Numerical Simulations of Gravity Waves' Effects on Airglow Emissions

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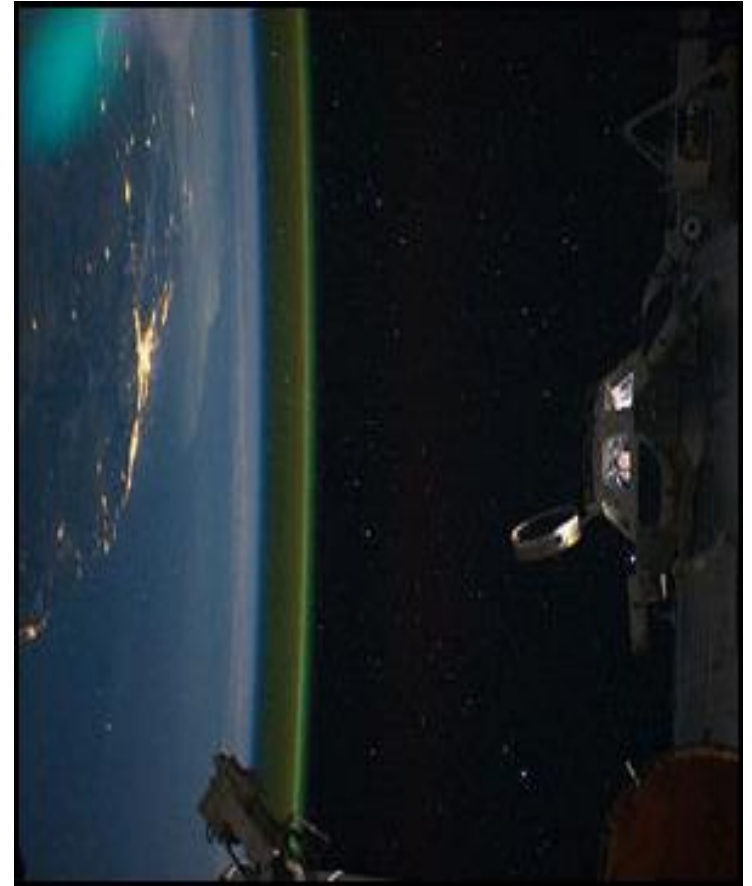**University Park, May 16- 20, 2016**

What is atmospheric airglow?

- Atmospheric airglow is weak emission of light by excited atoms or molecules above 80 km. In the MLT region, various airglow emissions are mainly emitted by neutral particles.

Airglow in the MLT region:

- Na layer (85 km), λ=589 nm
- OH Meinel bands (87 – 92 km), λ=600-2000 nm
- Green line O(1s) (97 km), λ=557.7 nm
- O2 (0-0) atmospheric bands (95 km), λ=762 nm, not observable from the ground
- O2(0-1), λ=864 nm

http://spaceflight.nasa.gov/gallery/images/station/crew-28/html/iss028e050185.html

Why Do We Study Atmospheric Airglow?

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

- Understanding the density and temperature variations caused by gravity waves provides important information for space vehicles.

- Understanding OH airglow variations provides a better guidance for heat-seeking flying objects because some of the OH airglow emissions are in the near infrared.

- Studying both gravity waves and airglow variations helps us gain a better understanding of the dynamical and chemical processes, and energetics in that region.

Our Approach: We use numerical simulations for virtual experiments with a dynamics model coupled with chemistry models

- A Spectral Full Wave Model (SFWM) simulates a propagating, dissipative gravity wave packet originating from the lower atmosphere [Hickey et al., 2000].

- It produces wave perturbed quantities (ρ', T', u', v') to be input to the chemistry models.

- The OHCD model consists of an OH chemistry model and the SFWM [Huang and Hickey, 2007; 2008] .

- The MACD model consists of a Multiple Airglow Chemistry model of O(1S) and O2(0,1) nightglow and the SFWM [Huang and George, 2014; Huang, 2015] .

- The OHCD and MACD models are 2-D, nonlinear, and time-dependent.

