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

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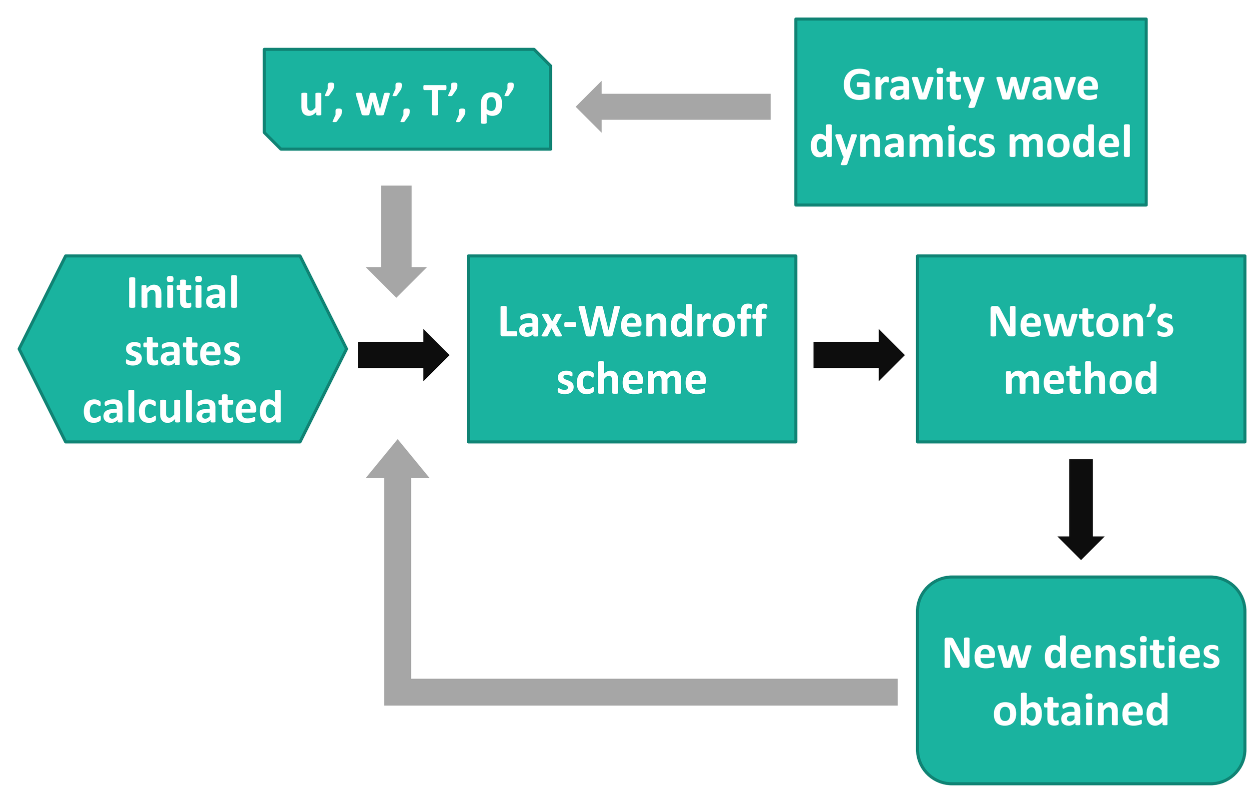
Introduction

- Because a change in the density of the species reacting in the airglow chemistry will undoubtedly produce changes in the airglow emissions, it is of great interest to investigate and assess the importance of the atmospheric reference model commonly used in modeling studies.
- The simulated wave-induced secular variations and fluctuations of O(^{1}S) greenline and O_2(0,0) atmospheric band change when different values are assigned to the branching ratios ε and α [Huang and George, 2014].
- There is currently a significant discrepancy in the values used for the branching ratios in the three-body recombination reaction. For instance, Hickey et al. [1993] use α = 0.8 and ε = 0.11, Snively et al. [2010] use α = 0.03, and Huang and George [2014] use α = 0.04 and ε = 7 × 10 $^{-5}$.

