A Missing Piece of the E-Region Puzzle: The Need for High-Resolution Photoionization Cross Sections and Solar Irradiance in Models

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Abstract

Most ionospheric models cannot sufficiently reproduce the observed electron density profiles in the E-region ionosphere, since they usually underestimate electron densities. Mitigation of this issue is often addressed by increasing the solar soft X-ray flux which is ineffective for resolving data-model discrepancies. We show that low-resolution cross sections and solar spectral irradiances fail to preserve structure within the data, which considerably impacts the radiative processes in the E-region, and are largely responsible for the discrepancies between observations and simulations. To resolve data-model inconsistencies, we utilize new high-resolution (0.001 nm) atomic oxygen (O) and molecular nitrogen (N₂) cross sections and solar spectral irradiances, which preserve autoionization and narrow rotational lines, allowing solar photons to reach lower altitudes and increase in the photoelectron flux. This work improves upon Meier et al. (2007) by additionally incorporating new high-resolution N₂ photoionization and photoabsorption cross sections in model calculations. Model results with the new inputs show increased O⁺ production rates of over 500%, larger than those of Meier et al. (2007) at 0.1 nm resolution, and total ion production rates of over 125%, while N₂⁺ production rates decrease by 15% ² in the E-region in comparison to the results obtained using the cross section compilation from Conway (1988). Low-resolution molecular oxygen (O₂) cross sections from the Conway (1988) compilation are utilized for all input cases and indicate that O₂⁺ is a dominant contributor to the total ion production rate in the E-region. Specifically, the photoionization contributed by longer wavelengths is a main contributor at 120 km.
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Key Points:

• Generated new high-resolution theoretical cross sections of O and N₂ for implementation in radiative transfer/photoionization rate models.
• Total photoionization rates increased in the E-region when utilizing the new high-resolution cross sections and solar spectral irradiances.
• O₂ is a dominant contributor in the E-region thus models need new high-resolution cross sections to address electron density discrepancies.

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Abstract

Most ionospheric models cannot sufficiently reproduce the observed electron density profiles in the E-region ionosphere, since they usually underestimate electron densities. Mitigation of this issue is often addressed by increasing the solar soft X-ray flux which is ineffective for resolving data-model discrepancies. We show that low-resolution cross sections and solar spectral irradiances fail to preserve structure within the data, which considerably impacts the radiative processes in the E-region, and are largely responsible for the discrepancies between observations and simulations. To resolve data-model inconsistencies, we utilize new high-resolution (0.001 nm) atomic oxygen (O) and molecular nitrogen (N₂) cross sections and solar spectral irradiances, which preserve autoionization and narrow rotational lines, allowing solar photons to reach lower altitudes and increase in the photoelectron flux. This work improves upon Meier et al. (2007) by additionally incorporating new high-resolution N₂ photoionization and photoabsorption cross sections in model calculations. Model results with the new inputs show increased O⁺ production rates of over 500%, larger than those of Meier et al. (2007) at 0.1 nm resolution, and total ion production rates of over 125%, while N₂⁺ production rates decrease by ∼15% in the E-region in comparison to the results obtained using the cross section compilation from Conway (1988). Low-resolution molecular oxygen (O₂) cross sections from the Conway (1988) compilation are utilized for all input cases and indicate that O₂⁺ is a dominant contributor to the total ion production rate in the E-region. Specifically, the photoionization contributed by longer wavelengths is a main contributor at ∼120 km.

Plain Language Summary

Most ionospheric models cannot sufficiently reproduce the observed electron density profiles in the E-region ionosphere and often attempt to mitigate the issue via unrealistic ad hoc modifications of the solar radiation flux. Here we address the low-resolution cross sections and solar spectral irradiances used as model inputs that are largely responsible for the discrepancy between models and observations. Low spectral resolution cross sections fail to accurately preserve structural features which allow solar photons to reach lower altitudes. We provide new high-resolution atomic oxygen (O) and molecular nitrogen (N₂) cross sections and solar spectral irradiances which preserve important structural features that allow photons to leak through and increase the photoelectron flux. Model results show increased O⁺ and total ion production rates of over 125% while a small decrease in the N₂⁺ production rate over calculations with historical data. Model outputs also indicate that O₂⁺ plays an important role in the total ion production rate, particularly at ∼120 km. These findings demonstrate that it is crucial to update ionosphere models with high-resolution photoionization and photoabsorption cross sections and high-resolution spectral irradiances.

1 Introduction

Accurate characterization of photoionization processes (including ionization frequencies and rates) is vital for understanding gases in the terrestrial atmosphere and its response to solar ionizing radiation. Ab initio models use solar spectral irradiances and photoionization and photoabsorption cross sections to compute the deposition of energy as a function of wavelength and altitude, eventually leading to the production of dayglow. However, essentially all ionospheric E-region models underestimate electron densities and fail to match observed electron density profiles (EDPs) (Maute, 2017; Sojka et al., 2014; S. Solomon, 2006). This puzzling outcome is often mitigated by ad hoc modifications to the solar radiation flux; however, these short term solutions do not properly address the underlying issue. The deficiency is related to the poor physical representation of the deposition of solar ionizing radiation in the lower thermosphere (90-150 km). This is a direct consequence of the low-resolution cross sections and solar spectral
irradiances that are implemented in models. Low-resolution cross sections and low-resolution irradiances do not permit sufficient penetration of solar radiation to lower altitudes and thus lead to a severe underestimation of E-region electron production rates (Meier et al., 2007). The scarcity of high-quality photoionization and photoabsorption cross sections and inadequate spectral irradiances have hampered the ability to properly model observations. In another example, the Chandra and XMM-Newton observatories currently provide an abundance of X-ray spectra of astronomical objects, but a lack of high-quality atomic data impedes the interpretation of these spectra. It is therefore necessary to produce and utilize high-resolution cross sections to accurately model observations and interpret spectra.

Photoionization cross sections contain hundreds of narrow autoionization lines which current ionospheric models neglect to include. These autoionization features are present as the result of photon absorption into the semi-bound states of an atom/molecule that resides above the ionization limit. The semi-bound electron can either return to a bound state with no ionization or jump into the continuum as an autoionization. The O cross section from Meier et al. (2007) included hundreds of autoionization lines that exhibited Fano-type line shapes characterized by very large increases adjacent to major dips at discrete wavelengths. These autoionization features produce windows and peaks in the cross sections that enable a net increased penetration of solar EUV radiation. Therefore, use of high-resolution cross sections which can resolve the line profiles and preserve the dips and peaks are needed to properly account for the solar ionizing radiation at lower altitudes.