The 2D OH Airglow Chemistry-Dynamics Model
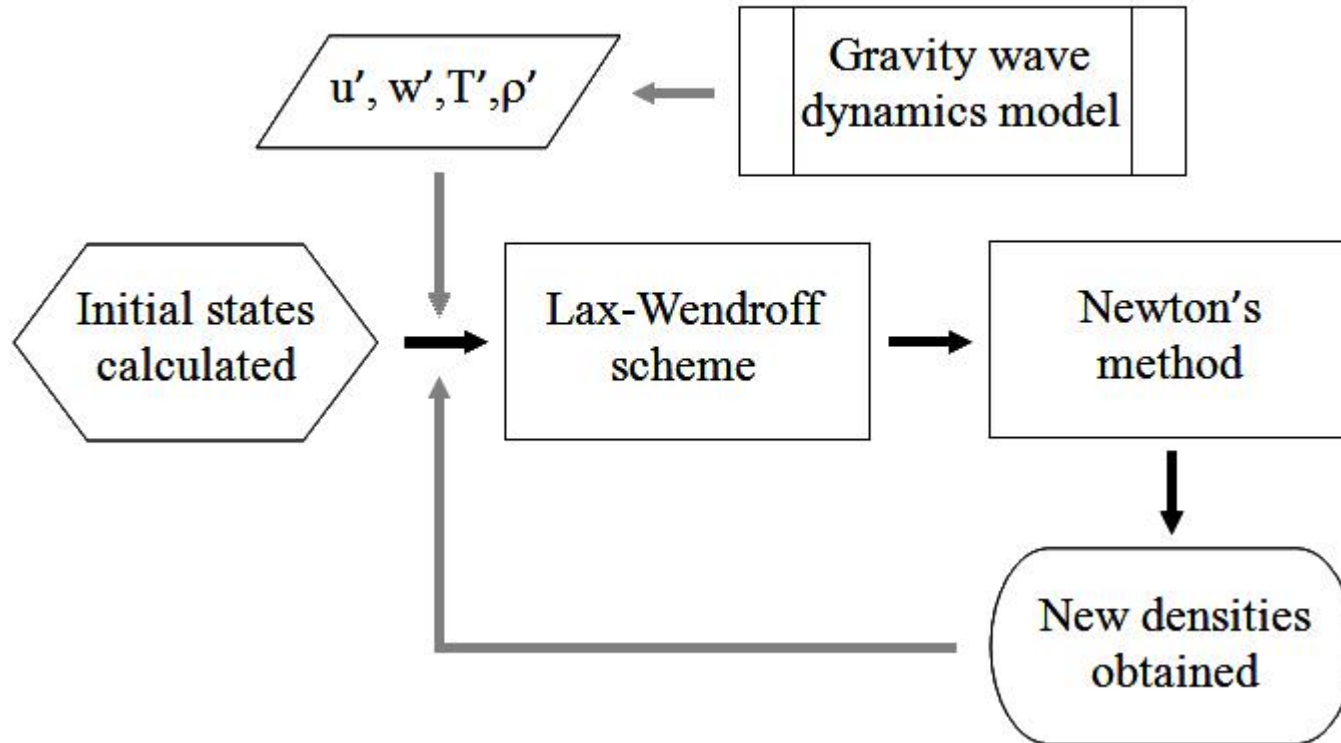
- We use Lax-Wendroff scheme to calculate flux and horizontal advection terms and Newton's method to calculate chemical P & L, and vertical advection terms.

- The chemistry models solve the continuity equation for each species and obtain the time evolution of the species.

