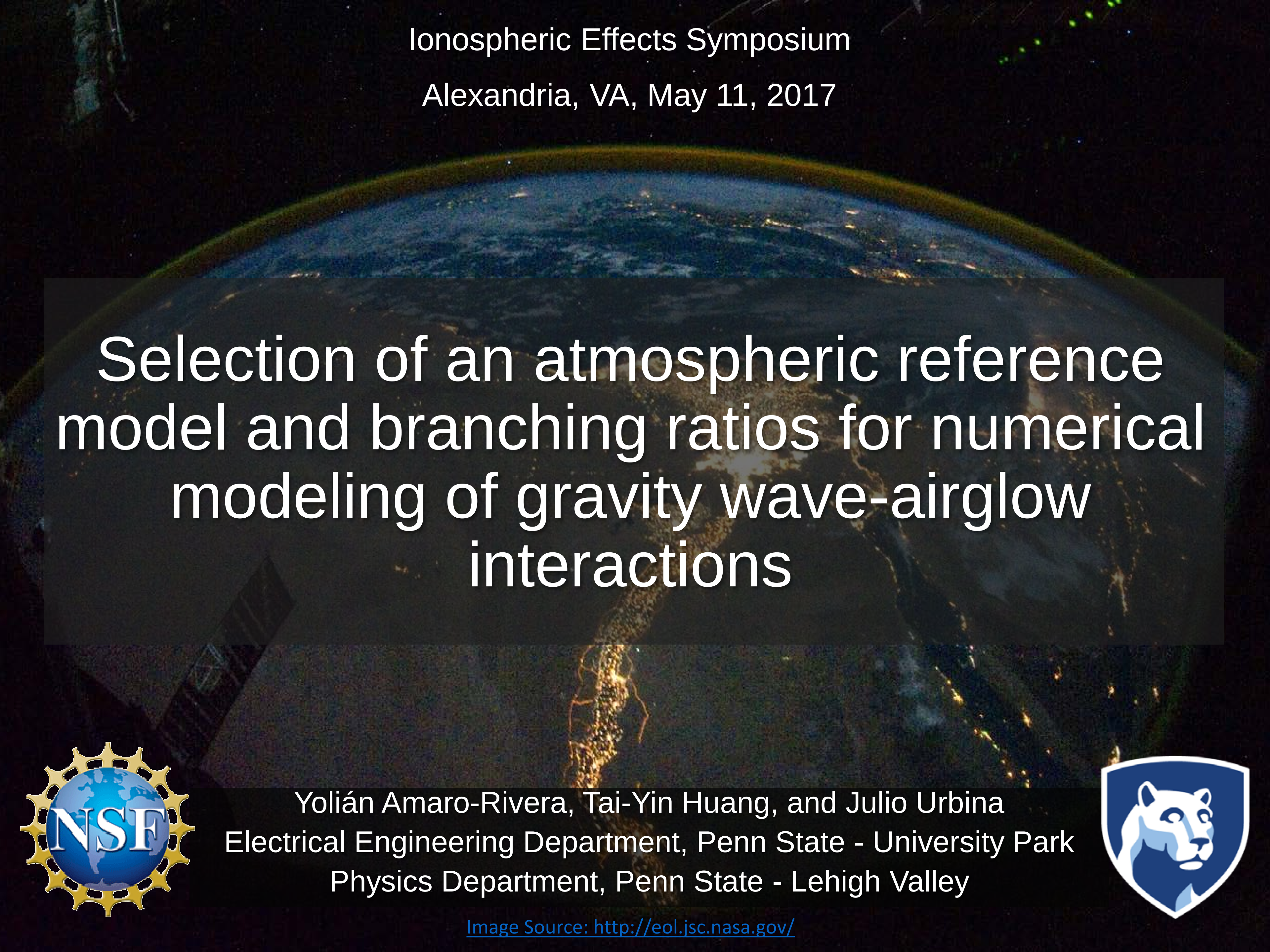

Ionospheric Effects Symposium

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Selection of an atmospheric reference model and branching ratios for numerical modeling of gravity wave-airglow interactions

Yolián Amaro-Rivera, Tai-Yin Huang, and Julio Urbina
Electrical Engineering Department, Penn State - University Park
Physics Department, Penn State - Lehigh Valley

Image Source: http://eol.jsc.nasa.gov/

Outline

Gravity Waves and Airglow

Chemistry Dynamics Model Description

Reference Model in Gravity-Wave Airglow Modeling

Determination of Branching Ratios

Conclusions

Gravity Wave-Airglow Interactions

- **Airglow is very sensitive to the atmospheric conditions** so understanding the variations helps us better understand our atmosphere.

- **Gravity waves can induce variations in atmospheric species and temperature**, leading to variations in airglow intensity & temperature.

- Studying **gravity wave-airglow interactions helps us gain a better understanding of the dynamical and chemical processes, and the energetics** in that region.

Airglow Emissions of Interest

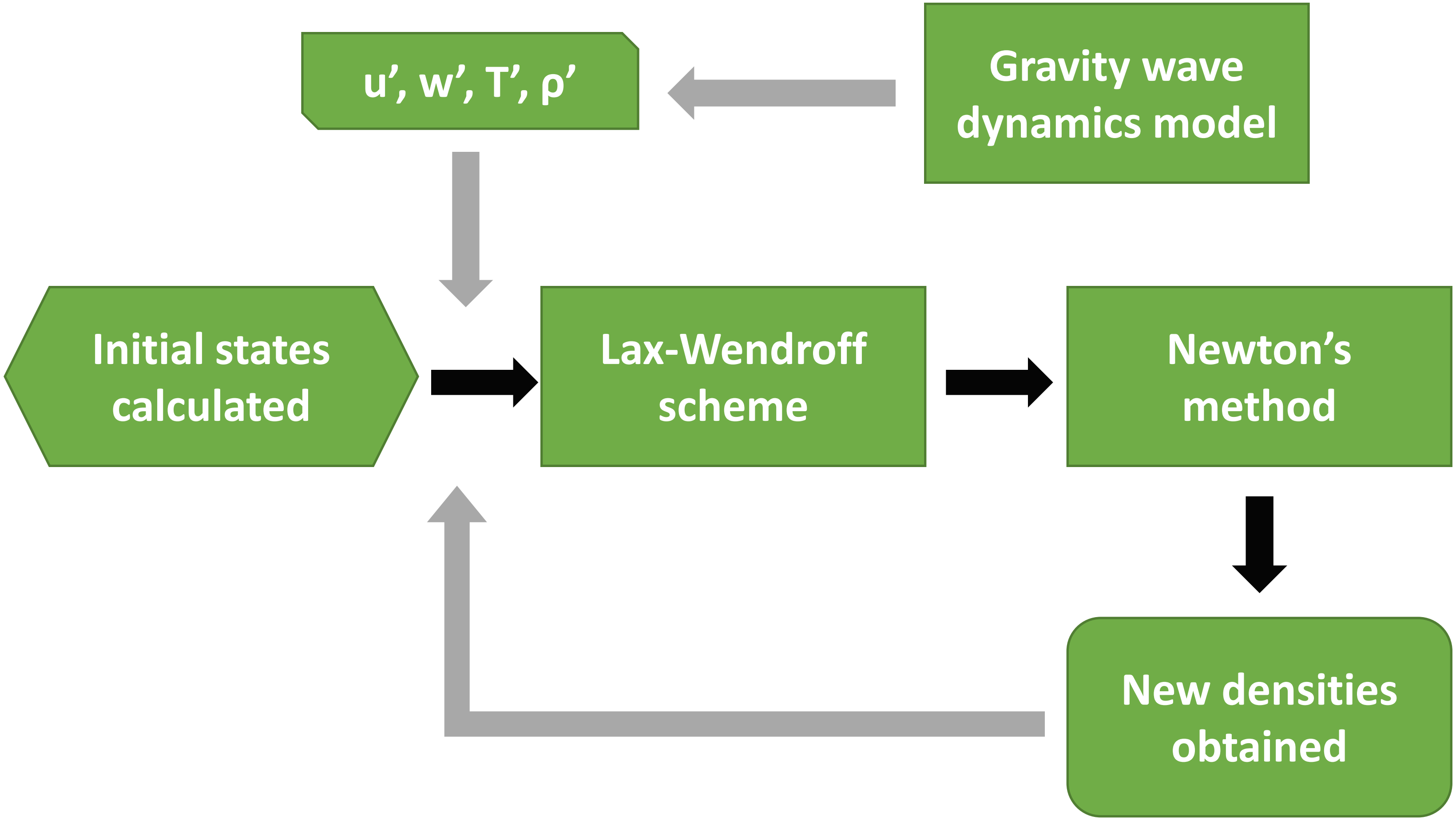
Green line O(^{1}S) (97 km), λ =557.7 nm

