“In this chapter, we recall electron impact ionization cross sections $Q_{\text{ion}}(E_i)$ calculated in chapter 2 and 3. Those cross sections are employed here to estimate macroscopic quantities like ionization Mean Free Paths and ionizing collision frequencies, for externally precipitated and secondary generated energetic electrons in the Earth’s ionosphere. Composite Ionization Mean Free Paths are also approximated. The study is extended to the calculation of ion production rates in the Mars and Titan’s ionosphere. We attempt to incorporate widely accepted quantum mechanical cross section data with the realistic systems, such as the ionospheres and the atmospheres of various planets. Thus we have adopted a micro-to-macro approach with implications to the Earth’s ionosphere along with the planets, their satellites, cometary coma and other astronomical bodies.”
6.1 Electron ionization: Earth's ionosphere - a Case study

Electrons play a vital role in physico-chemical processes of the ionosphere and upper atmosphere of the Earth and other planets and satellites, including comets. Fundamental physical-chemical processes are initiated by the electron induced reactions [1]. Electron impact processes play a major role in two naturally occurring atmospheric phenomena, viz., auroral emissions due to excitations of neutral species by the energetic electrons in polar upper atmosphere, and ionizations of constituents producing neutral and ionic fragments [2, 3]. The e- impact ionization is also important in the cometary coma [4] and night side Martian ionosphere [5]. Apart from the solar radiation Earth, Planets and solar system objects are constantly immersed in the flow of solar wind, consisting of electrons, protons and ions. The solar wind particles and galactic or extra galactic cosmic rays interact with the constituents of the planetary atmospheres and give rise to various electron induced atomic-molecular processes.

Photo-electrons produced by solar EUV and X-rays can also induce excitations and ionization of the constituent atoms/molecules. The relativistic electrons and cosmic rays can produce high energy secondary electrons, themselves capable of ionizing the constituents. An extensive work has been done by Bhardwaj and Gladstone [6] for auroral electron precipitation in giant planets, and by Haidar et al. [7] on the interactions of photo-electrons with various constituents of the
Martian atmosphere for modeling the chemistry. Present calculations can be incorporated in such models to include electron impact ionization processes.

The concentration of photo-electrons is $\sim 10^3$-$10^4$ per cc in the ionospheric D and E regions on the Earth with energy peak distribution around 50-70 eV [8]. At auroral latitudes this amount is $\sim 10^3$ per cc in the D region and $\sim 10^5$ in the E region having energy $\sim 1$-$10$ keV [9]. The number density of electrons in the solar wind is only $\sim 5$ per cc at 1 astronomical unit (AU), with energy distribution having peak around $\sim 12$ eV [10], which is close to the ionization potential of many atomic-molecular species in the Earth’s atmosphere. In short, there are enough electrons, primary and secondary as well, with the energy sufficient to induce impact ionization in the planetary atmospheres, their satellites (Titan, Io etc), comets and other astronomical bodies.

Almost all the planets and their satellites have a neutral atmosphere, composed of different species in different proportions. On the Earth $N_2$ ($\sim 78.29\%$) and $O_2$ ($\sim 20.8\%$) dominate at lower altitude (D region) and atomic O, N, He prevail at high altitudes $\sim 200$ km [11]. The Venus atmosphere has $CO_2$ ($\sim 96.5\%$) and $N_2$ ($\sim 3.5\%$). The Titan’s atmosphere is the only Nitrogen rich atmosphere ($\sim 98.4\%$) besides the Earth in our solar system, also having $CH_4$ ($\sim 1.4\%$) and $N_2^+$ in Titan torus. Cometary coma also contains neutrals like $H_2O$, $CO_2$, $CO$, $O$, $N_2$ & $H$ [4]. Many of these neutral species have been investigated by us in our theoretical calculations on the e-impact ionization and cumulative excitation processes along with elastic scattering [12-23]. Therefore the focus of the present chapter
is on deriving cross sections together with bulk parameters of the e-impact ionization with the ionospheric molecules N\textsubscript{2} and O\textsubscript{2} [11] along with atomic oxygen (ground as well as excited metastable states) found at ~100 km on the Earth. Table 6.1 shows the concentrations (per cc) of major neutral species available at different altitudes, as obtained from MSIS-E-90 (Mass Spectrometer Incoherent Scatter Radar) atmospheric model [11].