Solar spectral irradiance models often bin the flux into 1 nm or broader bands in order to maximize computational efficiency at the expense of preserving the structure in the solar spectrum (S. C. Solomon & Qian, 2005). Models such as the Time Dependent Ionospheric Model (TDIM; Schunk and Walker, 1973; Schunk, 1988) which use EVE (Extreme Ultraviolet Variability Experiment) solar flux measurements at ∼0.1 nm resolution, predicted electron densities that were 20% lower than observed implying a photoionization rate that is low by about 36% (Sojka et al., 2014). Meier et al. (2007) showed that such models produce serious errors in the E-region. Their analysis of high-resolution (0.001 nm) O cross sections that include more than 300 autoionization lines, demonstrated that photoionization rate estimates in the E-region can be low by as much as a factor of 3 when using solar spectral irradiances and cross sections modeled at 1.0 nm as opposed to a spectral resolution of 0.001 nm. The high-resolution cross sections possess autoionization features and dips in the continuum that allow photons to “leak” through to lower altitudes enabling a net increased penetration of solar EUV radiation to the E-region and thus increased ionization. To examine the increased ionization, sufficiently high-resolution solar spectra of the same spectral resolution as the high-resolution cross sections are necessary to determine the E-region electron density.

Determining the appropriate atomic cross sectional data over a range of energies and temperatures necessitates a predominantly theoretical approach. Experimental measurements are essential to validate theoretical studies, particularly in the case of complex heavy ionic systems. However, experimental studies are often limited in the range and resolution of energy, and charge states investigated. In order to model the dynamics of the interaction of photons with atomic systems, large $R$-matrix (Tayal & Zatsarinny, 2016; McLaughlin et al., 2011, 2013; Abdel-Naby et al., 2013; Scully et al., 2006) calculations have been performed to accurately predict both the whole state energies and the resulting photoabsorption (Sant’Anna et al., 2011) and photoionization spectra (Gharaibeh et al., 2011).

While other works by Bautista et al. (2022) and Bergemann et al. (2021) show $R$-matrix calculations of O photoionization cross sections, they are limited to a few of the O I lines while our work provides a more extensive analysis including 34 atomic oxygen states. Gorczyca et al. (2013) also presented an O I photoabsorption cross section, de-
determined via $R$-matrix calculations, for energies of interest in X-ray spectral modeling in order to resolve discrepancies in molecular O abundances between spectral models. Tashiro (2010) used the United Kingdom (UK) $R$-matrix codes (Morgan et al., 1998) to calculate N$_2$ photoionization cross sections; however, it was simply intended to demonstrate the ability of his newly implemented photoionization code, and the photon energy range was rather limited. Therefore, until now, no detailed high-resolution O and N$_2$ theoretical photoionization cross sections have been available to examine the discrepancies in the photoionization rates, and thus electron densities. This work satisfies this deficiency.

In this paper we first discuss the computational methodology for obtaining high-resolution theoretical cross sections using the $R$-matrix method. This is followed by a discussion of the photoionization and photoabsorption cross sections used as inputs in photochemistry models (with a detailed description pertaining to how these are extended to lower and higher wavelength regimes provided in the Supplemental Materials). We then discuss the solar flux models and methods used to generate high-resolution solar spectral irradiances. In the following section we examine the model outputs of two radiative transfer/photoionization codes using the new high-resolution inputs. In the final section we summarize the most significant insights from the study.

2 Computational Methodology

In this work, the $R$-matrix method is used to treat photoionization of atomic oxygen and molecular nitrogen. Specifically, $e^- - O^+$ and $e^- - N_2^+$ collision problems are calculated by the $R$-matrix method to extract the photoionization cross sections. The $R$-matrix theory of electron-atom and electron-molecular collisions (P. G. Burke & Robb, 1976; K. Burke P.G. Berrington, 1993; P. G. Burke, 2011) is based on the variational principle, in which the electron configuration space is divided into inner and outer regions. The boundary between the inner and outer regions is known as the $R$-matrix boundary radius. This radius should be large enough to contain all the density of the target atom or molecule. In the outer region, the scattering process is approximated as a single electron dynamics, neglecting the exchange of target and scattering electrons. In the inner region, the dynamics of all the electrons in the system, the target electrons plus the scattering electron, are treated as in usual quantum chemistry computations. This means the exchange effect of target and scattering electrons and some degree of correlation effect are properly considered in the inner region. In this method, we first solve the inner region problem which is equivalent to quantum chemistry computation within a restricted space, where the system is confined within a box radius, and its eigenstates form a discrete basis. These eigenstates carry information of the scattering electron. In addition, the wavefunctions of the bound states, i.e., neutral O atom or N$_2$, are also obtained from these eigenstates. Then, the scattering problem in the outer region is solved to obtain wavefunctions of the outgoing photoelectrons, based on the eigenstates calculated in the inner region. Photoionization cross sections are calculated by evaluating dipole transition moments between the wavefunctions of the bound states obtained in the inner region, and the wavefunctions of the photoelectrons constructed in the outer region calculation.

The target states included in the scattering calculations are represented by configuration-interaction (CI) wavefunctions. The target and continuum orbitals are orthogonalized using Schmidt orthogonalization. The continuum molecular orbitals are then orthogonalized among themselves using symmetric or Lowdin orthogonalization to remove the linearly dependent functions.

Inside the $R$-matrix sphere, the inner region, the total wavefunction for a given symmetry is expanded in basis states. The $(N+1)$ scattering system, where $N$ is the num-
ber of electrons in the target atom or molecule, in the inner region is represented by a

CI-type basis expansion;

\[ \Psi_{k}^{N+1} = A \sum_{i} \phi_{i}^{N}(x_{1}, ..., x_{N}) \sum_{j} \xi_{j}(x_{N+1}) a_{ijk} + \sum_{m} X_{m}(x_{1}, ..., x_{N}, x_{N+1}) b_{mk} \]  

where A is an antisymmetrization operator, \( x_{p} \) is the coordinate of the \( p \)th electron, 
\( \phi_{i}^{N} \) is the \( i \)th target state, \( \xi_{j} \) is the continuum orbital basis of the scattering electron, and 
\( k \) represents a particular \( R \)-matrix basis function. The continuum orbital basis, unlike

a bound orbital basis function, does not vanish on the boundary. \( X_{m} \) are \((N+1)\) electron correlation functions constructed from the bound orbitals to ensure the complete-

ness of the basis function when the continuum orbital basis is orthogonalized to the bound

electron basis. It further allows us to include correlation effects that arise from virtual

excitations to higher electronic states. The coefficients \( a_{ijk} \) and \( b_{mk} \) are determined by

matrix diagonalization, resulting in the \( R \)-matrix eigenstates in the inner region.

