RESOLVING E-REGION DATA/MODEL DISCREPANCIES: THE ROLE OF HIGH-RESOLUTION CROSS SECTIONS AND PHOTOIONIZATION RATES

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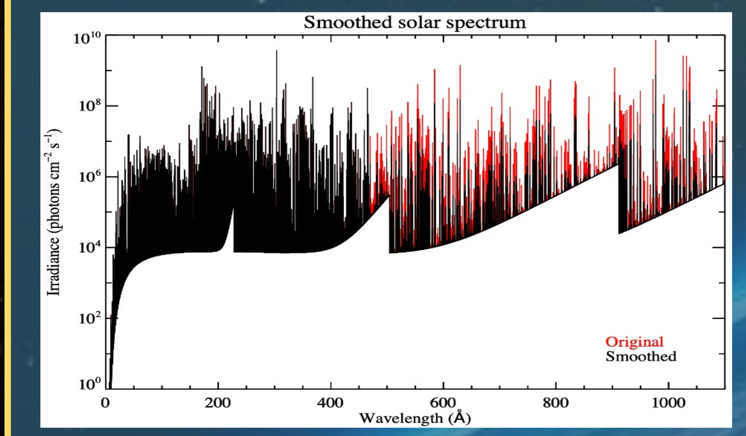
Motivation

Long-standing fundamental deficiencies in essentially all ionospheric E-region models perennially underestimate electron densities and are unable to match observed electron density altitude profiles. Mitigation of these issues is often addressed by increasing the solar soft x-ray flux; however, this quick fix is simply ineffective for resolving data-model discrepancies. We believe that these model deficiencies are the effect of poor physical representation of the deposition of solar ionizing radiation in the lower thermosphere. This is unequivocally driven by the use of low-resolution cross sections and low-resolution solar spectral irradiance models, which fail to preserve structure within the data that directly impacts radiative processes in the E-region. Accurate photoionization rates are therefore vital for the study and understanding of ionospheres, specifically high-resolution cross sections that preserve autoionization lines which allow solar photons to leak through to lower altitudes. To resolve data-model discrepancies, we utilize new high-resolution (0.01 Å) atomic oxygen (O) and molecular nitrogen (N_2) photoionization and electron impact cross sections and smoothed solar spectral irradiances in order to account for the increase in the photoelectron flux at lower altitudes caused by the penetration of high-resolution photoionizing solar radiation. Model results with these new inputs show increased production rates in the E-region in comparison to results using Conway [1988] inputs and are in better agreement with measurements taken at the Arecibo Observatory. Current findings indicate that molecular oxygen (O_2) plays a dominant role in photoionization production rates in the E-region. Therefore it is crucial to update the ab initio ionospheric models with high-resolution photoionization cross sections.

Methodology

In addition to previously updated O and N_2 photoionization cross sections accounting for 37 states, newly calculated high-resolution O and N_2 electron impact cross sections are incorporated into CPI's Atmospheric Ultraviolet Radiance Integrated Code [AURIC; Strickland et al., 1999]. The new cross sections are updates for 19 states currently used in AURIC. We also utilize a smoothed high-resolution solar spectrum, provided by H. Warren of the U.S. Naval Research Lab, to simulate realistic conditions (Figure 1).