Table 6.1: Concentration of major species available at different altitudes [11]

<table>
<thead>
<tr>
<th>Species</th>
<th>Concentration/cc</th>
<th>Species</th>
<th>Concentration/cc</th>
</tr>
</thead>
<tbody>
<tr>
<td>N\textsubscript{2}</td>
<td>2.66\times10\textsuperscript{14}</td>
<td>N\textsubscript{2}</td>
<td>9.04\times10\textsuperscript{12}</td>
</tr>
<tr>
<td>O\textsubscript{2}</td>
<td>7.06\times10\textsuperscript{13}</td>
<td>O\textsubscript{2}</td>
<td>2.08\times10\textsuperscript{12}</td>
</tr>
<tr>
<td>Ar</td>
<td>3.09\times10\textsuperscript{12}</td>
<td>0</td>
<td>3.76\times10\textsuperscript{11}</td>
</tr>
</tbody>
</table>

In section 6.2, we first highlight our quantum mechanical calculations on the e-impact ionization of atomic-molecular targets, and then go over to the bulk quantities like, macroscopic cross section, ionization Mean Free Path (MFP) together with the composite ionization MFP, and ionizing collision frequency for the electrons in a gas medium. Many of these bulk quantities were estimated in the past for slow electrons. In the present chapter these are calculated for ionizing collisions, from the reliable quantum mechanical cross sections derived from our method [12-23].
The various e− impact processes are important to understand the complex properties of various planetary atmospheres. The underlying scattering theory adopted here rests on complex interaction potential formalism, describing simultaneous elastic and inelastic scattering of electrons. Historically, understanding the planetary atmospheres has been a primary motivation for studying electron-molecule collisions in theory and in laboratory. The basic calculations discussed presently can help to develop the theoretical models for understanding bulk processes in the different environments.

6.2 Theory and formalism

The microscopic calculation of electron-molecule ionization rests on our quantum mechanical approximation CSP-ic [12-23]. The details of the cross section calculations are already discussed in chapter 2 and hence not repeated here. We simply move on to the application of these cross sections.

An attempt has been made presently to incorporate the ionization cross section \( Q_{\text{ion}} \), as an input parameter to carry out calculations of various bulk parameters, viz., the so-called macroscopic cross section \( \Sigma_{\text{ion}} \), ionization Mean Free Path (MFP) \( \Lambda_{\text{ion}} \) together with the composite ionization MFP, and ionization collision frequency \( \nu_{\text{ion}} \). All these quantities are functions of energy of the incident electrons in a given medium (Earth’s ionosphere etc). The macroscopic cross section for ionization \( \Sigma_{\text{ion}} \) is defined as

\[
\Sigma_{\text{ion}} = N Q_{\text{ion}}
\] (6.2.1)
Where, $N$ is the number of atoms/molecules per unit volume in the medium. If $I_E$ is the ionization energy of the target (constituent) atom/molecule then $I_E \cdot \Sigma_{ion}$ is a measure of the energy lost in ionization, by the electrons per unit path length.

The MFP of ionizing collisions in a bulk medium is given as,

$$\Lambda_{ion} = \frac{1}{\Sigma_{ion}} \quad (6.2.2)$$

The composite MFP $\Lambda_{comp}$ of electrons in a bulk composite medium can be obtained by considering different gases or species (1, 2, 3 etc) with different concentration e.g. in the Earth’s ionosphere. Thus,

$$\frac{1}{\Lambda_{comp}} = \frac{1}{\Lambda_1} + \frac{1}{\Lambda_2} + \frac{1}{\Lambda_3} + \ldots \quad (6.2.3)$$

Where, $\Lambda_i$ is the ionization MFP of the $i^{th}$ constituent species in the medium.

Now, in the case of mono-energetic electrons the ionization collision frequency $\nu_{ion}$ can be defined by,

$$\nu_{ion} = N \cdot Q(E_i) \cdot \nu \quad (6.2.4)$$

Where, $\nu$ is velocity of the incident electrons. Considering Shkarofsky [24] with the notation of Itikawa [25], when the electrons are considered as having energy distribution, the effective ionization collision frequency $< \nu_{ic} >$ becomes

$$< \nu_{ic} > = \frac{4}{3\sqrt{\pi}} \int_{I_E}^{\infty} \nu_{ion} \cdot e^{-\frac{3}{E}} dE \quad (6.2.5)$$
In equation (6.2.5), \( \varepsilon = E_i/kT \), with \( k \) as the Boltzmann constant and \( T \) is electron temperature in \(^{0}\text{K}\). Here Maxwellian distribution of energetic electrons is assumed as an approximation in the Earth’s ionosphere.

