative recombination, radiative recombination, collision mechanism, etc.(Richards, 2011; Whitten and Poppof, 1964).

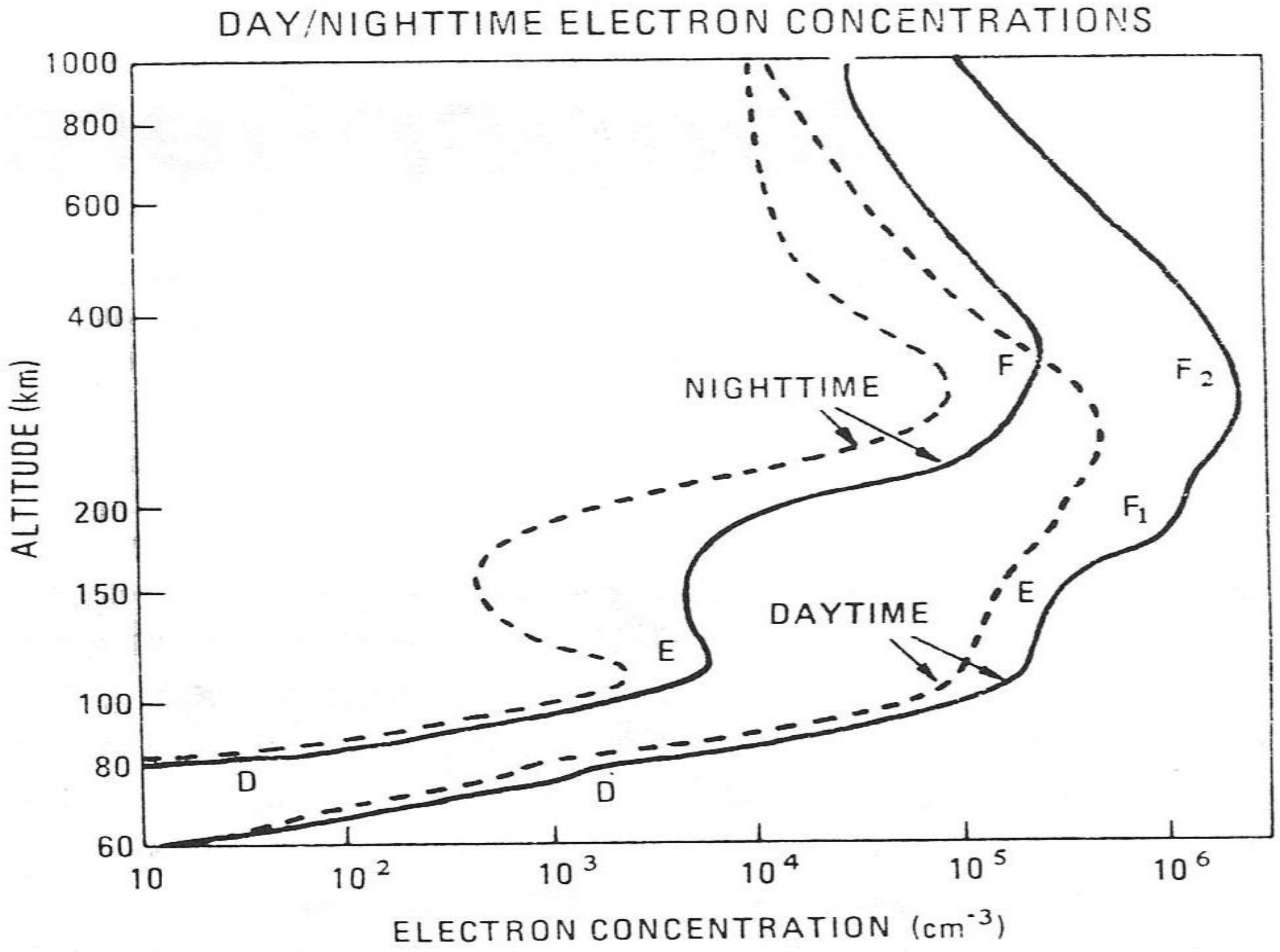

Figure 1. Electron density in the Earth ionosphere.