O_2(0-0) atmospheric bands (95 km), λ=762 nm

O_2(0-1), λ=864 nm

OH Meinel bands (87 – 92 km), λ =600-2000 nm

2D Airglow Chemistry Dynamics Model



Gravity wave dynamics model

u’, w’, T’, ρ’

Initial states calculated

Lax-Wendroff scheme

Newton’s method

New densities obtained

Boundary and Initial Conditions

Upper Boundary:	130 km
Lower Boundary:	70 km
Horizontal Grid Spacing:	1 km
Vertical Grid Spacing:	0.1 km
Lateral Boundary:	periodic
Time Step:	3 secs
Wave Forcing:	set at 10 km
Reference Model:	GS data, MSIS-90, MSIS-00

Multiple Airglow Chemistry Dynamics (MACD)

- 2-D, nonlinear, time dependent
- 5 minor species are considered: O, O2C, O2B0, O2B1, and O1S

Three versions of the MACD model:

1. **MACD**: uses O from Garcia and Solomon (1985) model and MSIS-90
2. **MACD-90**: uses MSIS-90
3. **MACD-00**: uses NRLMSIS-00

Initial profiles of O2C, O2B0, and O2B1 are obtained from the chemical balance

OH Airglow Chemistry Dynamics (OHCD)

- 2-D, nonlinear, time dependent
- 6 minor species are considered: O, O3, H, HO2, OH, and OH*

Three versions of the OHCD model:

1. **OHCD**: uses O and H from Garcia and Solomon (1985) model and MSIS-90
2. **OHCD-90**: uses MSIS-90
3. **OHCD-00**: uses NRLMSIS-00

Initial profiles of O3, OH, OH*, and HO2 are obtained from the chemical balance

Recent Work using MACD and OHCD Models

- Gravity wave effects in O(1S), O_2(0,0), and OH(8,3) airglow emissions [Huang and George, 2014].

- Airglow temperature variations, phase relationships, and Krassovsky ratios [Huang, 2015].

- Effect of CO_2 increase and 11-year solar cycle in airglow emissions [Huang 2016, 2017].

- Reference model in gravity wave- airglow numerical models [Amaro-Rivera et al. 2017].

A reference model that provides initial profiles of atmospheric species and temperature is needed for numerical modeling of gravity wave-airglow interactions.

The Continuity Equation & Initial Tendency

In our models, we remove the initial tendency from the continuity equation to isolate the wave-induced effects. The continuity equation after removing the initial tendency is

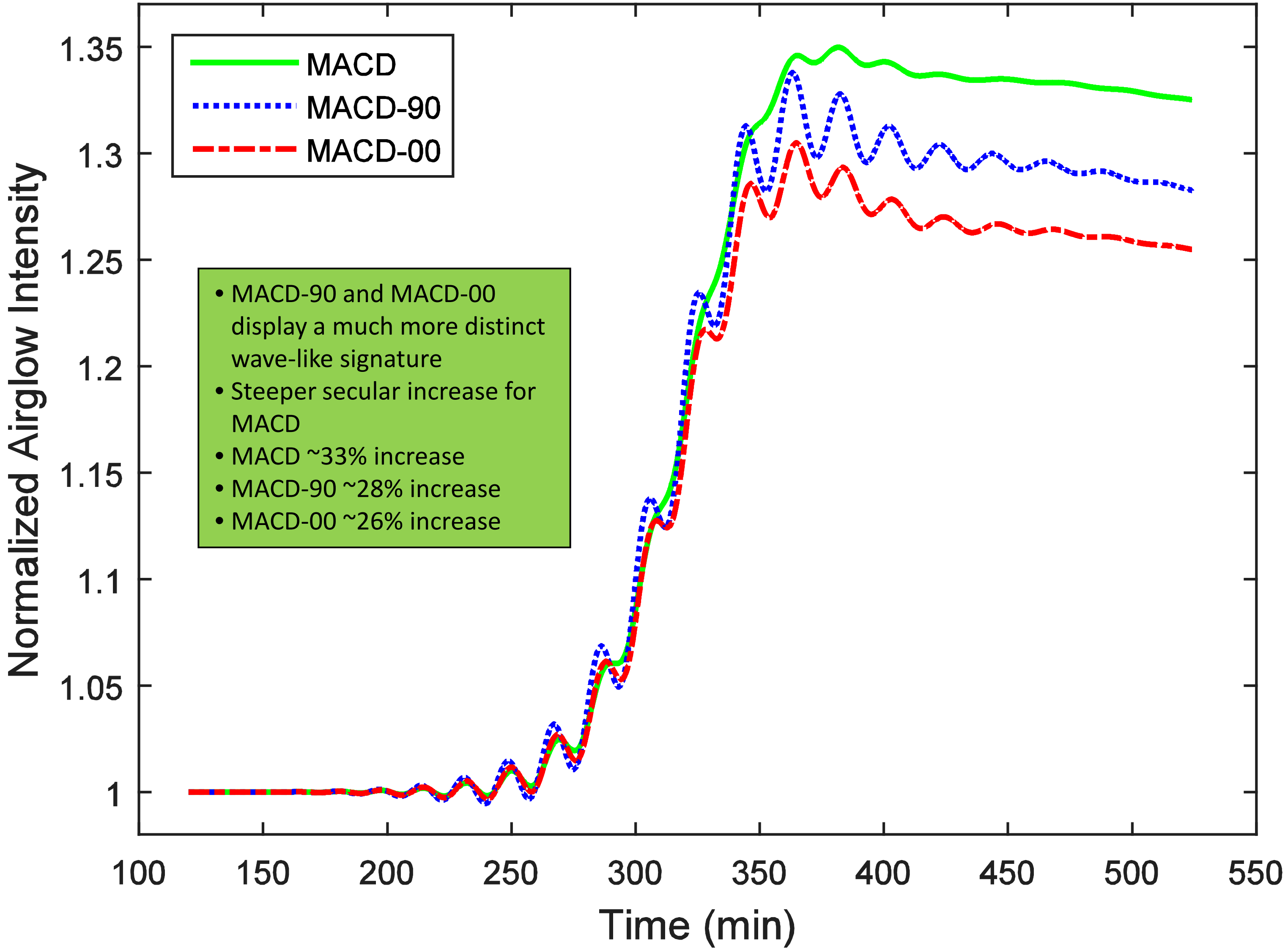
$$\frac{\partial n}{\partial t} = P - nL - \nabla \cdot (n\vec{V}) - (\frac{\partial n}{\partial t})_{t=0}$$