One more bulk parameter that can be derived using the ionization cross section and that will be considered later on in this chapter is the ion production rates (IPR) \( P_j(z) \) in the planetary ionospheres. This is defined as,

\[
P_j(z) = n_j(z) \int_{E_{th}}^{E} F(z,E)\sigma_j(E) \, dE \quad \text{(in } \text{cm}^{-3}\text{s}^{-1}) \tag{6.2.6}
\]

Where, \( n_j(z) = \text{Concentration of } j^{th} \text{ neutral species in gaseous state, at altitude } z \)

\( F(z, E) = \text{Flux of ionizing electrons, at energy } E_i \)

\( \sigma_j(E) = \text{Electron ionization cross section for target } j^{th}, \text{ as already calculated} \)

6.3 Results and discussions

In this section, we have discussed the cross section calculations for the present study and then their application in deriving various macroscopic parameters in a specific bulk medium.

6.3.1 Electron atom-molecule ionization cross sections

Electron interactions and ionization of \( \text{N}_2 \) has been extensively studied in theory and in laboratory [15] in view of its importance in the planetary and satellite atmospheres. Collisions of the electrons with \( \text{N}_2 \) molecules can give rise to a wide variety of processes. The parent as well as dissociative ionization of this
molecule plays an important role in the Earth’s ionosphere, aurora etc. Thus N\textsubscript{2} in its ground electronic state offers a very good test of the present methodology.

![Figure 6.1](image)

Figure 6.1: Total ionization cross section \( Q_{\text{ion}} \) (Å\(^2\)) for e\(^{-}\) impact on N-atom and N\textsubscript{2}-molecule: Solid line-present \( Q_{\text{ion}} \) for N\textsubscript{2} molecule, Star-Krishnakumar and Srivastava [26], Circles-Rapp et al. [27], Dash dot- Itikawa et al.[28], Dot- present \( Q_{\text{ion}} \) for N atom, Dark box- Brook et al.[29].

In Figure 6.1 our CSP-ic ionization cross sections are exhibited along with comparisons. The top curve, solid line, shows the results of the cross sections \( Q_{\text{ion}} \) for the e\(^{-}\) impact on N\textsubscript{2} peaking around 90 eV. The Present \( Q_{\text{ion}} \) results are in good agreement with experimental results of Krishnakumar and Srivastava [26] above 100 eV, while the experimental results of Rapp et al. [27] are on higher side at the peak. The present cross sections are also compared with the recommended data of Itikawa et al. [28], which are lying lower than the present
values above 100 eV. Our results of $Q_{\text{ion}}$ for the e-impact on N$_2$ are in a good general agreement with the other recommended theoretical data. For the sake of clarity of figures we have compared the $Q_{\text{ion}}$ data only with available experimental results unless specified otherwise.

Role of the atomic nitrogen cannot be ignored for the calculation of ionization cross section in the Earth's ionospheric E region, considering its concentration. In Figure 6.1, bottom curve with dotted line indicates our total ionization cross sections $Q_{\text{ion}}$ for atomic nitrogen. The experimental results of Brook et al. [29] are fairly in agreement with our results beyond 30 eV. Below the electron energy 30 eV, the experimental ionization data are well above the theoretical curve. In fact, the experiments of [29], show ionization signals even at atomic (ground state) ionization threshold i.e. 14.53 eV. This indicates the presence of the metastable excited species in the experimental atomic N beam of [29]. Our calculations of ionization shown in bottom of Figure 6.1 are entirely based on the ground state of the N atoms and hence the discrepancy is understood.

Next, O$_2$ is the second most dominant molecule in the Earth’s ionospheric D region. In Figure 6.2, the uppermost curve, solid line, shows the CSP-ic results of the total ionization cross sections $Q_{\text{ion}}$ for the e-impact on O$_2$, peaking around 100 eV. The present total ionization cross sections $Q_{\text{ion}}$ are compared with the experimental results of Krishnakumar and Srivastava [30] and Rapp and Englander-Golden [31]. At the low energies the present results are slightly higher than that of [30] and [31] but there is an overall good agreement at the
peak position and higher energies. Several other recommended and theoretical data on O\textsubscript{2} are not presented in the Figure 6.2, to preserve clarity, since overall agreement is quite satisfactory.