The role of O+ and H2 particles on the Earth's ionosphere chemistry is very important according to density changes in the upper and lower ionospheric height so many researchers have done studies on these particles. In these studies, theoretical models have been used to investigate the effects of artificially injected H2 gas on plasma densities in the ionospheric F region and the overlying protonosphere. It has been found that the release of modest amount H2 gas can produce significant perturbations in the ionosphere and protonosphere (Bernhardt et al., 1975).

Also the effect on ionosphere of O^+ and H_2 was separately investigated by them and no attempt was made the effects on the earth ionosphere by combining kinetic theory-based models with the cross sections in the 0.02-0.1 eV collision energy range and state to state rate constants values for the $O^+ + H_2 \rightarrow OH^+ + H$ reaction that have been obtained using a quantum wave packet method.

In this presentation, total reaction rate constants and cross sections obtained for the reaction (Gómez-Carrasco et al., 2014) previously;

$$'\boldsymbol{O^+ + H_2 \rightarrow OH^+ + H}'$$

and used to investigate the effects in the ionosphere.

2. Methodology

The theoretical analysis of ionosphere chemistry modification must be carried out due to a large number of factors, such as the great increases in the energy regime of the earth ionosphere system, the change in density and temperature during the collision and the abrupt disconnections. Also several statistical quantities such as potential energy barrier and total number of reactive collisions must be taken in to account and so shall find quantitative relationships between statistical quantities characterizing molecular collisions (such as mean free path, etc.) and basic physical properties of the gas (such as concentration, temperature, height, etc.). These terms are closely related to each other and to other fundamental molecular quantities.

2.2. Total Collision Number

A chemical reaction is explained as a simple collision with the following relative velocity dependent cross section.

$$g_0 = \sqrt{\frac{2U_0}{m^*}} = \sqrt{\frac{8kT}{\pi m}} \qquad (1)$$

Where g_0, is the velocity of relative motion which is sufficient to overcome the potential energy barrier:

$$U_0 = \sqrt{\frac{4kT}{\pi}} \tag{2}$$

Z_{12} which is the number of reactive collisions per unit volume can be calculated. This can be done by substituting the cross section of the chemical reaction (Gombosi, 1994):

$$\mathrm{Z_{12} = 4\pi K_{12}\sigma_0 n_1 n_2 \left(\frac{m^*}{2\pi kT}\right)^{3/2} \int_{g_0}^{\infty} dg g^3 e^{-\frac{m^* g^2}{2kT}}} \tag{3}$$

This equation is valid for both the forward and the reverse reaction. The main difference between this two reactions is that the forward reaction involves the collision of different (unlike) molecules, therefore K_{12}=l, while the reverse reaction involves the collision of two like molecules, therefore K_{12} = l/2.

The threshold velocity can be expressed in terms of the barrier potential energy:

$$Z_{12} = K_{12}\sigma_0 n_1 n_2 \sqrt{\overline{v_1^2} + \overline{v_1^2}}\, e^{-\frac{U_0}{kT}}\left(1 + \frac{U_0}{kT}\right) \tag{4}$$

3. Results

The reaction dynamics of the ‘$\boldsymbol{O^+ + H_2 \rightarrow OH^+ + H}$’ reactive reaction have been investigated in this study. All parameters are calculated for the Elazig (38.40^{0}N, 39.12^{0}E) coordinates and year, day and time are taken as 2009, equinox, local time (12:00) respectively, together with the ionospheric temperature and density data are obtained from IRI (International Reference Ionosphere) website (Blitza, 2012, 2014; IRI Web Program).

O^+ is active particle, while H_2 molecule is stationary in this reaction. Also, we need to match the reaction formation temperature with ionospheric temperature.

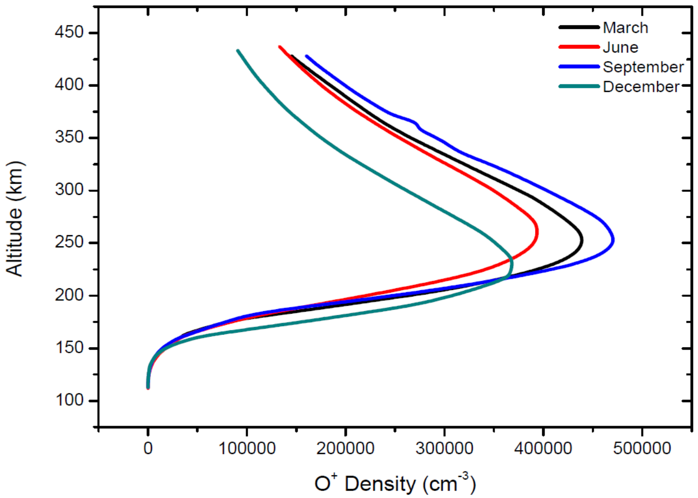

Figure 2. Variation of O^+ density with the ionospheric height.