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

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	$O + O + M \longrightarrow O_2(b^1\sum_g^+) + M$	$\varepsilon k_1 ; \varepsilon = 7 \times 10^{-5}$	Campbell and Gray (1973)
R_3	$O + O + M \longrightarrow O_2(c^1\sum_u^-) + M$	$\alpha k_1 ; \alpha = 0.04$	Campbell and Gray (1973)
R_4	$O_2(c^1\sum_u^-) + O_2 \longrightarrow O_2\left(b^1\sum_g^+\right) + O_2$	$k_2 = 5 \times 10^{-13}$	Greer et al. (1981)
R_5	$O_2(c^1\sum_u^-) + N_2 \longrightarrow O_2\left(b^1\sum_g^+\right) + N_2$	$k = 0$	Slanger (1978)
R_6	$O_2(c^1\sum_u^-) + O \longrightarrow O_2(b^1\sum_g^+) + O$	$\gamma k_3 ; \gamma = 0.0,$ $k_3 = 3 \times 10^{-11}$	Greer et al. (1981)
R_7	$O_2(c^1\sum_u^-) + O \rightarrow O_2 + O(1s)$	$\delta k_3 ; \delta = 0.2$	Greer et al. (1981)
R_8	$O_2(c^1\sum_u^-) + O \longrightarrow O_2 + O$	$(1 - \gamma - \delta)k_3$	Greer et al. (1981)
R_9	$O_2(c^1\sum_u^-) \longrightarrow O_2 + h\nu$	$A_1 = 0.02$	Slanger (1978)
R_{10}	$O_2(b^1\sum_g^+) + N_2 \longrightarrow O_2 + N_2$	$k_4 = 5 \times 10^{-13}$	Kalogerakis et al. (2002)
R_{11}	$O_2(b^1\sum_g^+) + O_2 \longrightarrow 2O_2$	$k_5 = 1.0 \times 10^{-11}$	Kalogerakis et al. (2002)
R_{12}	$O_2(b^1\sum_g^+) + O \longrightarrow O_2 + O$	$k_6 = 4.5 \times 10^{-12}$	Pejakovic et al. (2005)
R_{13}	$O_2(b^1\sum_g^+) \longrightarrow O_2 + h\nu(total)$	$A_2 = 0.083$	Vallance Jones (1974)
R_{14}	$O(1s) + O_2 \rightarrow O + O_2$	$k_7 = 4 \times 10^{-12}e^{-865/T}$	Slanger et al. (1972)
R_{15}	$O(1s) \rightarrow O + h\nu(total)$	$A_3 = 1.35$	Nicolaides et al. (1971)
R_{16}	$O_2(b^1\sum_g^+) \longrightarrow O_2 + h\nu(0-1)$	$A_3 = 0.058$	Krupenie (1972)
R_{17}	$O(1s) \rightarrow O + h\nu(5577)$	$A_5 = 1.18$	Nicolaides et al. (1971)

The OH(8,3) Nightglow Chemistry in the OHCD Model

Reaction	Rate Coefficient	Enthalpy

1. $O + OH(v=0) \longrightarrow H + O_2$ $4 \, x10^{-11}$ $\Delta E_1 = -16.77$

2. $H + O_2 + M \longrightarrow HO_2 + M$ $2.1 \, x10^{-32} \exp(290/T)$ $\Delta E_2 = -49.1$

3. $O + HO_2 \longrightarrow OH(v=0) + O_2$ $4 \, x10^{-11}$ $\Delta E_3 = -53.27$

4. $O + O + M \longrightarrow O_2 + M$ $4.7 \, x10^{-33} \left(300/T\right)^2$ $\Delta E_4 = -119.4$

5. $O + O_2 + M \longrightarrow O_3 + M$ $1.0 \, x10^{-34} \exp(510/T)$ $\Delta E_5 = -25.47$

6. $H + O_3 \longrightarrow OH^*(v=8) + O_2$ $1.4 \, x10^{-10} \exp(-470/T)*0.27$ $\Delta E_6 = -76.90$

7. $H + O_3 \longrightarrow OH(v=0) + O_2$ $1.4 \, x10^{-10} \exp(-470/T)*0.73$

8. $OH^*(v=8) \longrightarrow OH(v=3) + h\nu$ 0.569

9. $OH*(v=8) + O \longrightarrow H + O_2$ $2.5 \, x10^{-10}$ $\Delta E_7 = -16.77$

10. $OH^*(v=8) + O_2 \longrightarrow OH(v-1) + O_2$ $8.0 \, x10^{-12}$

11. $OH^*(v=8) + N_2 \longrightarrow OH(v-1) + N_2$ $7.0 \, x10^{-13}$

Rate constants are in units of cm^6s^{-1} for termolecular reactions and cm^3s^{-1} for bimolecular reactions; enthalpies in kcal/mole

The Continuity Equation & The Initial Tendency

The continuity equation for minor species is $\quad \dfrac{\partial n}{\partial t} = P - nL - \nabla \cdot (n \vec{V})$

In our models, we first calculate the initial tendency

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

Then we remove the initial tendency from the continuity equation to isolate the wave-induced effects. The continuity equation after removing the initial tendency is

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

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.