The standard \( R \)-matrix method has also been extended to include the effects of cou-
pling of the bound states to the target continuum, using the \( R \)-matrix pseudo state (RMPS)

method (P. G. Burke, 2011; Bartschat et al., 1996; Gorczyca & Badnell, 1997; Mitnik

et al., 1999). In our version of the RMPS method, used in the photoionization of atomic

oxygen, the target continuum states are represented by a set of Laguerre pseudo states.

Details of the \( R \)-matrix calculation for valence photoionization on atomic oxygen

are similar to previous work by Meier et al. (2007). We used 34 \( \text{O}^{+} \) states as target states

in the close-coupling expansion, obtained from the configurations \( 2s^{2}2p^{4}, 2s2p^{4}, \) and \( 2s^{2}2p^{2}3l \)

\((l = s, p \) and \( d)\). The K-shell photoionization of atomic oxygen was treated as in the work

by McLaughlin et al. (2013), where additional 1s-hole configurations were considered, 

resulting in 910 levels. The radius of the \( R \)-matrix sphere was taken to be 7.3 \( a_{0} \). We

neglect relativistic effects in our work and perform all calculations in LS coupling. All

atomic \( R \)-matrix results were obtained based on the Belfast suite of codes (Berrington


The \( R \)-matrix calculation on photoionization of nitrogen molecule was performed

based on target molecular orbitals (MO’s) obtained by the complete active space self cons-
istent (CASSCF) calculation on \( \text{N}_{2}^{+} \) molecular ion using the MOLPRO suite of codes

(Werner et al., 2012; Werner & Knowles, 1985; Knowles & Werner, 1985). We used the

cc-pVTZ basis set (Dunning, 1989) and full-valence active space was employed for the

CASSCF calculation. The continuum orbitals up to \( g \) \((l = 4)\) partial waves were rep-

resented by Gaussian-type molecular orbitals, centered at the center of gravity of the molecule.

The radius of the \( R \)-matrix sphere was taken to be 10 \( a_{0} \). All molecular calculations were

performed in the fixed nuclei approximation, using modified version of the UK Molec-

ular \( R \)-matrix Scattering package (Morgan et al., 1998; Tashiro, 2010).

3 Cross Sections

New high-resolution atomic oxygen and molecular nitrogen photoionization cross

sections are produced using the method described in the previous section at spectral res-

olution (0.0001-0.02 nm). The cross sections can be implemented in aeronomy models

such as the Atmospheric Ultraviolet Radiance Integrated Code [AURIC; Strickland et

al. (1999)] to compute volume production rates, electron density profiles, and additional

model outputs. AURIC requires that model inputs such as the photoionization cross sec-

tions and solar spectrum be on the same spectral resolution grid. Therefore, we discuss

the creation of new high-resolution cross sections to match the wavelength grid of the

high-resolution solar spectrum provided by H. Warren and colleagues (Warren, 2005) at

the Naval Research Laboratory (discussed in further detail in Section 4). The high-resolution

-5-
Table 1. Resolution Acronym Definitions

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
<th>Resolution</th>
<th>Citation</th>
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<tbody>
<tr>
<td>LR</td>
<td>Conway (1988) low-resolution cross sections</td>
<td>0.05 nm (0.1 - 10 nm) &amp; 0.1 nm (10-105 nm)</td>
<td>Conway (1988)</td>
</tr>
<tr>
<td>ILR</td>
<td>Conway (1988) low-resolution cross sections interpolated onto the high-resolution grid</td>
<td>0.001 nm (0.1-105 nm)</td>
<td>Conway (1988)</td>
</tr>
<tr>
<td>HR</td>
<td>New high-resolution data interpolated onto the NRLEUV high-resolution grid</td>
<td>0.001 nm (0.1-105 nm)</td>
<td>This Work</td>
</tr>
<tr>
<td>BHR</td>
<td>New high-resolution data binned onto the low-resolution grid</td>
<td>0.05 nm (0.1 - 10 nm) &amp; 0.1 nm (10-105 nm)</td>
<td>This Work</td>
</tr>
<tr>
<td>Original</td>
<td>New high-resolution R-matrix calculations on a variable grid</td>
<td>0.0001-0.02 nm variable resolution (0.1 - 105 nm)</td>
<td>This Work</td>
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The wavelength grid has a fine 0.001 nm bin size from 0.1-105 nm in comparison to current cross sections with resolutions typically ranging from 0.05-0.1 nm. The new cross sections are compared to the low-resolution compilation by Conway (1988), which were previously used in AURIC. To do so, we bin the high-resolution cross sections onto the low-resolution grid comprised of 0.05 nm bins from 0.1-10 nm and 0.1 nm bins from 10-105 nm. Figures corresponding to the cross sections in the following passages are labeled thusly: the new high-resolution cross sections interpolated onto the high-resolution grid are represented by HR and those binned onto the low-resolution grid are designated as BHR while the original low-resolution Conway (1988) cross sections are labeled as LR and the low-resolution data interpolated onto the high-resolution grid is represented by ILR (Table 1).

The new partial cross sections (the cross section for a given state in the species), excluding the O K-shell, require a linear shift in energy to match the NIST ionization potential (IP). This is done by applying a uniform shift to the partial cross sections based on accepted values from the literature for each species as the states and resonance peaks may have different accuracy. Small deviations in the IP from experimental values exist and thus the uniform shift should pose negligible differences to the individual states. For example, the NIST Chemistry WebBook lists ionization energies of 15.5802-15.5812 eV from optical spectroscopy (Trickl et al., 1989; Ogawa & Tanaka, 1962; Worley, 1943; Worley & Jenkins, 1938), 15.58-15.61 eV from photoelectron spectroscopy (Kimura et al., 1981; Lee & Rabalais, 1974; Natalis, 1973; Hotop & Niehaus, 1970; Potts & Williams, 1974; Katrib et al., 1973), and 15.58-15.7 eV from electron impact techniques (Stephan et al., 1984; Grade et al., 1983; Armentrout et al., 1981; Sahini et al., 1978) for N$_2$. Likewise, NIST also lists O IP values ranging from 13.0-14.0 eV from various experimental methods (Lide, 1992; Kelly, 1987; Banon et al., 1982; Paule, 1976). The specific shift in the photon energy of the partial cross sections is discussed the Supplemental Materials.
As discussed in Sections 3.1 - 4, cross sections and solar spectra are processed and placed on the corresponding high- and low-resolution grids via interpolation and binning. Additionally, the new high-resolution cross sections are supplemented by ancillary data to extend the wavelength range and incorporate other datasets that preserve autoionization features at transitional wavelengths near the limits of the new data. Following Kirby et al. (1979), it is necessary to preserve the integrated cross section when data are obtained from multiple sources of varying resolution and have been mapped to a different resolution. We impose the same requirement to conserve the integrated cross section by implementing flux preserving interpolation, or binning, which guarantees that the integrated cross section on the original (finer) grid over a specific wavelength interval is equivalent to the integrated cross section on the coarser grid over the same wavelength interval. The discussion in the following sections and the Supplemental Materials details these steps in the process while Section 5 presents the impacts the new cross sections have on atmospheric model calculations.