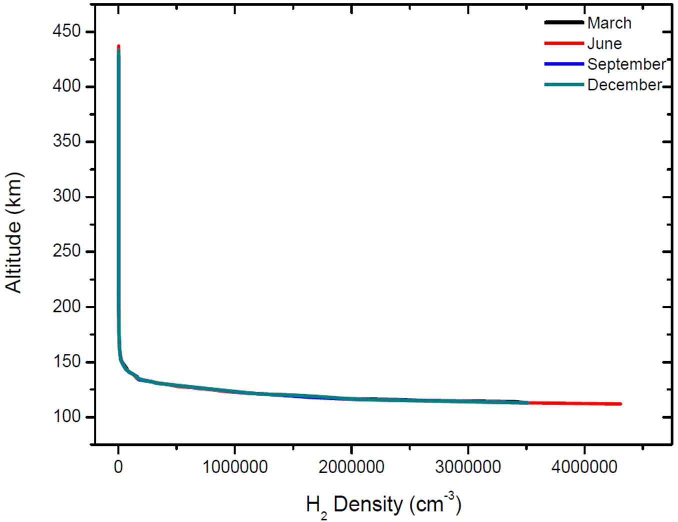

Figure 3. Variation of H_2 density with the ionospheric height.

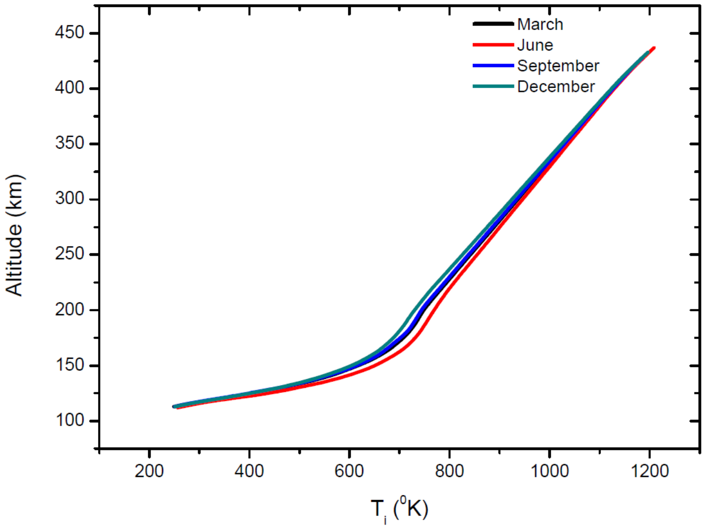

Figure 4. Ion temperature change in the ionosphere.