![Figure 6.2: Total ionization cross section \(Q\text{\textsubscript{ion}}(\text{Å}^2)\) for e-impact on O-atom and O\textsubscript{2}-molecule;](image)

Solid line-present \(Q\text{\textsubscript{ion}}\) for O\textsubscript{2} molecule, Triangle-Krishnakumar and Srivastava [30], Star-Rapp and Englander [31], Dot- present \(Q\text{\textsubscript{ion}}\) for O atom, Diamond-Thomson et al. [32], Dash dot dot-Total ionization cross section \(Q\text{\textsubscript{ion}}\) of \(^1\text{S}\) state, Dash- Total ionization cross section \(Q\text{\textsubscript{ion}}\) of \(^1\text{D}\) state, Short dash dot- Total excitation cross section \(\Sigma Q\text{\textsubscript{exc}}\) for atomic O in ground state.

Atomic oxygen is the primary constituent for the color formation of aurora in the polar ionospheres. The electrons with the other charged particles, upon collision with the atomic O, can give rise to various excited states of O and lead to the metastable states as well. The de-excitation of these states can give rise to auroral green and red color. The curves with dash dot dot line and with dashed
line in Figure 6.2 show respectively our ionization cross section for the metastable excited states $^1S$ and $^1D$ of atomic O. The metastable calculations present a novel feature of our investigations, perhaps the first ever, and hence no comparable data are available. The nearest comparison is with the ground state O, which we consider next.

The dotted curve in Figure 6.2 shows the present total ionization cross sections for atomic O purely in its ground state. The present results on O (ground state) are in good agreement with the experimental data of Thomson et al. [32]. Lastly, the lower most curve, with dash dot line in Figure 6.2 shows our calculations of cumulative electronic excitation cross section $\Sigma Q_{exc}$ on atomic O, which is an important outcome of our CSP-ic method. There is thus a good general accord on our theoretical results for atomic and molecular oxygen as well. With this confidence we next go over to the computations of bulk or macroscopic parameters.

### 6.3.2 Macroscopic parameters

In an attempt to incorporate these valuable and widely accepted quantum mechanical cross section data into the realistic systems, such as the ionosphere/atmosphere of various planets, we have applied a micro-to-macro approach. That is, we employ our $Q_{ion}$ to derive macroscopic cross sections $\Sigma_{ion}$, and ionization Mean Free Paths and ionizing collision frequencies in the Earth's atmosphere and other specific cases.
6.3.2.1 Mean free paths

Figure 6.3: Ionization Mean free path $\Lambda_{\text{ion}}$ of $e^-$ in the Earth’s atmosphere at 80 km altitude (Lat.:70° N, Long.: 100° W)
Dash dot- $\Lambda_{\text{ion}}$ for $N_2$, Dash- $\Lambda_{\text{ion}}$ for $O_2$, Dot- $\Lambda_{\text{ion}}$ for Ar, Solid line- Composite $\Lambda_{\text{ion}}$ in m

Calculations on the ionization mean free path $\Lambda_{\text{ion}}$ carried out using equation (6.2.2) with the quantum mechanical cross section for ionization as an input parameter in equation (6.2.1). The MFP are shown graphically in Figure 6.3. The required concentration or number density of the constituents is as shown in Table 6.1 above.

In Figure 6.3, the curve with dash dot line shows the ionization mean free path $\Lambda_{\text{ion}}$ for the electron collisions with the available neutral $N_2$ at the given location in our atmosphere. Similar calculations have also been carried out for $O_2$ and Ar
and shown in Figure 6.3. As we are interested in mean free path for ionization, the exhibited results start from the ionization potential of the concerned target atom/molecule and calculated up to 10 keV. As can be seen from Figure 6.3, the minimum ionization mean free path $\Lambda_{ion}$ of electrons, purely for the available concentration of N$_2$ is 0.13 meter and the minimum occurs at energy 100 eV. The minimum MFP reflects the maximum of the cross section $Q_{ion}$. In the case of O$_2$ the minimum $\Lambda_{ion}$ is 0.49 meter and for Ar it is 11.63 meter. The ionization MFP for electrons increases with decreasing concentration of neutral species i.e. from N$_2$ to Ar. Apart from the individual ionization MFP, we have also calculated composite ionization-MFP, vide equation (6.2.3), for our composite atmosphere, composed of 78.28% N$_2$, 20.8% O$_2$ and 0.9% Ar. The lower most curve in Figure 6.3 shows the composite MFP and it exhibits minimum value of 0.10 meter at energy 100 eV.