Boundary and Initial Conditions

- Upper boundary at 130 km, in diffusive equilibrium

- Lower boundary at 70 km, constant number densities

- 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 from MSIS-90.

- Initial number densities of O and H at 18 N are from observations [Garcia and Solomon, 1985].

- The rest of the species are obtained from the requirement of chemical equilibrium.

Current Topics of Investigation

- Secular variation and fluctuation of minor species

- Secular variation and fluctuation of airglow emissions and airglow temperatures

- Exothermic heating variations

- Phase relationship

- Krassovsky ratio

- Species and airglow variations induced by the increase of CO_2 and solar variation

Wave-induced variations of minor species

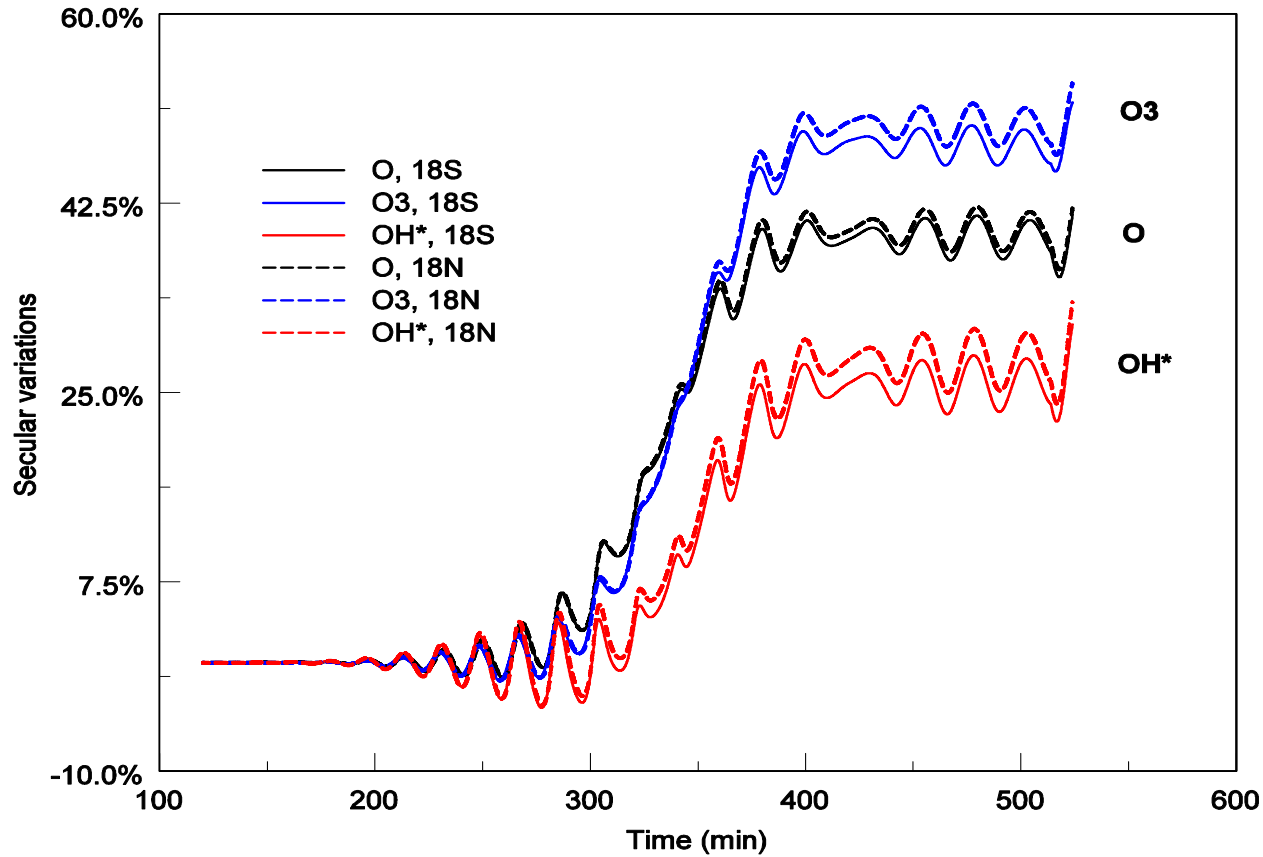## Initial and final profiles - OH chemistry