Chemistry Dynamics Model



Boundary and Initial Conditions:

- Lower boundary: 70 km
- Upper boundary: 130 km
- Lateral boundary: periodic, separated by one horizontal wavelength
- Vertical grid spacing: 0.1 km
- Horizontal grid spacing: 1 km
- Time step: 3 sec
- Wave forcing set at 10 km
- Major gases N_2 and O_2 and temperature at 18°N are obtained from MSIS-90 and NRLMSIS-00

Atmospheric reference model in gravity waves- airglow studies

I. Objective of the study

- Assess the impact of atmospheric reference model in gravity wave-airglow simulations.

II. Importance to the field

- Provides insight for the interpretation of airglow observations and for investigation of energy & momentum transfer in the atmosphere.

III. Case Study

This study presents the up-to-date model simulation results of gravity wave-induced airglow intensity variations and a comparison to previous results.

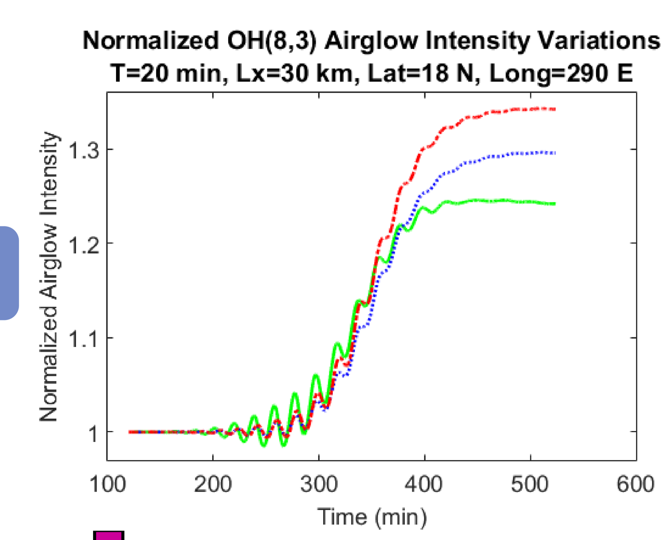
Multiple Airglow Chemistry Dynamics (MACD)

- 2D, nonlinear, time dependent
- **MACD**: uses O from GS model [1] & MSIS-90
- **MACD-90**: uses MSIS-90
- **MACD-00**: uses NRLMSIS-00

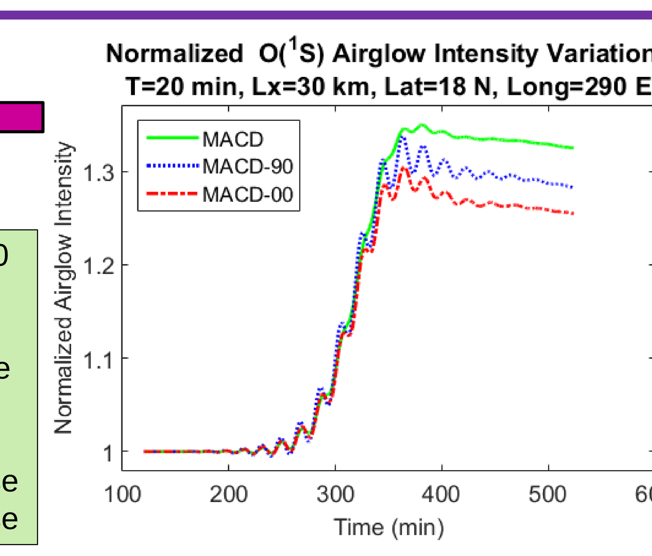
OH Airglow Chemistry Dynamics (OHCD)

- 2D, nonlinear, time dependent
- **OHCD**: uses O and H from GS model [1] & MSIS-90
- **OHCD-90**: uses MSIS-90
- **OHCD-00**: uses NRLMSIS-00