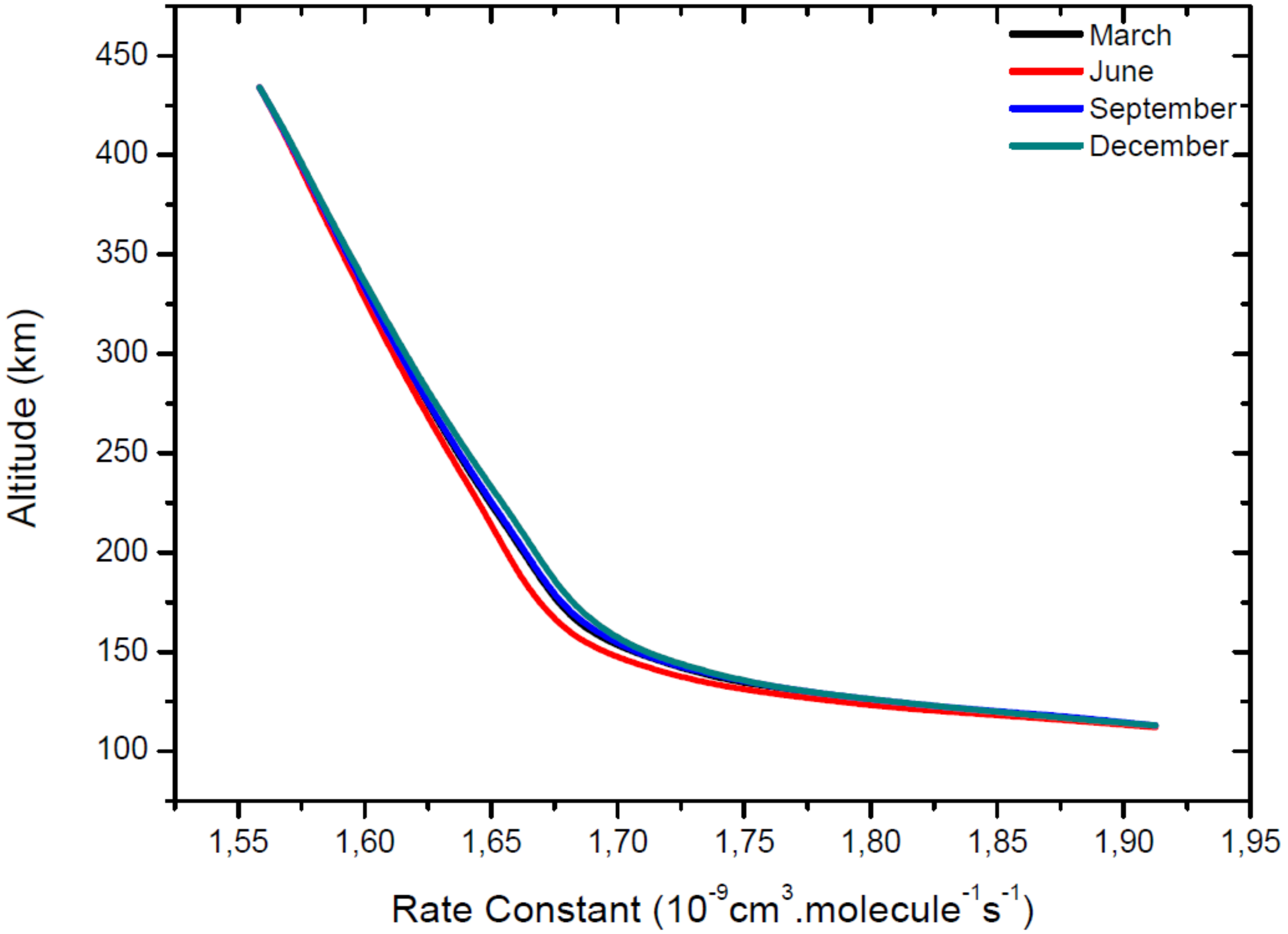

Figure 5. Rate constant variation with altitude.