3.1 O Photoionization and Photoabsorption Cross Sections

Through the application of the RMPS method as described in Section 2, we obtained the valence and K-shell photoionization of atomic oxygen (Figures 1 – 9). All of the figures depicting cross sections and solar spectral irradiances are plotted with decreasing wavelengths from left to right which correspond to increasing energies when considering the values in energy space. In Figures 1 – 7 we show the cross sections for the six dominant states as identified by Conway (1988), the absorption (ABS) cross section (also shown in Figure 8), and relegate the remaining 29 states to a newly constructed pseudo state shown in Figure 9. The pseudo state was created to incorporate the contribution from the additional 29 states that were not previously explicitly included in the Conway (1988) compilation, and thus absent from the original AURIC input file, but which do not require individual tabulations since the states are not important contributors. The new HR photoionization cross sections are constructed from the native high-resolution (0.0001 – 0.02 nm) RMPS computations, supplemented with low-resolution cross section data from the Conway (1988) (hereafter LR) compilation at lower wavelengths where high-resolution R-matrix data are unavailable. The R-matrix methodology is usually accurate enough through 20-50 eV above the ionization threshold depending on the choice of basis function, R-matrix boundary radius, and so on, therefore additional data are needed at the lower wavelength regime. Details regarding the treatment of the cross sections are provided in the Supplemental Materials.
Figure 1. **Atomic Oxygen Photoionization Cross Sections.** (Left) The total and partial RMPS high-resolution photoionization cross sections interpolated onto the high-resolution solar spectrum grid vs wavelength. (Right) The RMPS high-resolution photoionization cross sections binned onto the low-resolution grid vs wavelength. The six dominant ionized states are shown in addition to the photoabsorption cross section (blue) and a pseudo state that incorporates the cross section of the remaining 29 partial states (orange).
Figure 2. $O^+\ 2s2p^3\ {}^4S_0$ Photoionization Cross Sections vs Wavelength. (Left) R-matrix calculations on the native grid (Original) and the low-resolution Conway (1988) compilation (LR) are shown. (Middle) The Conway low-resolution data interpolated onto the high-resolution NRLEUV grid (ILR) and the high-resolution data interpolated onto the NRLEUV grid (HR) are shown. (Right) The LR and the new binned high-resolution onto the low-resolution grid (BHR) are shown.
Figure 3. $\text{O}^+\ 2s2p^1\ ^2\text{D}_0$ Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figure 4. $^{2}P_{0}$ Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figure 5. $\text{O}^+\ 2s2p^1\ ^4\text{P}$ Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figure 6. $\text{O}^+ \, 2s2p^1 \, ^2P$ Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figure 7. $\text{O}^+\text{ K-shell Photoionization Cross Sections vs Wavelength}$. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figure 8. O⁺ Photoabsorption Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figures 2 – 9 illustrate the photoionization and photoabsorption cross sections interpolated onto the high-resolution (0.001 nm) fine grid (middle plot in panels) and binned onto the low-resolution solar spectrum wavelength grid (right plot in panels). The left panels show the new high-resolution cross sections on the variable native grid along with the LR cross sections, which were the previous default AURIC inputs. Figure 8, shows the Original total photoabsorption cross section which represents the sum of the original R-matrix O\(^+\) photoionization cross sections on the native grid. Data from the R-matrix calculations provided reliable data down to about 10 nm. The newly constructed cross sections contain a great deal more structure from the inclusion of autoionization lines that are absent in the LR cross sections and which are partially preserved when the new data are binned onto the low-resolution wavelength grid. While differences in the HR (BHR) and ILR (LR) cross sections are dominated by these new autoionization features, the new \(^4\)P and \(^2\)P state cross sections are systematically lower than the LR values (Figures 5 and 6). The high- and low-resolution pseudo states (Figure 9) also exhibit a “hump” at low wavelengths that results from smoothly fitting over the gap in the high-resolution absorption data (Figure 8) from 5.7 nm down to 4.1 nm. Although this side effect is present, incorporating the remaining 29 O\(^+\) states into the pseudo state allows us to preserve the ionization lines present at these lower wavelengths.
Figure 10. $N_2^+$ X Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.

Figure 11. $N_2^+$ A Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.
Figure 12. \( \text{N}_2^+ \) B Photoionization Cross Sections vs Wavelength. (Left) Original grids, (middle) high-resolution NRLEUV grid, and (right) low-resolution grid.

### 3.2 \( \text{N}_2 \) Photoionization Cross Section

Utilizing the \( R \)-matrix method (Schneider, 1995; Gillan et al., 1995; Tennyson, 2010; P. G. Burke, 2011) we derive the \( \text{N}_2^+ \) X, A, and B state photoionization cross sections (Figures 10 – 12) which are dominant contributors to the total \( \text{N}_2 \) photoionization cross section. Details regarding the treatment of the cross sections are provided in the Supplemental Materials.

Figures 10 – 12 illustrate the photoionization cross sections interpolated onto the high-resolution (0.001 nm) fine grid and binned onto a standard low-resolution solar spectrum wavelength grid. The newly constructed cross sections contain considerably more structure from the inclusion of autoionization lines that are absent in the LR cross sections. As in the case of the atomic O cross sections, much of the autoionization structure is preserved when the new \( \text{N}_2 \) cross sections are binned onto a low-resolution wavelength grid. At high wavelengths, the new cross sections differ by about an order of magnitude in comparison to the LR cross sections particularly for the X and B states (Figures 10 & 12).