Secular variations are obtained by performing a running average, with the window size equal to one forcing wave period, to separate the total variation into two parts:

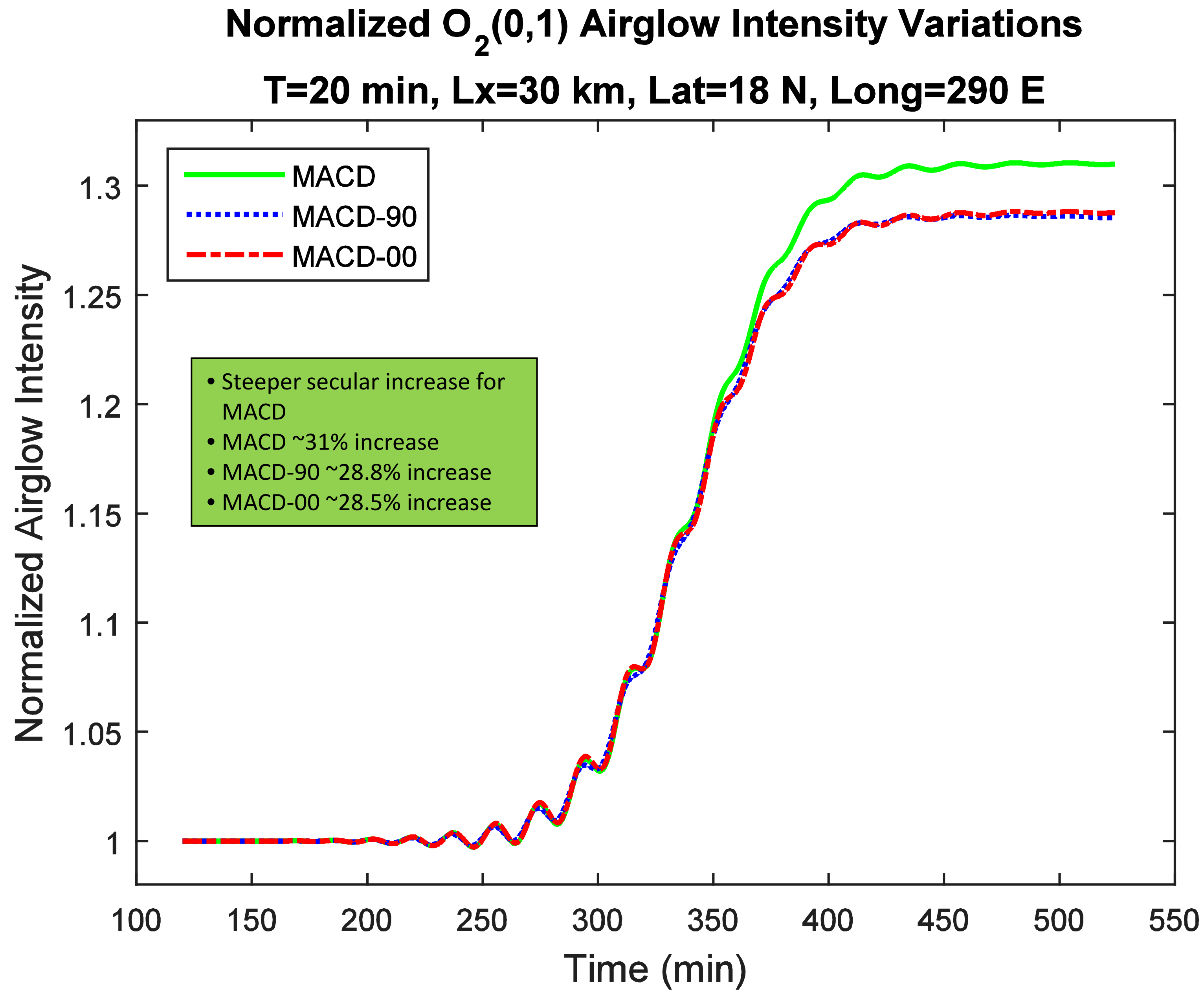
Total variation= secular part + fluctuating part

The fluctuating part oscillates at the forcing wave period while the secular part is the quantity that remains after the running average.

Normalized O(^{1}S) Airglow Intensity Variations
T=20 min, Lx=30 km, Lat=18 N, Long=290 E



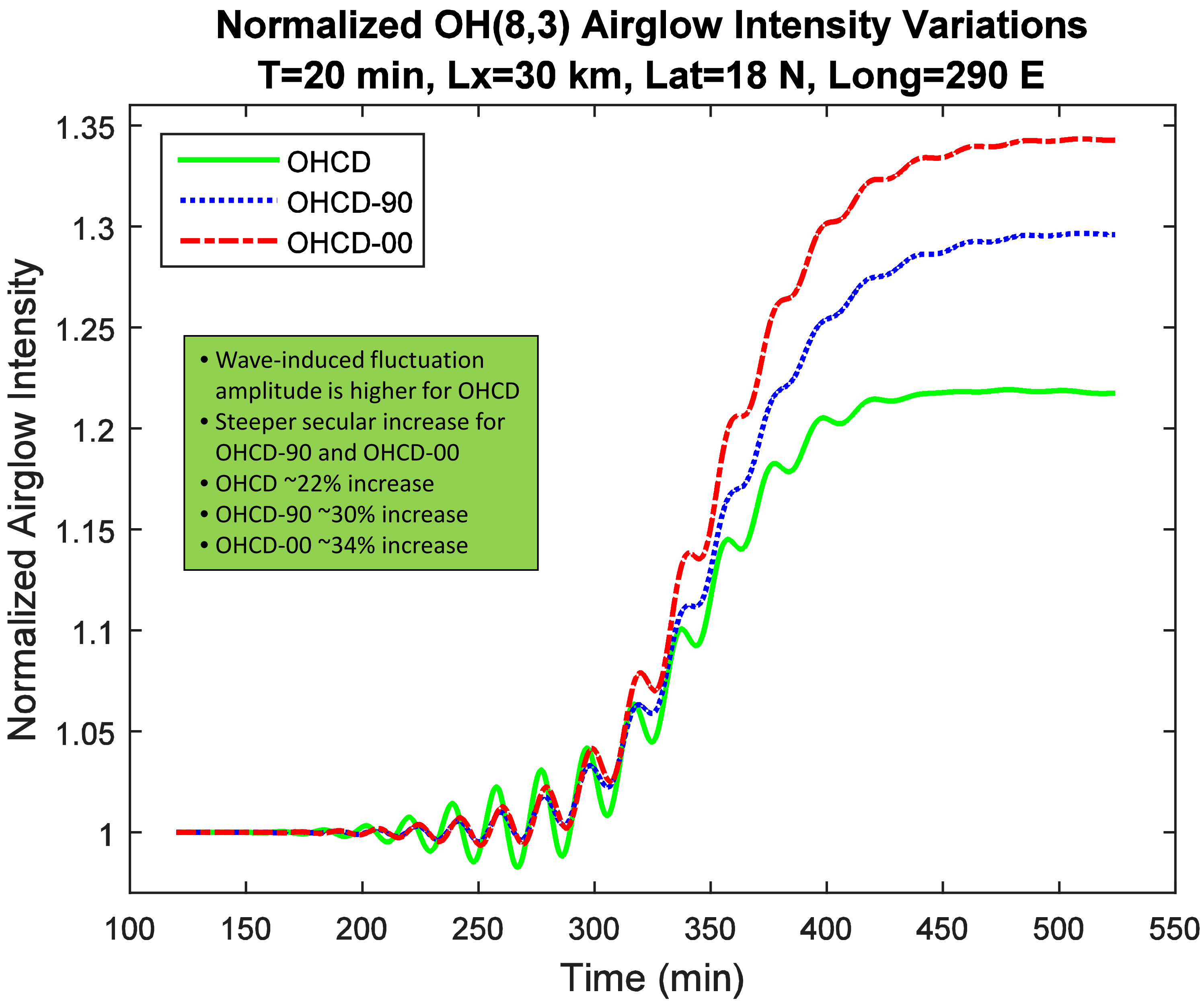
- MACD-90 and MACD-00 display a much more distinct wave-like signature
- Steeper secular increase for MACD
- MACD ~33% increase
- MACD-90 ~28% increase
- MACD-00 ~26% increase