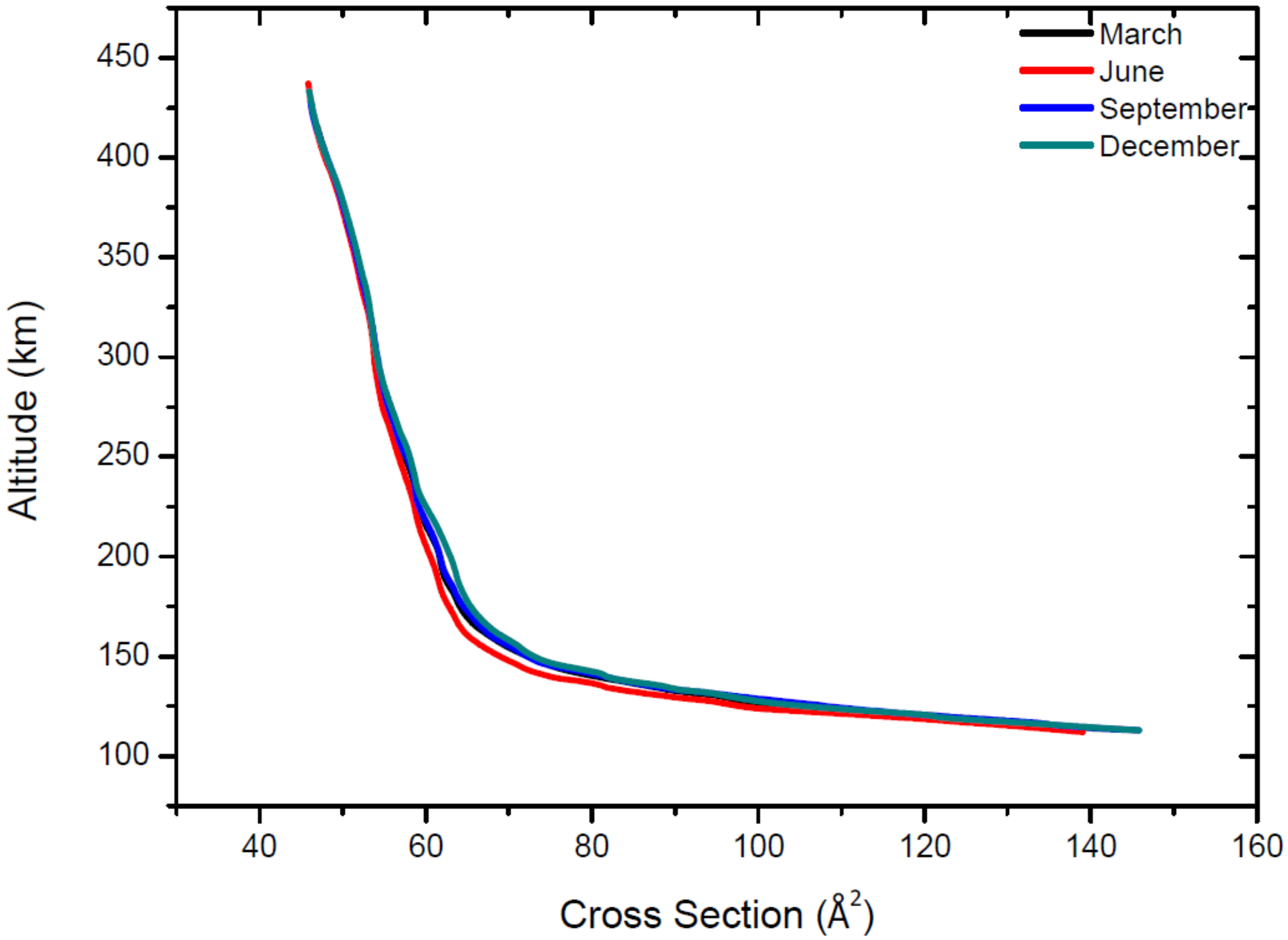

Figure 6. Cross section change in the ionosphere.