Next let us consider the altitude of 100 km, in our ionospheric E region in the polar atmosphere (Lat.:70° N, Long.: 100° W). In this case also we have calculated the ionization MFP $\Lambda_{ion}$ for the dominant neutral species for the impact electrons in the energy range starting from $I_E$ of the neutral target to 10 keV.

Since O, N$_2$ and O$_2$ are the dominant species in this region with the concentrations shown in Table 6.1, these are included for finding of ionization MFP $\Lambda_{ion}$ and the results are shown in Figure 6.4. The curve with solid line shows $\Lambda_{ion}$ of electrons purely for the available concentration of N$_2$. It shows a minimum value of 4.19 meters at incident energy 100 eV. For O$_2$ this value is 18.22 meters.
(dashed curve) while for atomic O it amounts to 179 meters (dotted curve) for the electrons with 100 eV energy.

![Image](image.png)

**Figure 6.4**: Ionization Mean free path $\Lambda_{\text{ion}}$ of $e^-$ in the Earth's atmosphere at 100 km altitude (Lat.: 70° N, Long.: 100° W)

Solid line-$\Lambda_{\text{ion}}$ for N$_2$, Dash-$\Lambda_{\text{ion}}$ for O$_2$, Dot-$\Lambda_{\text{ion}}$ for O, Star-Composite $\Lambda_{\text{ion}}$ ($\Lambda_{\text{comp}}$) in m

The composite ionization MFP is also calculated for the bulk medium available at this location. The composite values follow almost the same trend as N$_2$, because of its dominant concentration among the available species. Similar calculation can also be made on the planetary and other atmospheres, such as that of Titan, with appropriate concentration of neutral components.

### 6.3.2.2 Ionizing collision frequencies

A lot of work was done, during 1960s and '70s, on the collision frequency of thermal electrons in the ionospheric D and E region [25, 33, 34]. Electron
collision frequency in the ionospheric D and E region depends on neutral particle concentration [35]. In the D region, only N₂ and O₂ play significant role in the calculation of collision frequency [25, 33, 36, 37] with Ar as minor constituent. The dissociation of O₂ starts to occur at about 90 km [38] and further towards the E region, the concentration of atomic oxygen increases rapidly above this height. In E region atomic O and N₂, O₂ have significant concentrations [11]. In our calculation of the effective ionizing collision frequency νᵢₑ we have considered the electrons capable of ionizing the available neutral species. As a primary approximation Maxwellian distribution of the electrons is assumed. As can be seen from the neutral concentration available from MSIS-E-90 [11] and from the effective species in concerned ionospheric region, N₂ may be the most effective neutral target to influence the effective ionizing collision frequency νᵢₑ. Thus we have computed νᵢₑ by considering the concentration of N₂ in ionospheric D and E regions at 80 km and 100 km of altitude respectively using equation (6.2.5), and the results are shown in Figure 6.5. The curve with the solid line shows νᵢₑ at 80 km altitude peaking to 1.5×10⁷ s⁻¹, for the electrons with 149 eV energy.

An important feature which makes the calculations rather visible is in terms of number of ion-pairs produced. With the ionization collision frequency obtained above, the corresponding maximum number of ion-pairs (electron plus positive ion) turns out to be 1.5×10⁷.
Figure 6.5: Ionizing collision frequency $\nu_{ic}$ (s$^{-1}$) of e$^-$ with N$_2$ at 80 km and 100 km altitude in the Earth’s atmosphere (Lat.:70° N, Long.: 100° W), Solid line- $\nu_{ic}$ at 80 km, Dot- $\nu_{ic}$ at 100 km.

In Figure 6.5 the lower curve with dotted line shows $\nu_{ic}$ at 100 km altitude peaking to $1.7 \times 10^6$ s$^{-1}$, for the electrons with 149 eV energy. The $\nu_{ic}$ is an order of magnitude lower in E region as compared to D region. This difference is attributed to the amount of neutral concentration available at those locations.

6.4 Ion production rates in the ionospheres of Mars and Titan: Results

With this perspective in mind and the sample calculations discussed above in section 6.2.2, we are now confident enough to move out of the mother Earth. Let us explore the application of our calculated ionization cross sections to other
environments to estimate another important bulk parameter viz. ion production rates (IPR) in the ionospheres such as in Mars and Titan (moon of Saturn).