Normalized O_2(0,1) Airglow Intensity Variations

T=20 min, Lx=30 km, Lat=18 N, Long=290 E

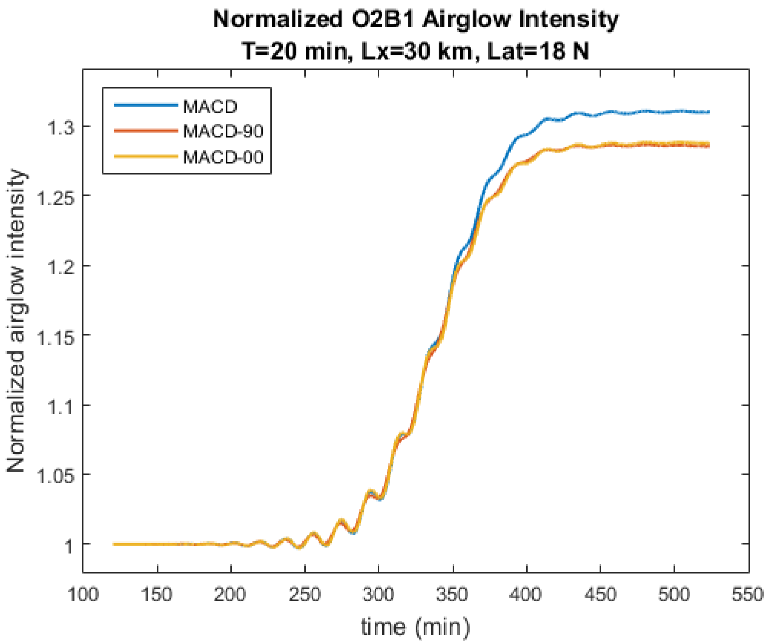
- Steeper secular increase for MACD
- MACD ~31% increase
- MACD-90 ~28.8% increase
- MACD-00 ~28.5% increase



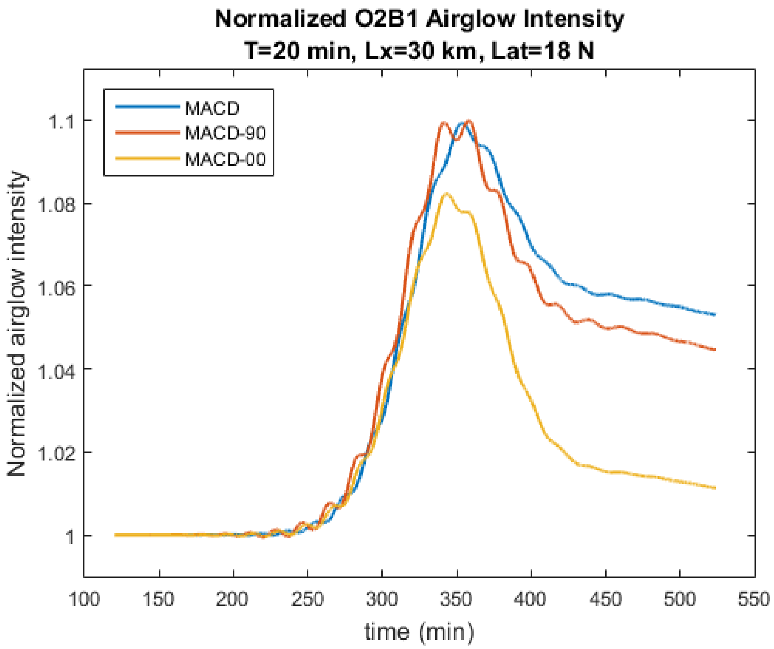
Normalized OH(8,3) Airglow Intensity Variations
T=20 min, Lx=30 km, Lat=18 N, Long=290 E

- Wave-induced fluctuation amplitude is higher for OHCD
- Steeper secular increase for OHCD-90 and OHCD-00
- OHCD ~22% increase
- OHCD-90 ~30% increase
- OHCD-00 ~34% increase

Rate coefficients are important!



α =0.04, ε=7x10^-5



α =0.04, ε=0.09

Branching Ratios Used in Literature

Reference	α	ε
Huang and George [2014]	0.04	7 x 10^{-5}
Snively et al. [2010]	0.03	-
Hickey et al. [1993]	0.8	0.11

In order to understand the wave dynamics or energetics, we first need to better understand airglow chemistry or rather an accurate set of airglow chemical reactions!