### 3.3 \( \text{N}_2 \) Photoabsorption Cross Section

Current models use low-resolution photoabsorption cross sections, which like low-resolution photoionization cross sections and solar spectra do not allow sufficient penetration of solar radiation down to lower thermospheric altitudes. Therefore, a new \( \text{N}_2 \) photoabsorption cross section is constructed to reflect the changes introduced by the new high-resolution \( \text{N}_2^+ \) X, A, and B states that preserve the structure allowing solar radiation to penetrate deeper into the atmosphere. To formulate the new cross section the states below the ionization threshold of the \( \text{N}_2^+ \) X state are first considered. The high-resolution photoabsorption cross section is constructed by interpolating the Conway data onto the high-resolution solar spectrum grid, removing the contribution from the former
Figure 13. \(N_2\) Photoabsorption Cross Section. \(N_2\) photoabsorption cross section constructed from the Bishop et al. (2007) model and digitized Carter (1972) interpolated onto a 0.1 nm (top) and a 0.001 nm (bottom) resolution grid.

X, A, and B states, and summing with the HR states described in Section 3.2. Likewise, to construct the low-resolution absorption cross section, the contribution from the former X, A, and B states is removed and the remainder is summed with the 3 partial state BHR cross sections.

The LR photoabsorption cross section lacks structure at larger wavelengths which has been reported from measurements and more recent models. Therefore, we incorporate a high-resolution \(N_2\) photoabsorption cross section for the \(\sim 73.0 - 105.0\) nm region computed using the method of Bishop et al. (2004, 2007) and measurements from Carter (1972) (Figure 13). The Bishop model generates the \(N_2\) photoabsorption spectrum for 6 singlet states \((b^1\Pi_u, b^1\Sigma_u^+, c^1\Sigma_u^+, c^1\Pi_u, o^1\Pi_u, \) and \(e^1\Sigma_u)\) using a pure rotation approximation. The cross section is generated on a 0.0001 nm grid and then interpolated onto the high- and low-resolution solar spectrum grids at 0.001 nm and 0.1 nm resolution, respectively, using a flux preserving interpolation technique that preserves the integrated flux as mentioned in Section 3. Comparison of the Bishop cross section with Guertler et al. (1977) (0.003 nm resolution) and Huffman (1969) (0.004 nm resolution) measurements show very good agreement above \(\sim 86.6\) nm with more noticeable discrepancies at lower wavelengths. There are strong absorption features below 86.6 nm (i.e. 83.5 nm (near \(b^1\Sigma_u^+ v' = 25\)), 84.2 nm (\(c^1\Sigma_u^+ v' = 7\)), 85.6 nm (near \(c^1\Sigma_u^+ v' = 6\)), and 86.5 nm (\(e^1\Pi_u v' = 0\)) which are not present in the Bishop photoabsorption cross section. To preserve these features and utilize the highest resolution photoabsorption cross sections available, we combine the modified HR absorption cross section below \(\sim 73.62\) nm (and below 73.9 nm for the BHR cross section) with digitized data from Carter (1972), and the high-resolution Bishop model (Figure 14). The Carter (1972) data are interpolated onto the high- and low-resolution grids using a flux preserving interpolation technique and spliced in at \(\sim 73.62\) (73.9) nm - 86.6 nm with the interpolated Bishop data.
Figure 14. $N_2^+$ Photoabsorption Cross Sections vs Wavelength. (Left) high-resolution NRLEUV grid and (right) low-resolution grid.

Incorporation of the Carter (1972) cross section below the ionization limit of the $N_2^+$ X state is necessary to preserve structure at longer wavelengths that is not observed in the new $N_2^+$ X, A, and B cross sections. However, while the Carter (1972) photoabsorption cross section provides coverage at wavelengths between $\sim 73$ nm and up to the ionization limit ($\sim 79.5$ nm), the data in this regime cannot be solely attributed to photoionization. Huffman et al. (1963) stated that the bands below the ionization threshold are diffuse, implying that there is predissociation in the bands both he and Carter measured. Figure 2 of Huffman et al. (1963) shows almost no change in the absorption coefficient at the ionization threshold, implying that the absorption cross section is much larger than the ionization cross section. We infer that the undulations in the Carter $N_2^+$ photoabsorption cross section are therefore predissociation into $N+N$ rather than ionization. Furthermore, Conway (1988) states that the ionization yield is 100% for wavelengths below 66 nm and thus below the photoionization threshold, predissociation rapidly decreases toward 66 nm. Samson et al. (1977) found that from 65 – 80 nm several discrete Rydberg absorption lines exist and can autoionize to an extent; however, the photoionization yield is generally less than 100% in this region. The data of Samson et al. do not indicate a significant difference between the absorption and ionization cross sections below 70 nm but the data do increase above 70 nm, where Carter data becomes available. This again suggests that the peaks in the Carter data are due to $N+N$ predissociation and the ionization cross section is close to the lowest values in the Carter
photoabsorption cross section. The much broader oscillations observed in the new high-resolution cross sections between 70 – 79.5 nm are due to autoionization, as Samson et al. (1977) suggest. Thus while the Carter N₂ absorption cross section should be used to construct the new high-resolution N₂ photoabsorption cross section, it is not suitable to apply to the new high-resolution N₂ photoionization cross section.

Figure 15. NRLEUV Solar Minimum Spectrum. (Top) The original high-resolution NRLEUV solar spectrum delivered by H. Warren is shown in red. The black solid line is the triple smoothed (at wavelengths > 46.8 nm, non-thermal region) high-resolution solar spectrum. (Bottom) The NRLEUV high-resolution solar spectrum is shown in red while the binned (low-resolution) solar spectrum is shown in black.
Figure 16. Solar Spectra Panel. From top to bottom the final solar spectrum for the minimum (F$_{10.7}$ = 70), moderate (F$_{10.7}$ = 150), and maximum (F$_{10.7}$ = 250) solar activity cases are illustrated. The solar spectra are derived by reconfiguring the NRLEUV delivered minimum, moderate, and maximum spectra onto the high- and low-resolution grids. The spectra are then scaled using Lean’s model for the specific F$_{10.7}$ radio fluxes noted in the panel. The final high- (red) and low- (blue) resolution solar spectra are used in model calculations.

4 Solar Flux Model & Spectra

The Naval Research Laboratory’s extreme ultraviolet (NRLEUV) spectral irradiance model of Warren (2005) is used to generate the high-resolution solar spectra. The
model contains \( \sim 50,000 \) emission lines, six continua, and can be evaluated at any spectral resolution. It uses a differential emission measure distribution calculated from spatially and spectrally resolved solar data for a variety of solar activity. To obtain accurate photoionization rates EVE observations are used, which measure the solar EUV irradiance from 0.1 to 105.0 nm at 0.1 nm resolution with 20\% absolute accuracy, to normalize a 0.001 nm NRLEUV solar spectrum. This is accomplished by partitioning the irradiance at each 0.1 nm EVE interval into 0.001 nm subintervals.