6.4.1 Ion production rates (IPR)

Basically our quantum mechanical calculations are done at a given electron energy $E_i$ and the theoretical cross sections are presented as a function of $E_i$. In a laboratory situation the experiments are done with mono-energetic beam of electrons, and the incident energy is varied suitably. In a natural environment like an ionosphere, what we have is a flux of incident electrons (e.g. photo-electrons) with an energy distribution, which is assumed to be Maxwellian, for simplicity. Photo-electron impact ionization cross sections are important in the modeling of planetary ionospheres, airglow and aurora. For this purpose first we will discuss, in detail, the IPR in the Martian ionosphere and then move on to the Jupiter and Titan atmospheres.

In the year 2013, planet Mars is receiving great attention due to opportunity for launching various exploratory missions. Over the Mars, the present IPR calculations have been carried out for the dominant neutral species i.e. CO$_2$, CO, O$_2$, N$_2$ and O along with the diurnal variation IPR. Also the similar IPR calculations have been carried out for N$_2$ on Titan.

D, E and F layers are modeled in the Martian ionosphere by Haider et al. [39]. It has been found that photo-ionization is a dominant process in the formation of F layer as against the photo-electrons, which produce $\sim$70% ionizations in this region. But, the ionospheric E layer is mainly produced by electron impact
ionization where the photo-ionization is a secondary process [39]. Thus, the presently calculated $Q_{\text{ion}}$ are used to derive the ion production rates in the ionospheric E region of interest for the possible estimation of the Martian ionospheric chemistry.

The hyperbolic electrostatic analyzer (HARP) electron spectrometer carried aboard the Phobos 2 spacecraft showed the availability of the electrons with the sufficient energy to ionize the neutral species [40]. The first theoretical study of photo-electron impact ionization at Mars was reported by Mantas and Hanson [41] using a time-independent Boltzmann equation. Photo-electron fluxes for both the horizontal as well as the vertical magnetic fields have been calculated by them at Martian equator and poles respectively. However the observations of strong localized crustal magnetic fields by the Mars Global Surveyor (MGS) have significantly changed the above mentioned scenario [42]. Further this remnant magnetic fields are the possible sources of the localized aurora observed on the planet Mars [43].

We have employed the vital inputs viz., ionization cross sections, photo-electron flux and the neutral densities to the IPR calculations as described below.

### 6.4.1.1 Ionization cross sections

Ionization cross sections ($Q_{\text{ion}}$) are the most fundamental quantity to be employed for the IPR calculations. Figure 6.6 depicts our calculated $Q_{\text{ion}}$ for various neutral species available at Mars, viz. CO$_2$, NO, N$_2$, O$_2$, CO, O and N [44]. The present ionization cross sections in Figure 6.6 are well matched with the
available experimental and theoretical data sets. Here for the sake of clarity, other comparative data sets are not included in the Figure 6.6.

![Graph showing ionization cross sections](image)

Figure 6.6: Ionization cross sections $Q_{\text{ion}}$ for the dominant neutral species in the Martian Atmosphere [44]

### 6.4.1.2 Photo-electron flux

The extreme ultraviolet (EUV) radiation from the solar electromagnetic spectrum is a key source for the energetics of the planetary upper atmospheres [41]. Knowledge of the absorption and the partition of this energy among the various atmospheric constituents is required to understand the thermal structure, neutral and ionic composition, dynamics, aurora-airglow processes and several other important aspects of planetary atmospheres. The EUV flux can generate the photo-electrons via the photo-ionization, having sufficient energy to ionize the available neutral species in the atmosphere.
For the present IPR calculations on Mars, we have adopted the photo-electron flux data of Mentas and Hanson [41]. Figure 6.7 depicts the photo-electron flux at Mars for different altitudes at the solar zenith angle (SZA) $\chi = 45^\circ$, which is reproduced from the original Figure in [41]. We are also interested in Titan for which the photo-electron flux has been adopted from Bhardwaj and Jain [45]. Analytical yield spectrum technique along with the Solar EUV Experiment and SOLAR2000 (S2K) model has been used by Bhardwaj and Jain [45] to calculate the presently adopted photo-electron flux over Titan at selected altitudes at $\chi = 60^\circ$ [45]. The flux distributions are shown in Figure 6.8.