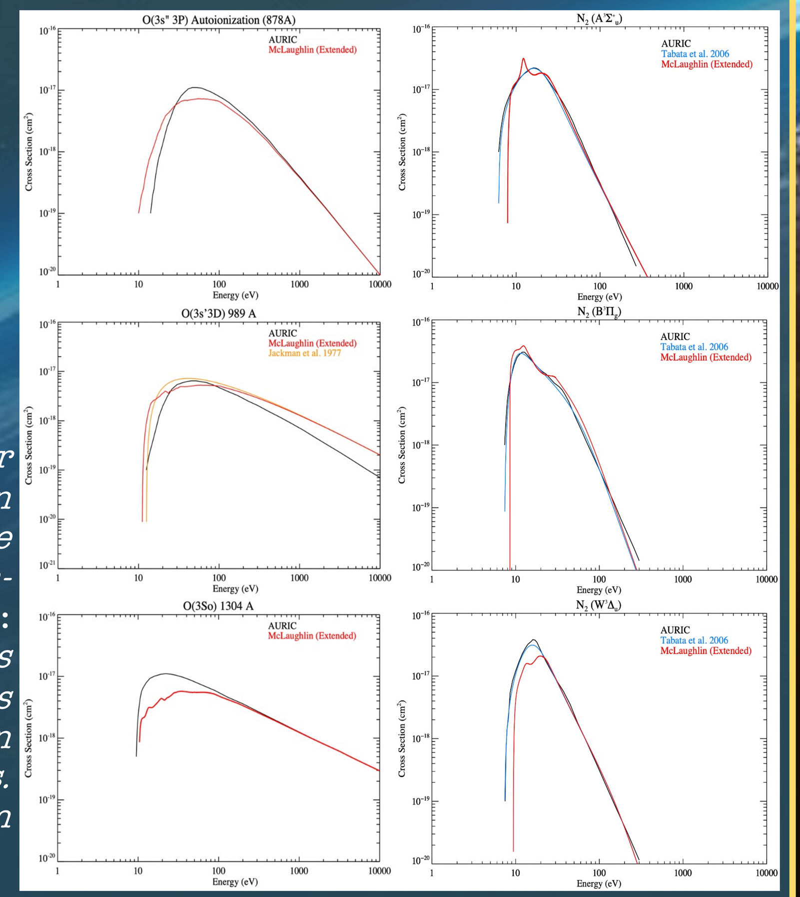


Figure 1 (Top): Original high-resolution solar spectrum delivered by H. Warren is shown in red. The black solid line is the triple smoothed (wavelengths > 468 Å) high-resolution solar spectrum. **Figure 2 (Right):** *Conway [1988] electron impact cross sections are shown in black. The red lines represent new theoretical high-resolution cross sections extended to higher energies. Orange and blue lines show analytic fits from Jackman et al. 1977 and Tabata et al. 2006.*

The R-matrix [Schneider 1995; Gillan et al. 1995; Tennyson 2010; Burke 2011] and R-matrix plus pseudo states [RMPS; Tayal et al. 2016; McLaughlin et al. 2011, 2013; Abdel-Nady et al. 2013; Scully et al. 2006] are used to calculate 8 N_2 and 11 O, respectively, high-resolution electron impact cross sections. Cross sections are extended to higher energies using analytic fits from Jackman et al. [1977] and Tabata et al. [2006] for O and N_2, respectively, and also by utilizing the Conway [1988] compilation (hereafter Conway1988). A selection of final cross sections incorporated into AURIC are shown in Figure 2. As illustrated in Figure 2, the updated O electron impact cross sections are typically of lower value than Conway1988. Several of the new N_2 electron impact cross sections are similar to Conway1988 while others are shifted down in value and in some cases the peak of the cross section is also shifted to higher electron energies (Figure 2). For the N_2 $A^3\Sigma_u^+$ state a new peak at lower energy is also seen in the structure of the cross section. The shape of the N_2 electron impact cross sections are generally similar to previous results from Itikawa et al. [2006], Gillan et al. [1996], Trajmar et al. [1983], and Borst [1972]. Overall, these cross sections show little structure and have minimal effect on calculations of ionization rates; however, AURIC results also incorporate previously updated high-resolution O and N_2 photoionization cross sections and do exhibit increased production rates in the E-region in comparison to results obtained with Conway1988 inputs.