For the low activity (solar minimum) case, the NRLEUV model uses EVE data at minimum solar activity and the CHIANTI database of atomic emission lines (Dere et al., 1997) to derive the EUV spectral irradiance. The spectrum is composed of various fits to an EVE spectrum: (1) an empirical fit to the various continua, (2) an empirical fit to the strongest optically thick lines, and (3) a superposition of a CHIANTI quiet Sun and active region spectrum. The high-resolution solar spectrum is triple smoothed above 46.8 nm to simulate realistic solar spectral line widths with FWHM of \( \sim 0.01 \) nm (Figure 15, top). To compare with the LR cross sections, a low-resolution solar minimum spectrum is constructed by binning the solar flux onto the low-resolution wavelength grid (Figure 15, bottom). The spectrum, which includes thousands of emission lines from the initial high-resolution model, may then be scaled with model data tuned for specific solar conditions such as the F10.7 cm radio flux, a reliable indicator of solar activity that is measured daily and used in forecasting space weather. Judith Lean’s solar EUV irradiance variability model (Lean et al., 2020; Woods et al., 2012; Lean et al., 2003) is used to simulate the solar activity for a spectrum with an F10.7 cm radio flux = 70. The NRLEUV derived high- and low-resolution solar minimum spectra are then scaled in increments of 0.1 nm (the lowest resolution of the two grids) to the integrated flux of Lean’s model spectra (Figure 16). Additional solar spectra for moderate and maximum solar activity cases are provided by S. Chabbra of NRL (private communication). The moderate and maximum solar activity spectra are similarly generated using the NRLEUV derived high- and low-resolution solar moderate (maximum) spectra scaled by Lean’s model spectra with an F10.7 cm flux = 150 (250) (Figure 16). The low-resolution solar spectra in Figure 16 appear shifted due to the \( \sim 100 \) factor increase in bin size from 0.001 nm to 0.1 nm resolution when binning the high-resolution solar spectra onto the low-resolution grid. The flux from 0 - 105 nm in the scaled spectra are conserved with differences in the integrated fluxes from 0 - 10 nm and 10 - 105 nm of less than \( \sim 0.6\% \). The total integrated flux for the new solar minimum, moderate, and maximum spectra are 2.93, 5.57, and 8.87 erg cm\(^{-2}\) s\(^{-1}\), respectively.

5 Photoionization Rates at High Spectral Resolution

5.1 AURIC

The need to incorporate high-resolution cross sections and solar spectra into photochemistry models prompted the generalization of the Atmospheric Ultraviolet Radiation Integrated Code [AURIC; Strickland et al. (1999)] to ingest data files with over 100,000 wavelengths. Following this update to the model, we replaced the current 0.05 - 0.1 nm resolution solar spectra used in AURIC with the high-resolution (0.001 nm) solar spectrum during solar minimum conditions supplied by H. Warren of NRL (private communication) scaled with a spectrum from Lean’s model (F10.7 = 70; Figure 16, top). AURIC comparisons presented herein represent model outputs using the Conway (1988) tabulation of cross sections, the newly computed high-resolution O and N\(_2\) photoionization and photoabsorption cross sections, and an MSIS 2.0 model atmosphere (Emmert et al., 2021). The scaled NRLEUV high-resolution solar spectrum with minimum solar activity is also implemented as a model input (please refer to Section 4 for details). AURIC also requires molecular oxygen cross sections. Here we use the Conway (1988) O\(_2\) cross sections on the low-resolution grid (LR) and interpolated onto the high-resolution grid (ILR) as model inputs. The O\(_2\) cross sections include states that dissociate into O+O...
\[(O^+)^+ = B^2\Sigma_g^+, \ 2\Pi_u + e^4\Sigma_m^-, \ 2\Sigma_u^+, \ \text{and K-shell; Conway, 1988}\) and we account for the ionization arising from these states independently of the total production for \(O_2^+\). Even though photoelectron ionization at \(\sim 110 \text{ km}\) is dominated by \(N_2^+\) (Siskind et al., 2022), we are investigating the impacts of high-resolution cross sections and solar irradiances on photoionization only, therefore, the photoionization rate and volume production rate values reported refer to the contributions from photoionization only (excluding photoelectron ionization contributions). Lyman alpha photoionization is not included in the analysis as the cross sections only extend up to 105 nm. We also note that AURIC rigorously includes ionization from solar photons and photoelectrons with vertical transport (Strickland et al., 1999).

Figure 17. \(O^+\) Photoionization Production Rates & Ratios. (Top) Photoionization production rates vs altitude for the dominant states in atomic oxygen. AURIC volume production rates using the HR (purple solid line) and BHR (yellow dashed line) cross sections are shown with the model results from the ILR (blue solid lines) and LR (red dashed lines) cross sections. (Bottom) Corresponding ratios of the volume production rates to the HR cross section case vs altitude. For reference, the ratio of the ILR/LR results are shown (solid black line). Ratios of photoionization rates of the ILR (solid blue line), BHR (dashed yellow line), and LR (dashed red line) cases to the HR case are shown.

Figures 17 - 19 illustrate AURIC model outputs for a combination of inputs. By comparing model results for the different cross sections and resolutions, we can analyze the impact of increasing the resolution versus the change resulting from differences in the cross section value. In the following sections model calculations using the low-resolution Conway cross sections and the low-resolution Conway data interpolated on the high-resolution solar spectrum grid are labeled as LR and ILR, respectively. Likewise, model calculations utilizing the new high-resolution cross sections and the new high-resolution cross sections binned onto the low-resolution grid are labeled as HR and BHR. Corresponding LR and ILR \(O_2\) data is used with the \(O\) and \(N_2\) BHR and HR cross sections, respectively, as model inputs. The ratios illustrated in Figures 17 - 19 are given with respect to the HR case, unless otherwise noted.

Figure 17 illustrates a significant divergence in the HR results in comparison to LR results for the \(O^+ 2s2p^3 \ ^4S_0\) state. Below approximately 175 km (E-region), the HR case has much greater volume ion production rates reaching a ratio of about 0.05 for the LR...
Figure 18. \( \text{N}_2^+ \) Photoionization Production Rates & Ratios for X, A, and B States.

(Top) Photoionization production rates vs altitude for the dominant states in molecular nitrogen utilizing the newly calculated \( \text{N}_2 \) cross sections from B. McLaughlin. AURIC volume production rates using the HR (purple solid line) and BHR (yellow dashed line) cross sections are shown with the model results from the ILR (blue solid lines) and LR (red dashed lines) cross sections. (Bottom) Corresponding ratios of the volume production rates to the HR cross section case vs altitude. For reference, the ratio of the ILR/LR results are shown (solid black line). Ratios of photoionization rates of the ILR (solid blue line), BHR (dashed yellow line), and LR (dashed red line) cases to the HR case are shown.