![Figure 6.7: Photo-electron flux at the selected altitude in the upper atmosphere of Mars (adopted from [41])]
6.4.1.3 Neutral density

Density of the neutral species available in the planetary upper atmospheres is a dominant input and a factor affecting the IPR. For Mars, species specific density measurements by neutral mass spectrometer aboard the Viking 1 and 2 landers are the first and the only in-situ neutral density measurements below 200 km [46], with the CO$_2$ as the most dominant neutral species. Atmospheric modeling has also played a major role in constructing the density profiles [39, 47]. In the present work the required neutral density profiles are adopted from Haider et al. [39, 45].

Figure 6.9 shows the densities of neutral CO$_2$, N$_2$, O$_2$, CO, NO, N and O in the Martian atmosphere.
Figure 6.9: Neutral densities of various species in the Mars atmosphere [39].

Figure 6.10: Neutral density of N$_2$ in the Titan atmosphere [48]
For the case of Titan, densities of the neutral $N_2$ have been acquired from the Cui et al. [48, 49] as depicted in Figure 6.10. Their [48] analysis is based on a large sample of Cassini/INMS (Ion Neutral Mass Spectrometer) measurements in the CSN (Closed Source Neutral) mode, obtained during 15 close flybys of Titan. Since $N_2$ is the most dominant species in the Titan atmosphere we aim to calculate IPR for the same.

### 6.4.2 Production of $CO_2^+$ in Mars and $N_2^+$ in Titan

This section describes our primary IPR calculations carried out for the $CO_2$ rich Martian and $N_2$ abundant Titanian atmospheres. The IPR is calculated using equation (6.2.6) as described in section 6.2.

For the IPR calculations at Mars, the required inputs, as already discussed in sections 6.4.1-3, viz. ionization cross sections, photo-electron flux and number density of $CO_2$ are obtained from Figure 6 [44], 7 [41] and 9 [39] respectively. Figure 6.11 shows our IPR calculations for $CO_2$ on Mars. The energy range under present consideration i.e. for $CO_2$, 13.77-100 eV and for $N_2$, 15.58-100 eV, allows for only parent/single ionization of the target molecules and hence the profile plotted in figure 6.10 is essentially the $CO_2^+$ production rates in the Martian atmosphere. The present calculations give the maximum $CO_2^+$ production rates of $1.36 \times 10^4 \text{ cm}^{-3} \text{s}^{-1}$ at the altitude of 128 km.
Figure 6.11: CO$_2^+$ production rates at Mars

Figure 6.12: N$_2^+$ production rates at Titan
The similar calculations are carried out for \( \text{N}_2^+ \) production rate over Saturnian moon- Titan. Basic inputs for IPR calculations are obtained from Figures 6 of [44], 8 of [45] and 10 of [48]. Our Figure 6.12 represents the \( \text{N}_2^+ \) production rate at selected altitudes in the Titan atmosphere. The present IPR calculations are limited to only three altitudes as the photo-electron flux data are available only for these altitudes. Though we are able to predict the height of maximum IPR at 900 km as can be seen from Figure 6.12, it may vary in between 900 to 1000 km.

### 6.4.3 Diurnal variation in the IPR (with Solar Zenith Angle)

Along with the altitude variation there must be IPR variations associated with the daily position of the Sun in the Martian sky, which is indicated by the zenith angle \( \chi \). Since the photoionization through EUV is the main source for the ionization of neutral species and photo-electron production, IPR does show dependence on the SZA. Presently we have made efforts to estimate the diurnal variation in the IPR with the varying SZA. Other dominant neutral species such as \( \text{CO}_2, \text{CO}, \text{N}_2, \text{O}_2 \) and \( \text{O} \), existing in the Martian atmosphere, are also included in the present calculations to have an overview of the detailed ion-neutral chemistry.

As already noted in section 6.4, three basic inputs to the IPR calculations namely ionization cross section, photo-electron flux and number densities are required. Further since we intend to study diurnal variation, we also require the photo-electron flux at different altitudes for different SZA. The \( Q_{\text{ion}} \) for \( \text{CO}_2, \text{CO}, \text{N}_2, \text{O}_2 \)
and \( O \) are calculated by our semi-empirical formalism as discussed in chapter 2 and as depicted in Figure 6.6. Essential photo-electron flux for five different solar zenith angles viz. \( 0^\circ \), \( 20^\circ \), \( 40^\circ \), \( 60^\circ \) and \( 70^\circ \) at different altitudes ranging from 115 through 160 km is obtained via private communication from Jain and Bhardwaj [50]. Figure 6.13 (a), (b), (c) and (d) shows the sample data for the photo-electron flux at SZA \( 0^\circ \), \( 40^\circ \), \( 60^\circ \) and \( 70^\circ \) respectively, employed in the present calculations. Flux data for SZA \( 20^\circ \) are not shown here.