The O_2(0,0) Atmospheric Band & O(1S) Greenline Chemistry in the MACD Model

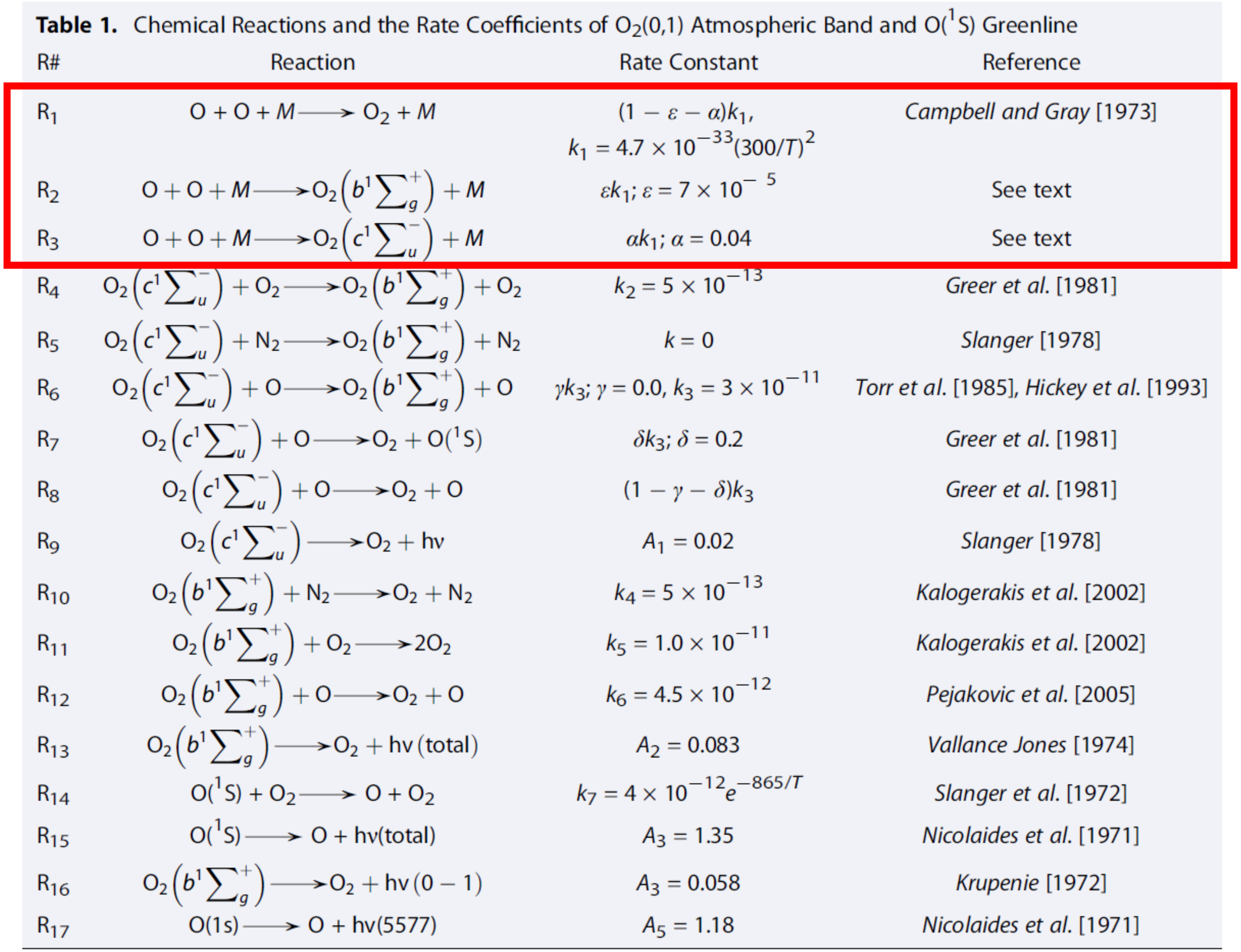
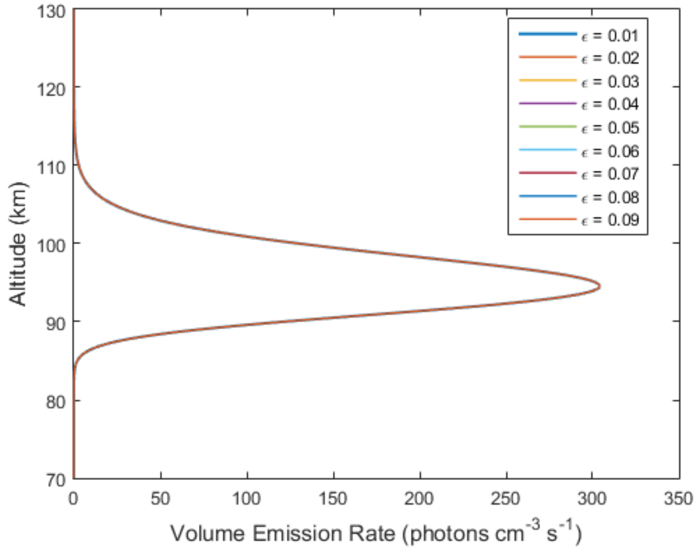


Table 1. Chemical Reactions and the Rate Coefficients of O_2(0,1) Atmospheric Band and O(^{1}S) Greenline

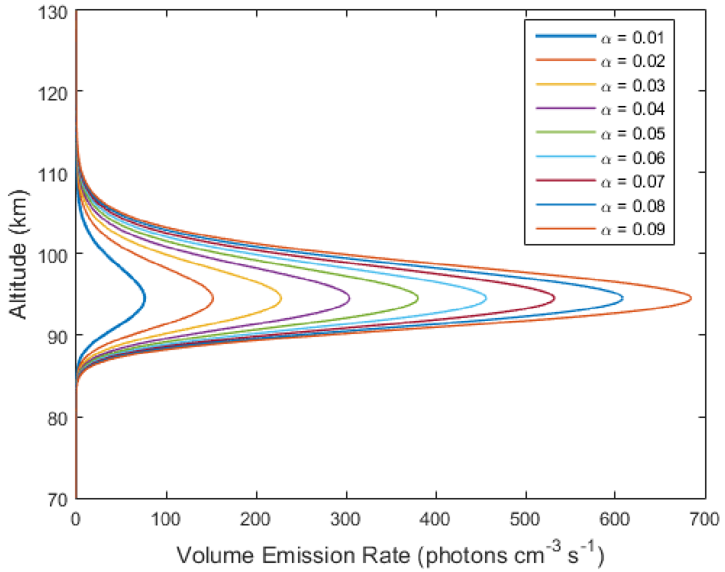
R#	Reaction	Rate Constant	Reference
R_1	$O + O + M \longrightarrow O_2 + M$	$(1 - \varepsilon - \alpha)k_1$, $k_1 = 4.7 \times 10^{-33}(300/T)^2$	*Campbell and Gray* [1973]
R_2	$O + O + M \longrightarrow O_2\left(b^1\Sigma_g^+\right) + M$	$\varepsilon k_1;\ \varepsilon = 7 \times 10^{-5}$	See text
R_3	$O + O + M \longrightarrow O_2\left(c^1\Sigma_u^-\right) + M$	$\alpha k_1;\ \alpha = 0.04$	See text
R_4	$O_2\left(c^1\Sigma_u^-\right) + O_2 \longrightarrow O_2\left(b^1\Sigma_g^+\right) + O_2$	$k_2 = 5 \times 10^{-13}$	*Greer et al.* [1981]
R_5	$O_2\left(c^1\Sigma_u^-\right) + N_2 \longrightarrow O_2\left(b^1\Sigma_g^+\right) + N_2$	$k = 0$	*Slanger* [1978]
R_6	$O_2\left(c^1\Sigma_u^-\right) + O \longrightarrow O_2\left(b^1\Sigma_g^+\right) + O$	$\gamma k_3;\ \gamma = 0.0,\ k_3 = 3 \times 10^{-11}$	*Torr et al.* [1985], *Hickey et al.* [1993]
R_7	$O_2\left(c^1\Sigma_u^-\right) + O \longrightarrow O_2 + O(^1S)$	$\delta k_3;\ \delta = 0.2$	*Greer et al.* [1981]
R_8	$O_2\left(c^1\Sigma_u^-\right) + O \longrightarrow O_2 + O$	$(1 - \gamma - \delta)k_3$	*Greer et al.* [1981]
R_9	$O_2\left(c^1\Sigma_u^-\right) \longrightarrow O_2 + h\nu$	$A_1 = 0.02$	*Slanger* [1978]
R_{10}	$O_2\left(b^1\Sigma_g^+\right) + N_2 \longrightarrow O_2 + N_2$	$k_4 = 5 \times 10^{-13}$	*Kalogerakis et al.* [2002]
R_{11}	$O_2\left(b^1\Sigma_g^+\right) + O_2 \longrightarrow 2O_2$	$k_5 = 1.0 \times 10^{-11}$	*Kalogerakis et al.* [2002]
R_{12}	$O_2\left(b^1\Sigma_g^+\right) + O \longrightarrow O_2 + O$	$k_6 = 4.5 \times 10^{-12}$	*Pejakovic et al.* [2005]
R_{13}	$O_2\left(b^1\Sigma_g^+\right) \longrightarrow O_2 + h\nu\,(\text{total})$	$A_2 = 0.083$	*Vallance Jones* [1974]
R_{14}	$O(^1S) + O_2 \longrightarrow O + O_2$	$k_7 = 4 \times 10^{-12} e^{-865/T}$	*Slanger et al.* [1972]
R_{15}	$O(^1S) \longrightarrow O + h\nu(\text{total})$	$A_3 = 1.35$	*Nicolaides et al.* [1971]
R_{16}	$O_2\left(b^1\Sigma_g^+\right) \longrightarrow O_2 + h\nu\,(0 - 1)$	$A_3 = 0.058$	*Krupenie* [1972]
R_{17}	$O(1s) \longrightarrow O + h\nu(5577)$	$A_5 = 1.18$	*Nicolaides et al.* [1971]