The total photoionization production rates for each species also demonstrate similar trends. In Figure 19, the top left panel illustrates the sum of the O\(^+\) VPR that originates from photoionization of atomic oxygen. The contribution from the dissociated states of O\(_2\)\(^+\), listed above, are shown as dotted lines in the O\(^+\) VPR panel; however, are not included in the totals or ratios. We find an overall increase in the O\(^+\) VPR utilizing the newly calculated partial cross sections with a maximum of 515 cm\(^{-3}\) s\(^{-1}\) at 189 km for the HR case and an increase of 172 cm\(^{-3}\) s\(^{-1}\) over the LR total VPR at 138 km.
total $O^+$ photoionization production rate ratios show increased volume production rates in the E-region below from 110-140 km with ratios less than $\sim 0.3$ for all the cases reaching a ratio of 0.14 at 115 km for the LR case. The total $N_2^+$ photoionization production rate demonstrates a large increase in magnitude for the HR case, reaching a peak of 800 cm$^{-3}$s$^{-1}$ at 180 km with ratios less than 0.75 for the LR and ILR cases above 207 km (33% increase). It is important to note that like $O_2$, several states in the $N_2$ cross section also dissociate or predissociate ($N_2^+ C^2\Sigma_u^+, F^2\Sigma_u^+, G^2\Sigma_g^+, E^2\Sigma_u^+, H^2\Sigma_g^+, H$, and K-shell). The contribution from the $N_2^+$ dissociated states are likewise shown as dotted lines in the middle left panel of Figure 19 and are included in neither the total $N_2^+$ VPR or ratio. Everything else being the same (same solar spectrum and resolution), the updated high-resolution $N_2$ photoabsorption cross section also impacts the VPR profile with deficits and enhancements at various altitudes. It is clear that the newly improved high-resolution cross sections result in larger production rates at higher altitudes in the F-region for $N_2$. Meier et al. (2007) also found that there was no accidental resonance overlap at the top of the atmosphere and we confirm that there are no major resonances with the updated cross sections from 300 km and above.

The large increase in the ionization rates produced by using the new high-resolution cross sections and solar spectrum may account for the magnitude discrepancy in the electron density profile (Buonsanto et al., 1995; S. C. Solomon & Qian, 2005; S. Solomon, 2006) (discussed in Section 1). Although these calculations use the Conway (1988) LR and ILR $O_2$ cross sections, we can infer the impact of the $O_2^+$ volume production rates.

As illustrated by the bottom panels of Figure 19, the total $O_2^+$ VPR (which excludes the dissociated states) when utilizing the new data (O & $N_2$ HR and BHR cases) produces a large increase in the total $O_2^+$ production rate with a ratio of less than 0.7 at $\sim$115-175 km, corresponding to an increase of over 40%. The LR case has a ratio of less than 0.4 at 135 km which correlates to an increase of over 150%.

Figure 20 shows the total photoionization production rate (left panel) and ratios (right panel) which do include the contributions from the dissociated $N_2^+$ and $O_2^+$ states. The total VPR for the HR and BHR cases are both larger in magnitude in comparison the LR and ILR cases above 110 km. The HR and LR both peak at 180 km with cross section values of 1529 and 1313 cm$^{-3}$ s$^{-1}$, respectively. The largest difference in magnitude is seen in the E-region at 126 km where the ratio drops to $\sim$0.43, corresponding to an increase of 133% in the HR VPR in relation to the LR case. While the BHR, ILR, and LR cases show two distinct peaks in the VPR altitude profile, the HR case exhibits a small tertiary peak at 126 km. This demonstrates that the increase in the VPR of the HR case is due not only to the new data from the partial cross sections but also as result of the finer resolution grid. The large difference in magnitude between the HR and LR cases at 126 km (515 cm$^{-3}$ s$^{-1}$) may produce an increase in the electron density profile when utilizing the HR cross sections.

### 5.2 Meier Photoionization Code

Meier et al. (2007) show that above 140 km the total photoionization rates for atomic oxygen when using high-resolution theoretical cross sections, regardless of the resolution of the solar flux grid, are relatively equal when the same cross sections are evaluated at bin centers (Figure 3 from Meier et al., 2007). The ionization rate ratio increases to 1.4 at $\sim$110 km and then drops to 1.0 at higher altitudes. Thus, according to Meier et al. (2007) the cross section resolution does impact the calculated photoionization rates between 100-140 km. In the analysis presented here the new BHR cross section can be compared to results from Figure 4 of Meier et al. (2007), with grid increments of 0.1 nm, although with the caveat that the resolution of the grid is not identical below 10 nm. Photoionization rate ratio results from Meier et al. (2007) Figure 4 for atomic oxygen show a ratio of $\sim$0.7 at about 115 km, indicating that the ionization rates for the 0.001 nm
Figure 19. Total Photoionization Production Rates & Ratios for each Species. (Left) Volume production rate results from AURIC with the newly incorporated high-resolution O and N\textsubscript{2} cross sections and solar irradiance spectrum for O\textsuperscript{+} (top), N\textsubscript{2}\textsuperscript{+} (middle), and O\textsubscript{2}\textsuperscript{+} (bottom). (Right) Volume production rate ratios for O (top), N\textsubscript{2} (bottom), and O\textsubscript{2} (bottom). These are the ratios with respect to the HR volume production rates. The ratio of LR and ILR is shown in black. Unity is shown in green.

The ratios shown in Figure 21 are of their LR cross sections with respect to the new high-resolution data. Likewise, the N\textsubscript{2}\textsuperscript{+} VPR peaks with a magnitude of 797 cm\textsuperscript{-3} s\textsuperscript{-1} at 184 km.
km with ratios less than 0.75 above 184 km. The $O_2^+$ VPR profiles also exhibit similar results, with $O_2^+$ VPR ratios of less than 0.7 at 114-176 km and a minimum ratio of $\sim$ 0.36 at 135 km. The shape of the $O_2^+$ VPR profile is also similar to the VPR results from AURIC which exhibit a bump above about 110 km, implying large increases in the ionization for tens of kilometers above this altitude. The total VPR produced from these calculations has a primary peak of 1505 cm$^{-3}$ s$^{-1}$ at 182 km with additional peaks of 1012 cm$^{-3}$ s$^{-1}$ at 129 km and 937 cm$^{-3}$ s$^{-1}$ at 108 km. The ratio of the total VPRs drops to 0.39 at 129 km which corresponds to an increase of 156% in the volume emission rate. These results are either identical or comparable with those obtained from AURIC with the largest difference arising from the discrepancy in the ionization of O at 137-138 km. The Meier photoionization code does not use flux-weighted cross sections, so that may also contribute to the differences seen in Figure 21. This demonstrates that both methods produce fairly consistent results with the updated high-resolution cross sections.