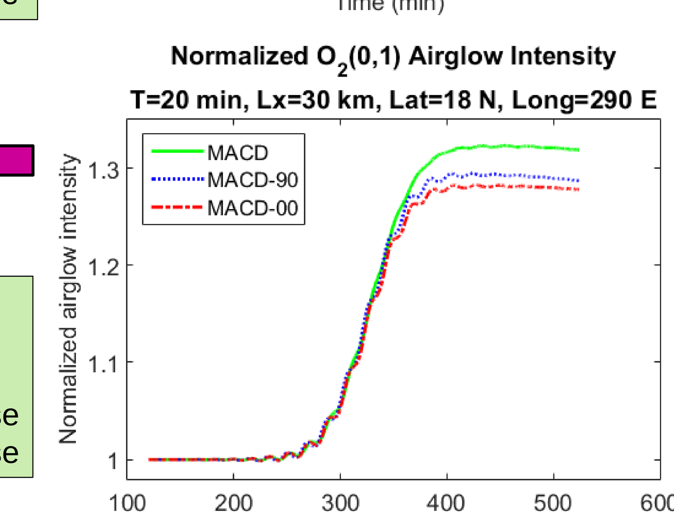
IV. Results



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



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



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

Using a numerical optimization approach to find branching ratios

I. Objectives of the study

- Estimate the set of branching ratios ε & α involved in the three-body recombination reactions.

II. Importance to the field

- Important for practical applications (i.e. atmospheric models) and to understand fundamental chemistry mechanisms.

III. Methodology

- CMA-ES
  - Bio-inspired algorithm
  - Performs real-valued single-objective optimization
  - Population-based strategy
  - Self-adaptive

Three-body recombination reactions

R#	Reaction	Rate Constant
R_1	$O + O + M \longrightarrow O_2 + M$	$(1 - \varepsilon - \alpha)k_1$, $k_1 = 4.7 \times 10^{-33}(300/T)^2$
R_2	$O + O + M \longrightarrow O_2\left(b^1\sum_g^+\right) + M$	εk_1; $\varepsilon =$?
R_3	$O + O + M \longrightarrow O_2\left(c^1\sum_u^-\right) + M$	αk_1; $\alpha =$?

IV. Observations

Ref	Source	Date	Lat, Long	Branching Ratios found by CMA-ES	
[2]	OXYGEN/S35	2/7/1981	67.9°N, 21.1°E	ε = 0.6720	α = 0.0930
	S310.10	8/24/1981	31.2°N, 131.1°E	ε = 0.2233	α = 0.0295
	ETON	3/23/1982	57.4°N, 7.4°W	ε = 0.2300	α = 0.0208
	OASIS	6/11/1983	32.4°N, 106.3°W	ε = 0.6378	α = 0.1476
	SOAP/WINE	2/10/1984	67.9°N, 21.1°E	ε = 0.1181	α = 0.0041
[3]	MULTIFOT	5/31/1992	2.3°S, 44.4°W	ε = 0.1445	α = 0.0225
[4]	WINDII	8/27/1992	20.8°S, 162.8°W	ε= 0.1082	α= 0.0157
		8/28/1992	21.4°S, 167.2°W		