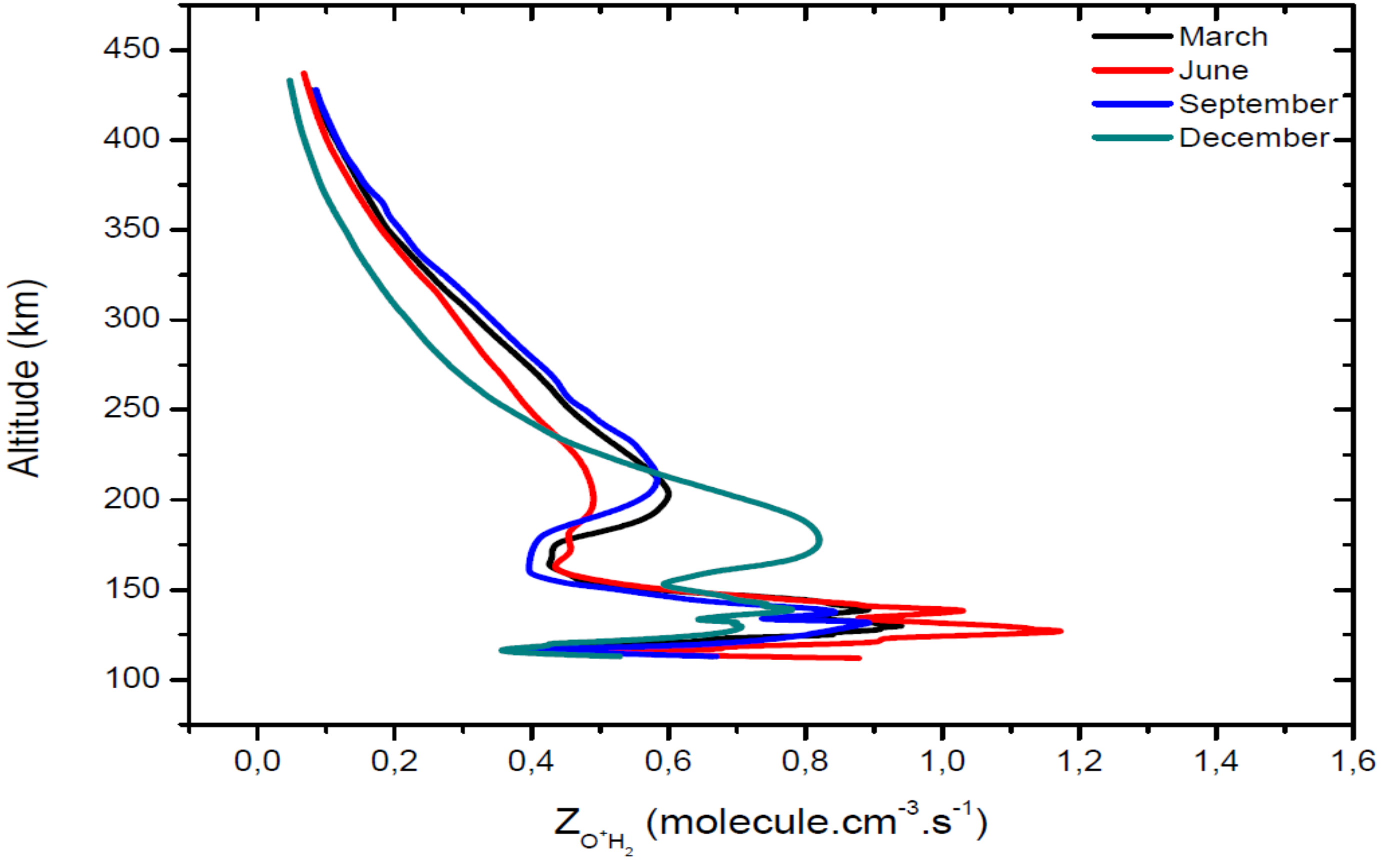

Figure 7. Variation of the total collision number of the reaction in the ionosphere.