**6 Discussion**

The incorporation of new high-resolution $N_2$ and O photoionization cross sections into models such as AURIC and the Meier photoionization code demonstrates that the preservation of structure found in the cross sections and solar spectrum is crucial to properly account for electron production in the E-region ionosphere and perhaps mitigate the sometimes worse discrepancies found in the D-region (Siskind et al., 2015, 2019). Our analysis indicates large increases (over 500%) in the total O ionization rate profile in the E-region and increases of over 33% in the total $N_2$ ionization rate in the F-region (above $\sim$ 200 km). Meier et al. (2007) found that the 1 nm binned solar flux and cross section cases were a factor of 3 lower (increase of $\sim$ 300%) than the high-resolution case at 120 km. While the new high-resolution solar spectrum may be responsible for an increase in the production rate at high altitudes (typically F-region), the driver of the increase in the ionization rate in the E-region is the new high-resolution O and $N_2$ cross sections. Although all of the O photoionization cross section states have been updated with the new theoretical partial cross sections, only a subset of the $N_2$ cross section states were revised (X, A, and B states), as well as the total photoabsorption cross section. The $O_2^+$

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*Figure 20.* Total Photoionization Rate & Production Rate Ratio. (Left) The total volume production rate for all 4 input cases for AURIC. (Right). The corresponding total volume production rate ratio from AURIC with respect to the new high-resolution cross section inputs.
Figure 21. Total Photoionization Production Rates & Ratios from Meier et al. (2007). (Top) Photoionization production rates as a function of altitude for O, N\textsubscript{2}, O\textsubscript{2}, and the total. The unbinned HR cross section results are shown in black. The LR cross section results, with a bin size of 0.1 nm, are shown in red. (Bottom) Photoionization rate ratios for O, N\textsubscript{2}, O\textsubscript{2}, and the total as a function of altitude are shown in red and unity is shown in black. The ratio represents the total production rate of the species (or total) from the binned LR cross sections / corresponding total production rate from the unbinned HR cross sections.

cross sections are the Conway compilation and have not been updated. Variations in the N\textsubscript{2} photoabsorption cross section, comprised of the revised high-resolution partial cross sections, experimental measurements, and high-resolution models, which preserve the rotational absorption lines, produced the largest impact on the calculated ionization rates in the E-region. Interestingly, the changes to the N\textsubscript{2} photoabsorption cross section had a greater impact on the O ion production rates than for N\textsubscript{2}\textsuperscript{+}. This is undoubtedly due to the enhanced penetration of solar radiation through the dips in the N\textsubscript{2} cross section.

Comparison to photoionization codes such as the upgraded Meier et al. (2007) code aid in validating AURIC model results. Results for O\textsuperscript{+}, N\textsubscript{2}\textsuperscript{+}, and O\textsubscript{2}\textsuperscript{+} demonstrate similar VPR magnitudes, overall shape of the profile, and ionization production rate ratios (Figures 19 and 21). As discussed in Sections 5.1 and 5.2, the results between AURIC and the Meier photoionization code are in relatively good agreement with the exception of the larger increase in the total O\textsuperscript{+} VPR from the Meier code at 137 km. The wider ionization peak, with larger VPRs extending to lower altitudes may account for the 500% versus 300% increase observed in the Meier et al. (2007) results. Both the O\textsuperscript{+} and O\textsubscript{2}\textsuperscript{+} ionization rate ratios drop below 0.4 in the 110-150 km altitude regime while the N\textsubscript{2}\textsuperscript{+} ionization rate ratios are typical greater than 1.0 within the same range, indicating that the source of the increase in the E-region ionization is O\textsuperscript{+} and O\textsubscript{2}\textsuperscript{+} ionization while N\textsubscript{2}\textsuperscript{+} rates drop when using the new high-resolution in comparison to the low-resolution cross sec-
tion. Comparison of model outputs with observations is also necessary to verify these findings. However, further validation of the model results with incoherent scatter radar measurements and additional models is beyond the scope of this paper and will be addressed in a companion paper (Sakib et al. 2023).

We find an overall increase in the total E-region ion production rate for the new high-resolution inputs in comparison to low-resolution inputs which meets the expectation that high-resolution cross sections and solar spectra allow photons to penetrate deeper into the atmosphere. Implementing high-resolution cross sections is important and therefore necessary to properly account for the electron production rate in the E-region. A preliminary test was also conducted at higher resolution (0.0001 nm) and showed differences of less than 1% in the total photoionization rate indicating that inputs utilizing the 0.001 nm resolution sufficiently characterize the peaks and valleys of the cross sections. Results presented here exposed how sensitive photoionization rate models are to the resolution of cross sections, primarily in how preserved autoionization lines impact model outputs.

We also show that O\(_2\) plays a dominant role in photoionization production rates in the E-region (Figure S2 in the Supplemental Materials), moreso than O and N\(_2\). Long wavelength photons (> 80 nm) are dominating the direct photoionization of O\(_2\) in the E-region. However, the resulting photoelectrons from soft X-rays can still have sufficient energy to produce photoelectrons with sufficient energy to cause collisional ionization, whereas the long wavelength photons do not, thereby amplifying the role of X-rays (S. C. Solomon & Qian, 2005). While the increase in the electron density magnitude with the HR model calculations does address one of the issues investigated, the discrepancy in the EDP peak is puzzling. The apparent loss of the lower E-region peak when using high-resolution inputs may also be attributed to broadening and an upward shift in the peak altitude of the O\(_2^+\) ion production rate; however, the cause for this phenomena is not currently understood. Therefore is it also necessary to incorporate high-resolution O\(_2\) cross sections in model calculations to properly account for the total ionization rate, and thus electron density, with respect to altitude. This work is currently being performed, will be incorporated for completeness into AURIC and be made available for other modeling codes in a future publication.

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Data Availability Statement

The O and N\(_2\) photoionization and photoabsorption cross sections, solar spectra, AURIC model outputs, and associated code needed to read the data files are publicly available via Soto et al. (2023). The Conway (1988) report and tabulated cross sections are available at https://apps.dtic.mil/sti/pdfs/ADA193866.pdf.

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