Results

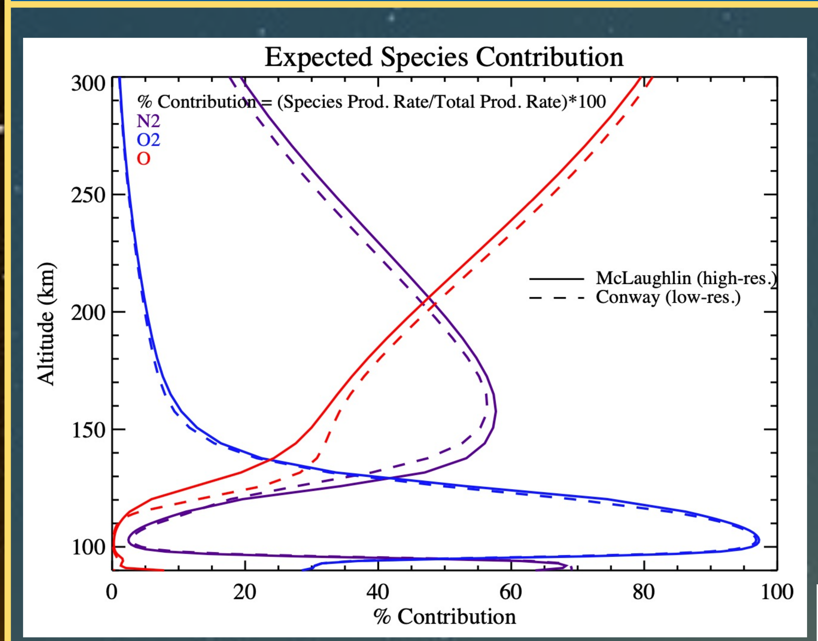


Figure 3 (Left): Expected species contribution as a function of altitude. The contribution for each species to the total ($O+N_2+O_2$) production rate from results utilizing the default Conway [1988] cross sections are shown as dashed red, purple, and blue lines for O, N_2, and O_2 respectively. Likewise, the contributions for each species to the McLaughlin total from results utilizing the high-resolution cross sections are shown as solid red, purple, and blue lines for O, N_2, and O_2 respectively. In the McLaughlin cross section results the default O_2 cross section from AURIC is currently being used in model calculations until it is updated through this study. From previous results, and the incorporation of the new cross sections, it is clear that O_2 plays a major role in the E-region.