Huang and George, 2014

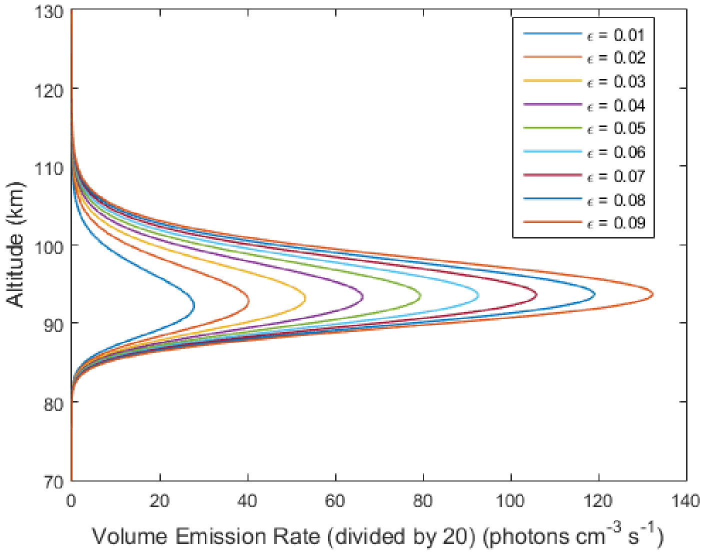
VER for O^1S with α = 0.04



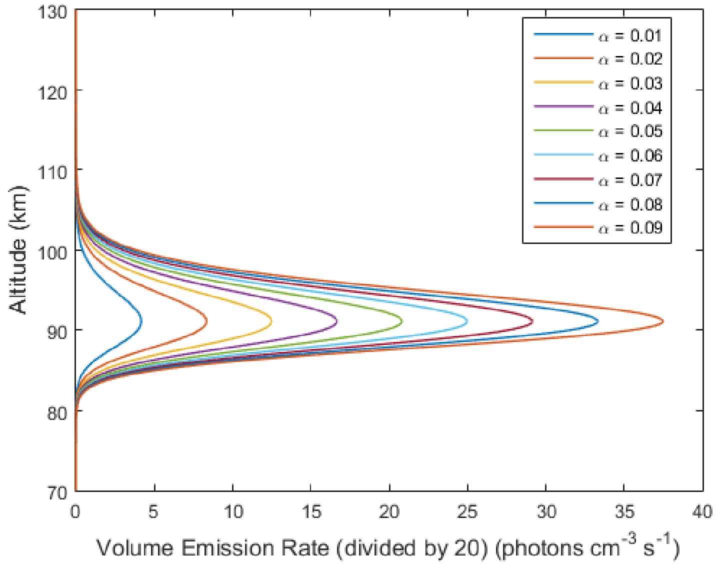
VER for O^1S with ϵ = 0.09

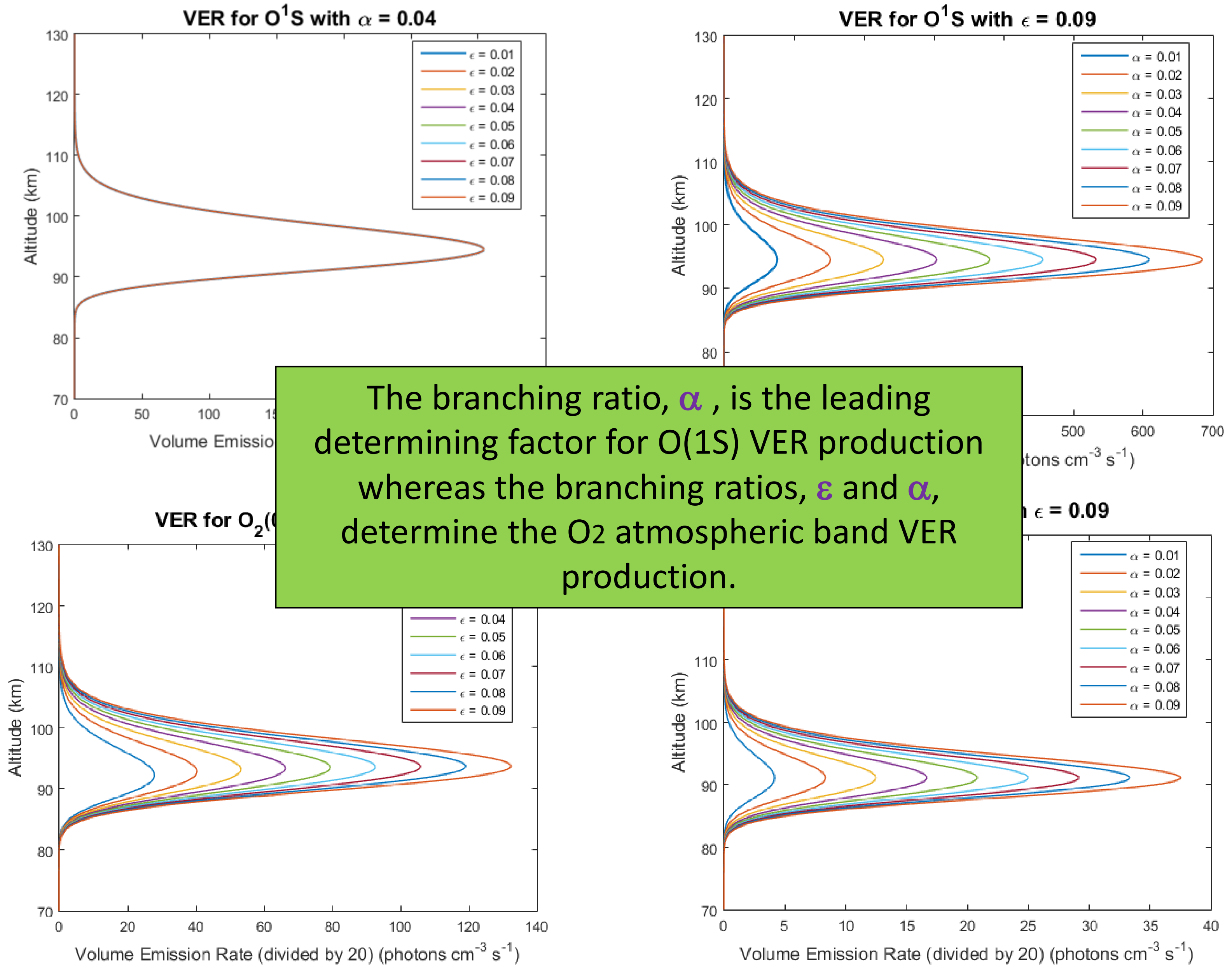


VER for $O_2(0,0)$ with α = 0.04



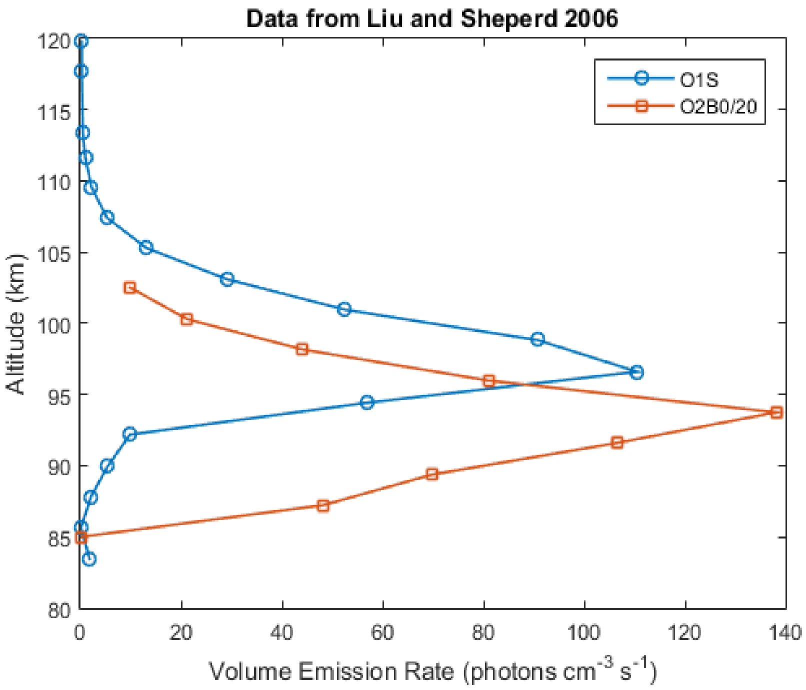
VER for $O_2(0,0)$ with ϵ = 0.09

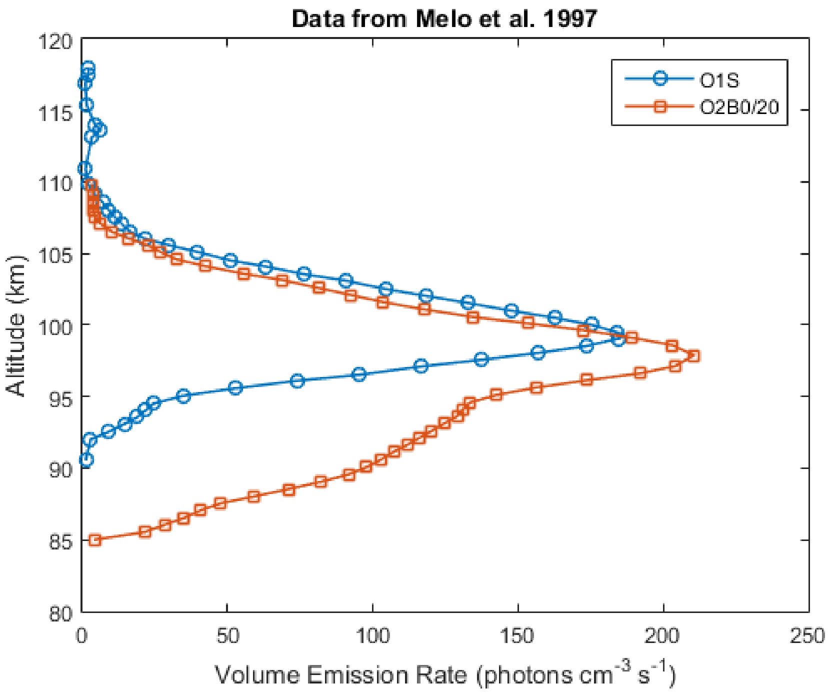




The branching ratio, α , is the leading determining factor for O(1S) VER production whereas the branching ratios, ε and α, determine the O2 atmospheric band VER production.