![Graphs showing photo-electron flux for different altitudes at SZA](image-url)

Figure 6.13: Photo-electron flux for different altitudes at SZA (a) \( 0^\circ \) (b) \( 40^\circ \) (c) \( 60^\circ \) and (d) \( 70^\circ \) at Mars [50]
The IPR calculated by us presently from these inputs are portrayed in Figures 6.14 (a)-(f). Figures 6.14 (a)- through (e) show the CO$_2^-$, CO$^+$, N$_2^+$ O$_2^+$ and O$^+$ production rates respectively at different altitude ranging from 115 km to 160 km for different SZA i.e. 0°, 20°, 40°, 60° and 70°. One can see from our results that for each of the species, the IPR increases with the decrease of SZA and that is what one expects. When the Sun is overhead, i.e. $\chi=0^\circ$, maximum ion production takes place [51,52]. This argument is in line with that of Chapman [51,52] stated way back in 1930′s. In order to obtain total IPR from the major neutral species on the Mars, individual IPR for the production of CO$_2^-$, CO$^+$, N$_2^+$, O$_2^+$ and O$^+$ are added together and the resultant total IPR is represented in Figure 6.14 (f).

We have also tried to investigate the prevailing trend in the decrease of IPR. For that purpose we have plotted the maximum IPR at different SZA and the trend we have obtained is plotted in Figure 6.15. A nice peak in the IPR is observed when the Sun is overhead in the sky of Mars. Thus, we confirm the expected IPR behavior over Mars.
Figure 6.14: variation of IPR with the SZA, (a) CO$_2$ (b) CO (c) N$_2$ (d) O$_2$ (e) O (f) Total
Figure 6.15: variation of maximum IPR with the SZA

6.5 Conclusions

In conclusion this chapter is devoted to planetary applications of our calculated ionization cross sections in order to derive various bulk parameters in a given (gaseous) medium. In the case of Earth's atmosphere, we have employed the reliable total cross sections \( Q_{\text{ion}} \) obtained in our method, to carry out calculations on ionization Mean Free Path \( \Lambda_{\text{ion}} \) and ionizing collision frequency \( \nu_{\text{ic}} \), using a micro-to-macro formalism (equations 6.2.2, 6.2.3, 6.2.4, 6.2.5). The present calculations are estimated for the D and E regions of high latitude ionosphere of the Earth. The composite ionization MFPs are also incorporated in this work. Up to our knowledge the present work is perhaps the first attempt to calculate
ionization MFPs and ionizing collision frequency for externally precipitated and the secondary generated energetic electrons, since previous studies were mostly confined to the low energy thermal electrons embedded in the ionosphere. It appears from literature that old ionization data of 1970s were employed for modeling, and quantum mechanical ionization cross sections such as reported here have not been employed to calculate various bulk quantities.

Another bulk parameter namely, ion production rate in the Martian and Titanian atmospheres, is discussed in the latter half of this chapter, where our efforts are aimed at applying calculated ionization cross section for this purpose. Our present work yields the CO$_2^+$, CO$^+$, N$_2^+$, O$_2^+$ and O$^+$ production rates at Mars for the available photo-electron flux at different solar zenith angles. To strengthen our understanding of the IPR variation, we have also estimated the prevailing trend in the variation of IPR with the SZA. Further we have also calculated the N$_2^+$ production rates in the Titan atmosphere. Though the present results are perhaps on a higher side as ion loss processes are not incorporated, we are led to a better understanding of the ionized species content in these environments which in turn gives rise to further complex chemistry.

It may be noted that the bulk medium considered in this chapter has been a gaseous medium. A separate treatment is required for electrons passing through a solid or a condensed-matter environment, as described in the chapter to follow.
Bibliography


See also [http://omniweb.gsfc.nasa.gov/vitmo/msis_vitmo.html](http://omniweb.gsfc.nasa.gov/vitmo/msis_vitmo.html)