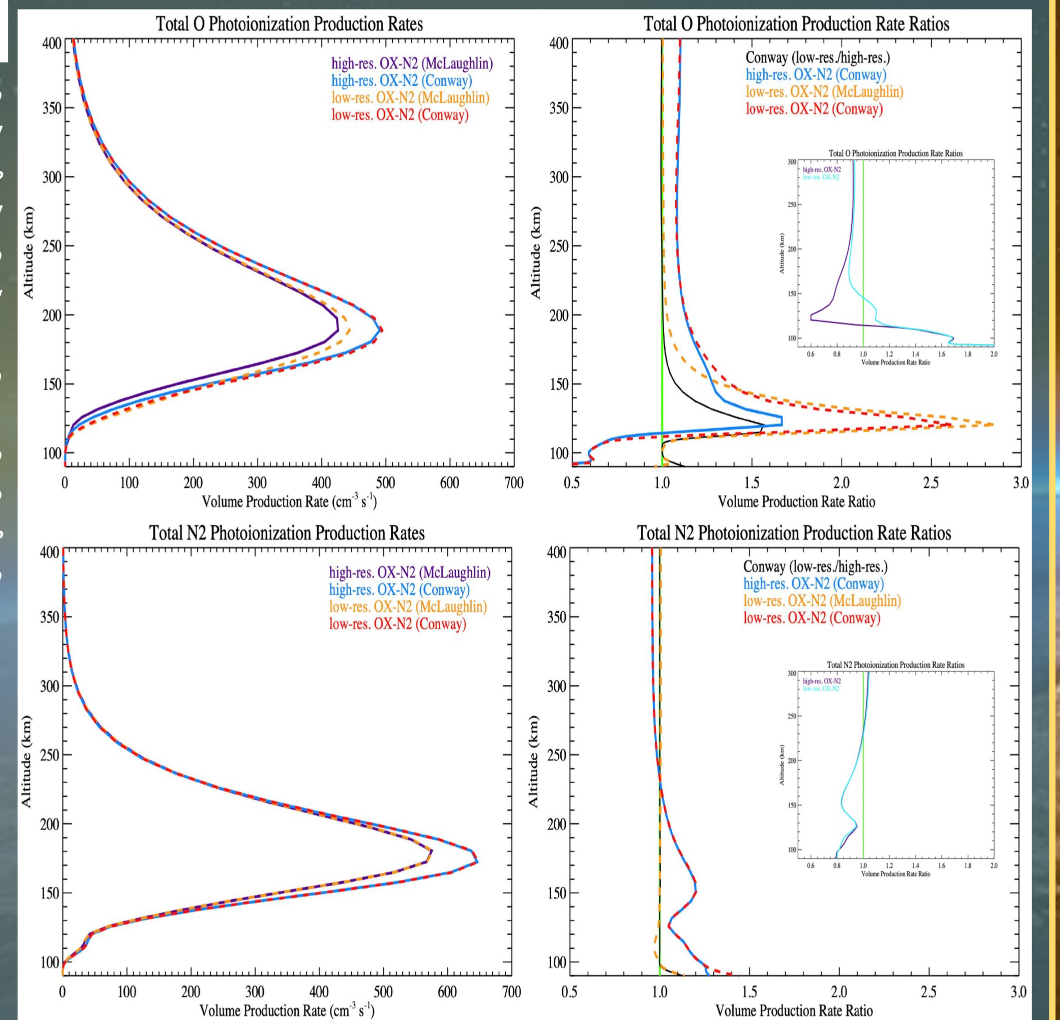


Figure 4 (Right): (Left) Volume production rate results from AURIC with newly incorporated high-resolution cross sections and solar irradiance spectrum for O (top) and N_2 (bottom). (Right) Volume production rate ratios for O (top) and N_2 (bottom). These ratios are with respect to the high-resolution McLaughlin volume production rates. The ratio of low-resolution Conway and high-resolution Conway is shown in black. The insets in the ratio plots on the right show the volume production rate ratios of O and N_2 for McLaughlin/Conway cross sections of like resolution. The high-resolution case is shown in purple and the low-resolution case is shown cyan. Unity is shown in green.