Airglow Measurements



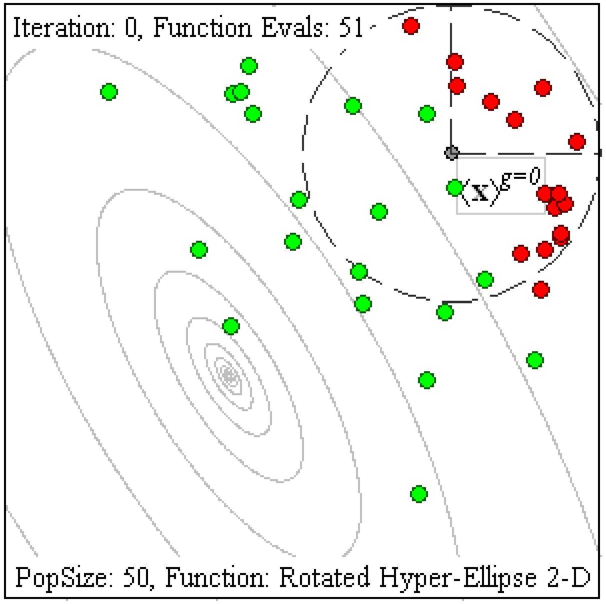


- Consecutive measurements of O1S and O2B0 airglow made with WINDII on Aug 27-28, 1992
- Latitude: 20.8S, Longitude: 162.8W
- Latitude: 21.4S, Longitude: 167.2W

- Simultaneous measurements of O1S and O2B0 airglow made with MULTIFOT rocket on May 31, 1992
- Latitude: 2.3S, 44.4W

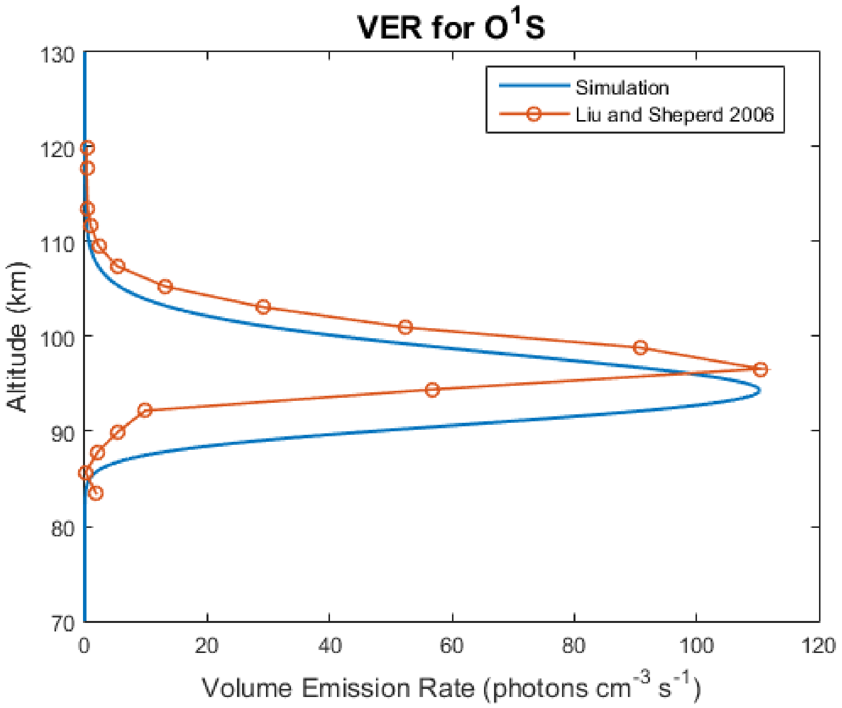
Determination of Branching Ratios using the Covariance Matrix Adaptation Evolution Strategy (CMA-ES)