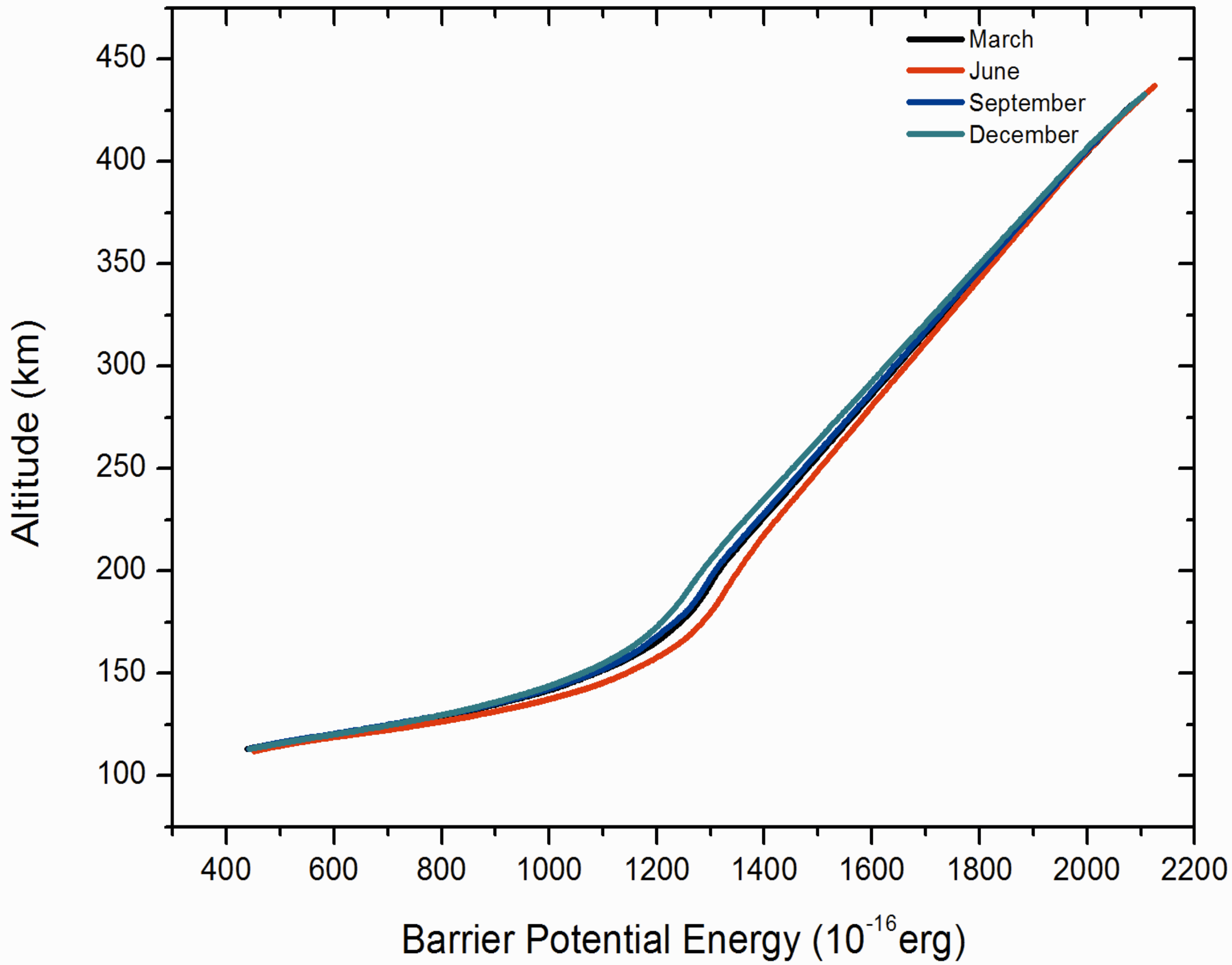

Figure 8. Variation of barrier energy and the ionospheric height.

4. Conclusion

In this study we have analyzed $'\boldsymbol{O^+ + H_2 \rightarrow OH^+ + H}'$ reactive reaction under ionospheric conditions.

$Z_{O^+H_2}$ has the maximum values at the lower height (about 100-150 km) and decrease with increasing height in upper ionosphere. Because H2 density is too much at the lower ionosphere and decreasing dramatically with the ionospheric height, the total collision number at the subionosphere has the greatest value and also O^+ ion density is very small at these altitudes.

As the altitude rises, the barrier energy also increases and there is no big difference between the months.

References

1.Brasseur, G.P., Solomon, S., 2005. Aeronomy of the Middle Atmosphere. Springer

2.Itikawa, Y., 2007. Molecular Processes in Plasmas Collision of Charged Particles with Molecules. Springer.

3.Mangla, B., Yadav, M., 2011. Chemistry of Upper Ionosphere- A Study. Int. J. Adv. Eng. Sci. 1, 1.

4.Richards, P. G., 2011. Reexamination of Ionospheric Photochemistry. J. Geophys. Res. 116, A08307.

5.Whitten, R.C., Poppof, I.G., 1964. Ion Kinetics in the Lower Ionosphere. J. Atmos. Sci. 21, 2.

6.Bernhardt, P. A., Park, C. G., Banks, P.M., 1975. Depletion of the F2 Region Ionosphere and the Protonosphere by the Release of Molecular Hydrogen. Geophys. Res. Lett. 2, 8, 341 344.

7.Gómez-Carrasco, S., Godard, B., Lique, F., Bulut, N., Klos, J., Roncero, O., Aguado, A., Aoiz, F., Castillo, J., Goicoechea, J., Etxaluze, M., Cernicharo, J., 2014. OH+ In Astrophysical Media: State-to-State Formation Rates, Einstein Coefficients and Inelastic Collision Rates with He. Astrophys. J. 794, 33, 16.

8. Gombosi, T.I., 1994. Gas Kinetic Theory. Cambridge University Press. Cambridge.

9. Bilitza, D., Brown, Steven A., Wang, Matthew Y., Souza, Jonas R., Roddy, Patrick A., 2012. Measurements and IRI Model Predictions during the Recent Solar Minimum. J. Atmos. Sol. Terr. Phys. 86, 99-106.

10. Bilitza, D., Altadill, D., Zhang, Y., Mertens, C., Truhlik, V., Richards, P., McKinnell, L.- A., Reinisch, B., 2014. The International Reference Ionosphere 2012 - a model of international collaboration. J. Space Weather Space Clim. 4, A07, 1-12. (URL< http://omniweb.gsfc.nasa.gov/vitmo/iri2012_vitmo.html >)

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