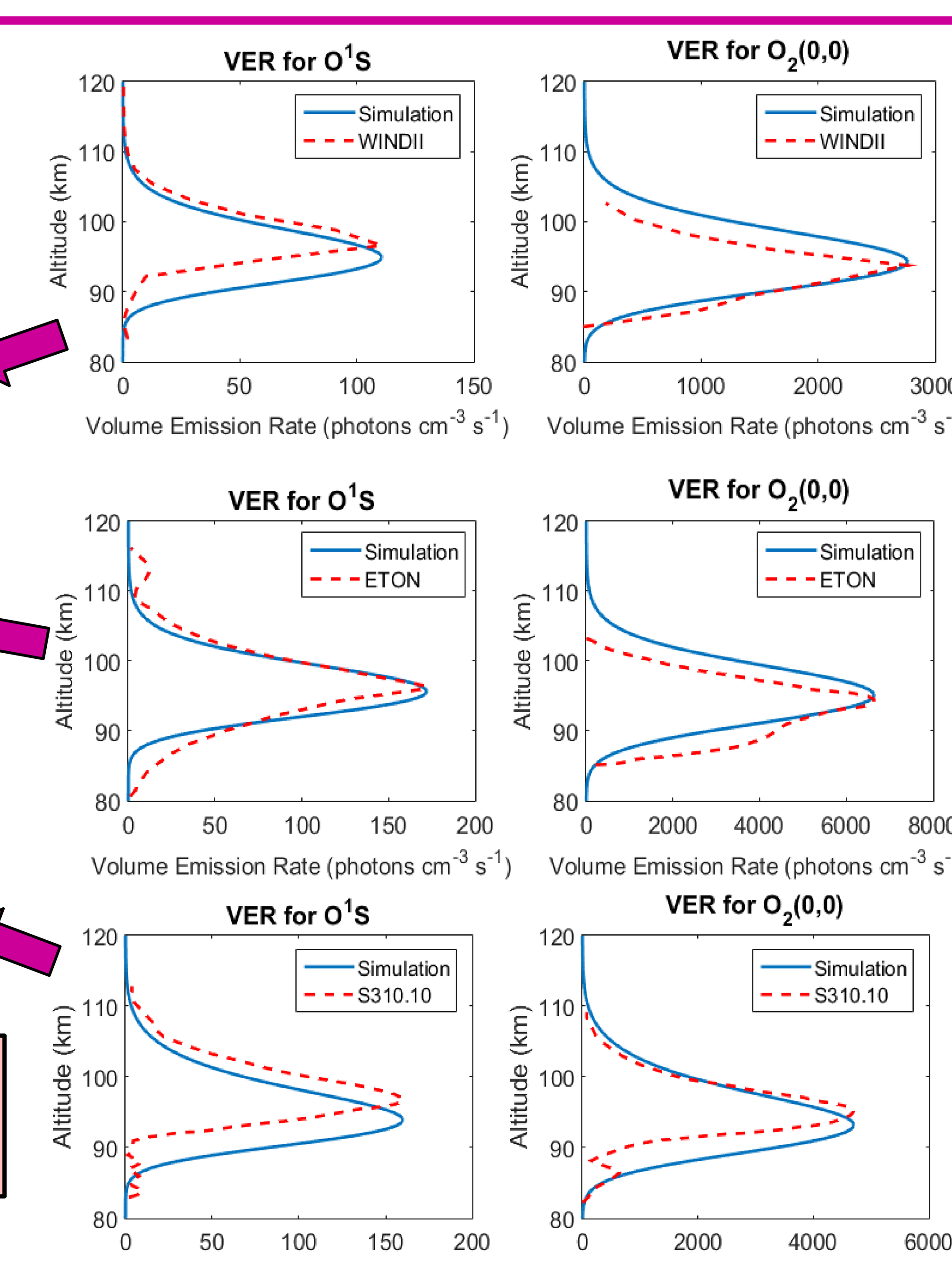
V. Results

- Good agreement between observations and simulation.
- O(^{1}S) altitude diff: 1.6 km
- O_2(0,0) altitude diff: 0.45 km

- O(^{1}S) simulated VER profile in good agreement with observations.
- O(^{1}S) altitude diff: 0.69 km
- O_2(0,0) altitude diff: 0.55 km

- O(^{1}S) altitude diff: 2.49 km
- O_2(0,0) altitude diff: 1.9 km

- Excellent agreement for the peak VER values
- Average branching ratios values: **ε = 0.1648** and **α = 0.0185**



Conclusions

- We present the up-to-date results of our numerical model.
- We show how changes in temperatures and species concentrations indeed have a great impact in the computed airglow intensities.
- Using a numerical optimization approach (CMA-ES), we match the simulated O(^{1}S) and O_2(0,0) VERs to VERs from observations to find optimal set of branching ratios.
- We found that the average values for the branching ratios were **ε =0.1648** and **α = 0.0185.**

References

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