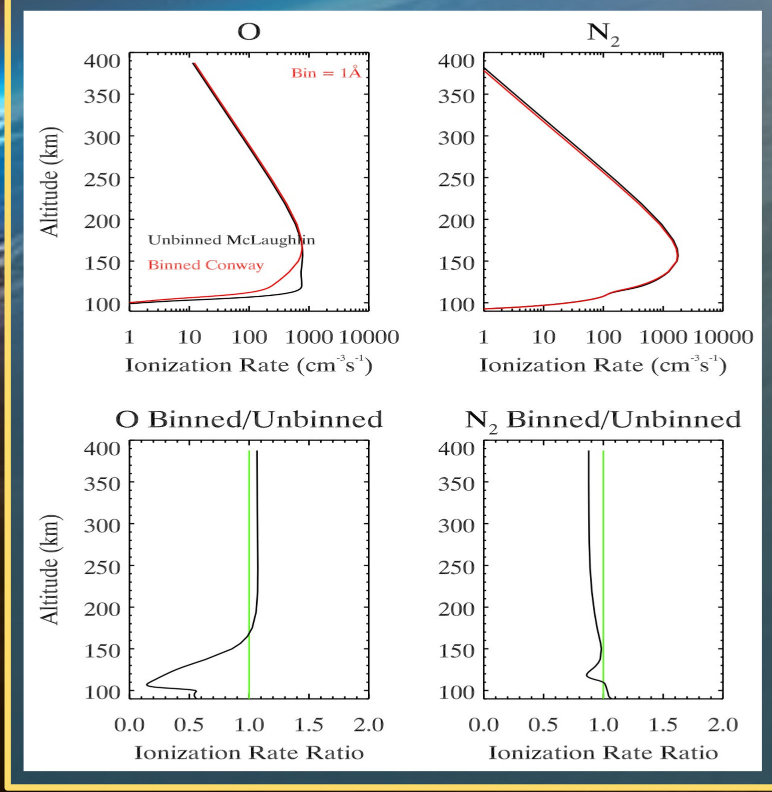


Figure 5 (Left): (Top) Total photoionization production rate as a function of altitude for O and N_2 from the Meier et al. 2007 ionospheric code. Results using the unbinned high-resolution McLaughlin cross sections are shown in black. Results using the low-resolution binned Conway cross sections, with a bin size of 1 Å, are shown in red. (Bottom) Photoionization rate ratios for O and N_2 as a function of altitude are shown in black and unity is shown in green. The ratio represents the total production rate of O (or N_2) from the binned Conway cross sections/corresponding total production rate from the unbinned McLaughlin cross sections.

Key Insights & Discussion

- **The expected contribution to the production rate in the lower E-region below ~130 km is expected to be primarily from O_2 (Figure 3).**
- **Volume production rate ratios determined using the AURIC code show increased ionization rates specifically for atomic O (Figure 4).**
- **New O and N_2 photoionization and electron impact cross sections greatly affect the O ionization rates, as calculated by the Meier et al. 2007 ionospheric code, below 170 km and N_2 ionization rates specifically at 120 km (Figure 5).**
- **Comparison to Arecibo ISR data illustrates good agreement between the AURIC model and Arecibo electron density measurements between 115 - 140 km (Figure 6).**

From AURIC results we are able to determine the expected contribution from each species to the total ($O+N_2+O_2$) volume production rate when utilizing the low-resolution Conway cross sections and high-resolution McLaughlin cross sections as model inputs. We find that N_2 and O dominate the volume production rates above 130 km and 200 km, respectively, while O_2 is expected to be the main contributor from 95-135 km (Figure 3). However, before reaching this altitude photons must pass through N_2 and O. Thus autoionization lines in those cross sections, which increase atmospheric transparency, may be of greater importance, but this has yet to be confirmed. Therefore, it is crucial to incorporate updated high-resolution O_2 photoionization cross sections once we complete theoretical calculations in order to accurately account for the production rates below ~135 km. Outputs from AURIC with updated high-resolution O and N_2 photoionization and electron impact cross sections indicate increased production rates up to ~40% in the E-region, specifically between 100-115 km in comparison to outputs utilizing the Conway [1988] cross sections (Figure 4). The inset plot in Figure 4, which depicts the volume production rate ratio of the McLaughlin/Conway cross section results of like resolution supports this for O showing a ~70% increase in the photoionization production rate when using the McLaughlin cross sections as model inputs for both resolutions. Production rates and ratios for N_2 do not illustrate a significant increase, only ~5% above 230 km. Comparison with results calculated using the Meier et al. [2007] ionospheric photoionization rate code, hereafter Meier2007, exhibit similar trends. Results calculated with Meier2007 show increased photoionization production rates for O when using the high-resolution McLaughlin cross sections below 170 km of up to 85% (Figure 5, left). Results for N_2 production rates calculated with Meier2007 also show increased photoionization production rates for N_2 of up to 15% between 110-120 km and typically ~ 10% above about 230 km (Figure 5, right). The ratio of the low-resolution Conway/high-resolution McLaughlin model results (red lines) in Figure 4 (right column) are comparable to Meier2007 results and illustrate similar shapes in the ratio profiles, however differ in magnitude. Overall, the high-resolution N_2 and O electron impact cross sections are not as important as photoionization cross sections in the grand scheme of model calculations for ionization rates. Validation of AURIC EDPs is an important step and we currently compare results to IRI-2016 [Bilitza et al. 2017] and FIRI-2018 [Friedrich et al. 2018] model results as well as observations from the Arecibo Observatory (Figure 6). However, validation with data from the Fast Auroral Snapshot (FAST) array of sensors, the Atmospheric Explorer E (AE-E) satellite, and the Constellation Observing System for Meteorology, Ionosphere, and Climate (COSMIC) radio occultation measurements is currently underway.