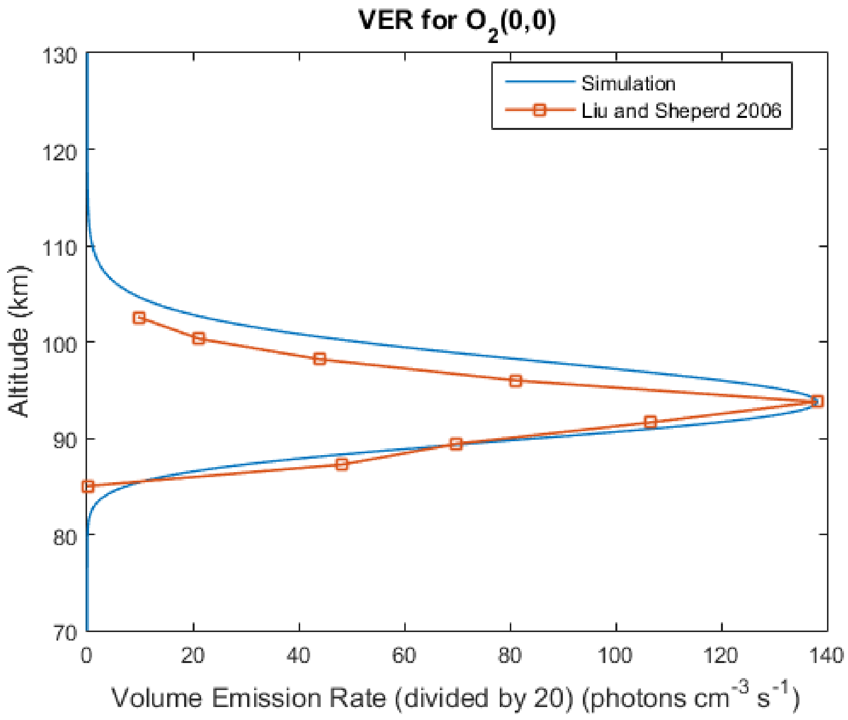
- CMA-ES
  - Performs real-valued single-objective optimization
  - Widely used algorithm
  - Population-based strategy
  - Self-adaptive



M. D. Gregory, Z. Bayraktar, and D. H. Werner, "Fast Optimization of Electromagnetic Design Problems Using the Covariance Matrix Adaptation Evolutionary Strategy," *IEEE Transactions on Antennas and Propagation*, Vol. 59, No. 4, pp. 1275-1285, April 2011.

CMA-ES (Best values: α=0.016 ε=0.109) WINDII

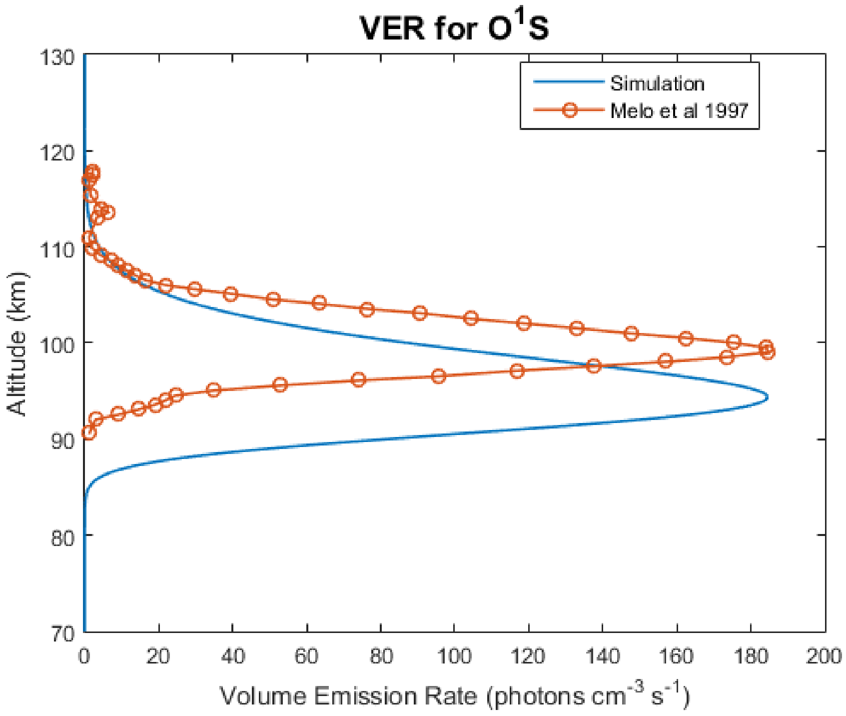


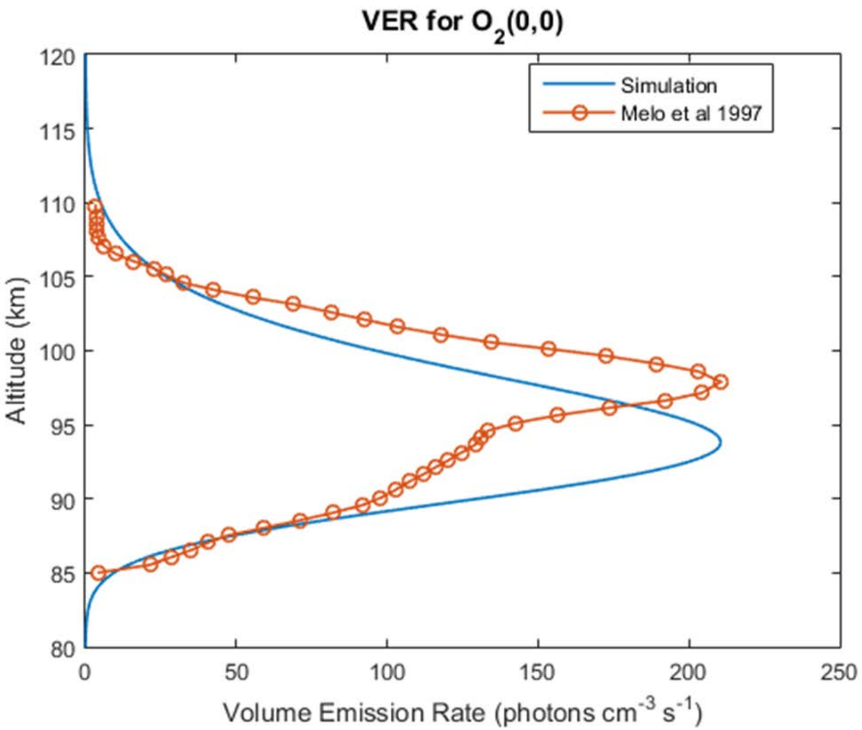


WINDII peak: 96.6 km
Simulation peak: 94.7 km

WINDII peak: 93.75 km
Simulation peak: 94.0 km

CMA-ES (Best values: α=0.018 ε= 0.121) MULTIFOT





MULTIFOT peak: 99.49 km
Simulation peak: 94.4 km

MULTIFOT peak: 97.89 km
Simulation peak: 94.0 km

Conclusions

- We present the results of our 2-D, nonlinear, time-dependent numerical models, Multiple Airglow Chemistry Dynamics (MACD) and OH Chemistry Dynamics (OHCD) when using different atmospheric reference models.
- We show how changes in temperatures and species concentrations indeed have a great impact in the computed airglow intensities.
- Using a numerical optimization approach, we match the simulated O(1S) and $O_2(0,0)$ VERs to the measured VERs from WINDII and MULTIFOT observations to determine optimal branching ratios.
- We found that the optimal values were $\alpha=0.02$, $\varepsilon=0.1$
- Future work includes expanding the MACD and OHCD models to study other airglow emissions.
- This includes incorporating chemical and dynamical processes that occur in the ionosphere.