Validation

Figure 6, compares AURIC electron density profiles (EDP) with measurements obtained from the Arecibo Observatory [Sojka et al. 2014] and illustrates agreement with incoherent scatter radar (ISR) observations, specifically from 115 - 145 km. FIRI-2018 appears to provide a good upper boundary constraint, and both IRI-2016 and FIRI-2018 characterize the peak of the Arecibo EDP for approximately noon time at ~ 110 km. Current AURIC outputs have a similar peak as that observed at Arecibo; however, shifted down vertically in altitude by about 5 km. We will be addressing this model discrepancy in future calculations to properly characterize the peak of observed EDPs. We will repeat the comparison using high-resolution cross sections and solar irradiance when the solar spectrum becomes available.

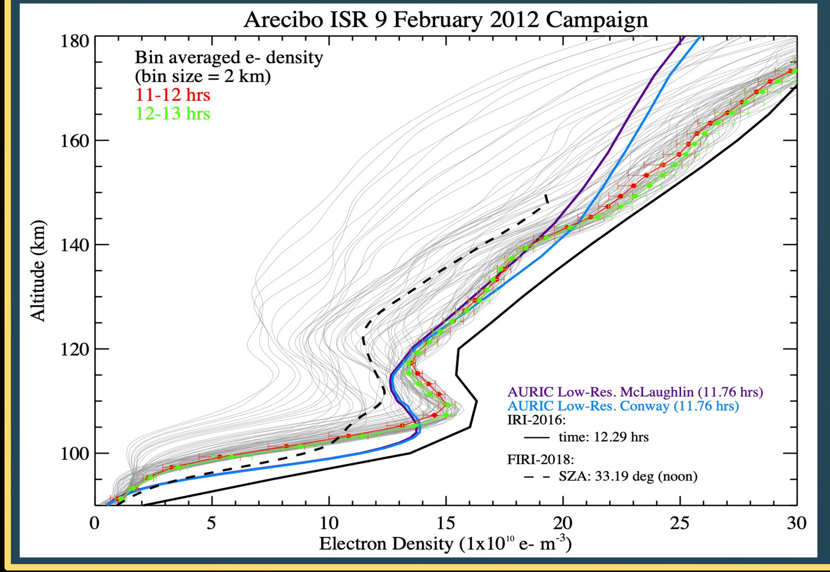


Figure 6: Comparison of model outputs using new cross sections to previous data. Arecibo Observatory electron density profiles (EDPs) from February 9, 2012 (Sojka et al. 2014) are shown in grey. The red and green solid lines show the mean EDPs in the time bins 11-12 hrs and 12-13 hrs, respectively. AURIC model results using an NRLEUV solar spectrum scaled by TIMED SEE for low-resolution McLaughlin cross section inputs and low-resolution Conway cross section inputs are shown as solid purple and blue lines, respectively. The dashed black line shows model results from the IRI-2016 code at 12.29 hrs while the solid black line illustrates the FIRI-2018 model results at solar zenith angle = 33.19 ° (representative of the SZA from AURIC model results).

Future Work

1. The next phase of the project includes calculation of theoretical molecular oxygen photoionization and electron impact cross sections for incorporation into the AURIC radiative transfer model. As indicated in Figure 3, ion production rates calculated with these cross sections are expected to dominated O and N_2 production rates in the E-region below ~130 km.
2. We will model the E-region ionosphere using AURIC and the updated high-resolution photoionization and electron impact O, N_2, and O_2 cross sections.
3. We will perform a detailed comparison between AURIC outputs and photoelectron fluxes measured by FAST and AE-E, and EDPs from COSMIC.
4. We will address discrepancies between measured and modeled EDPs from AURIC model outputs to properly account for electron deposition as a function of altitude in the E-region.

More to Come!

We are developing a web-based version of the AURIC model for public use to produce outputs at low- and high-resolution. The web-based version will eventually be made available on the CPI website.

Further questions? Please don't hesitate to reach out!
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Please check out our digital poster for additional plots and details!