T=20 min, Lx=30 km, Lat=18 N
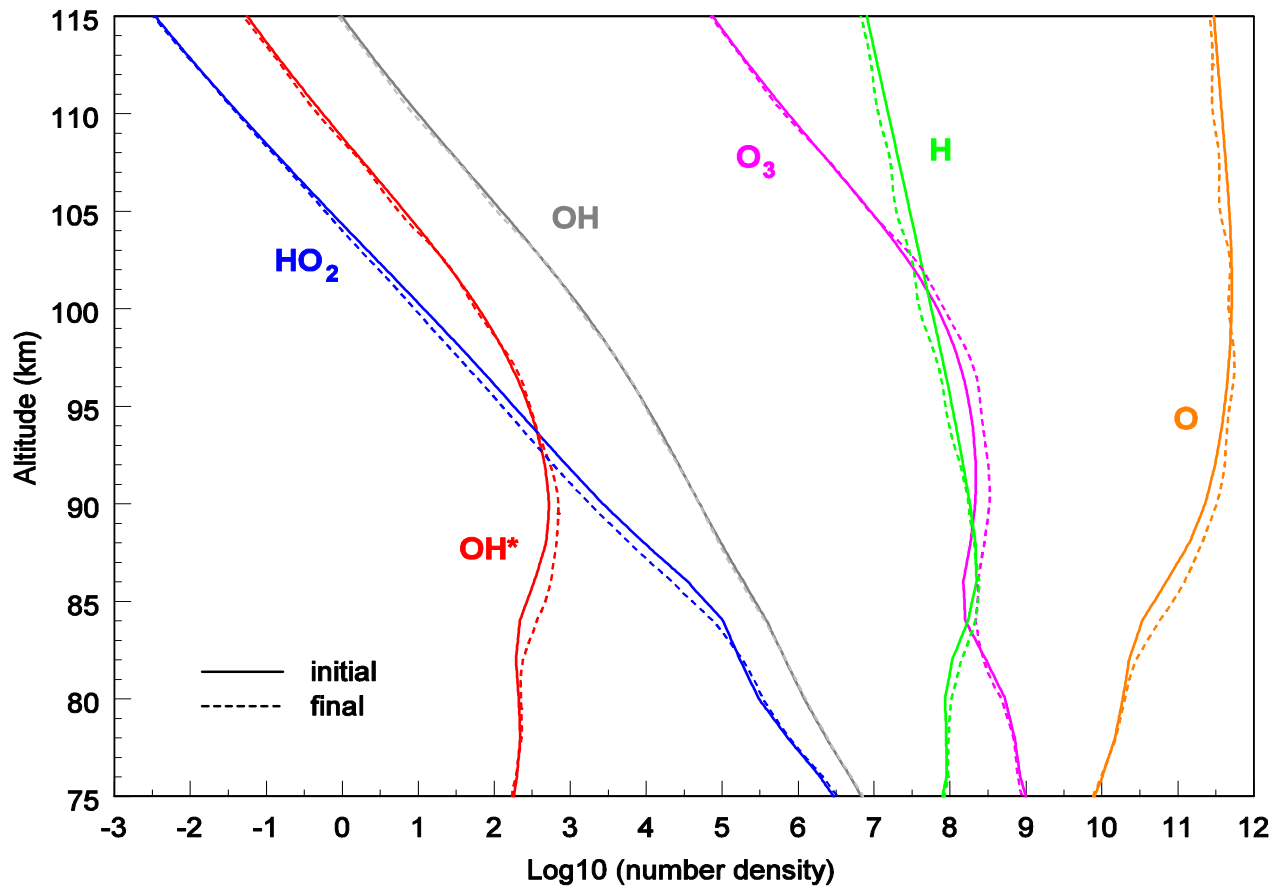
From OHCD

Wave-induced variations of minor species

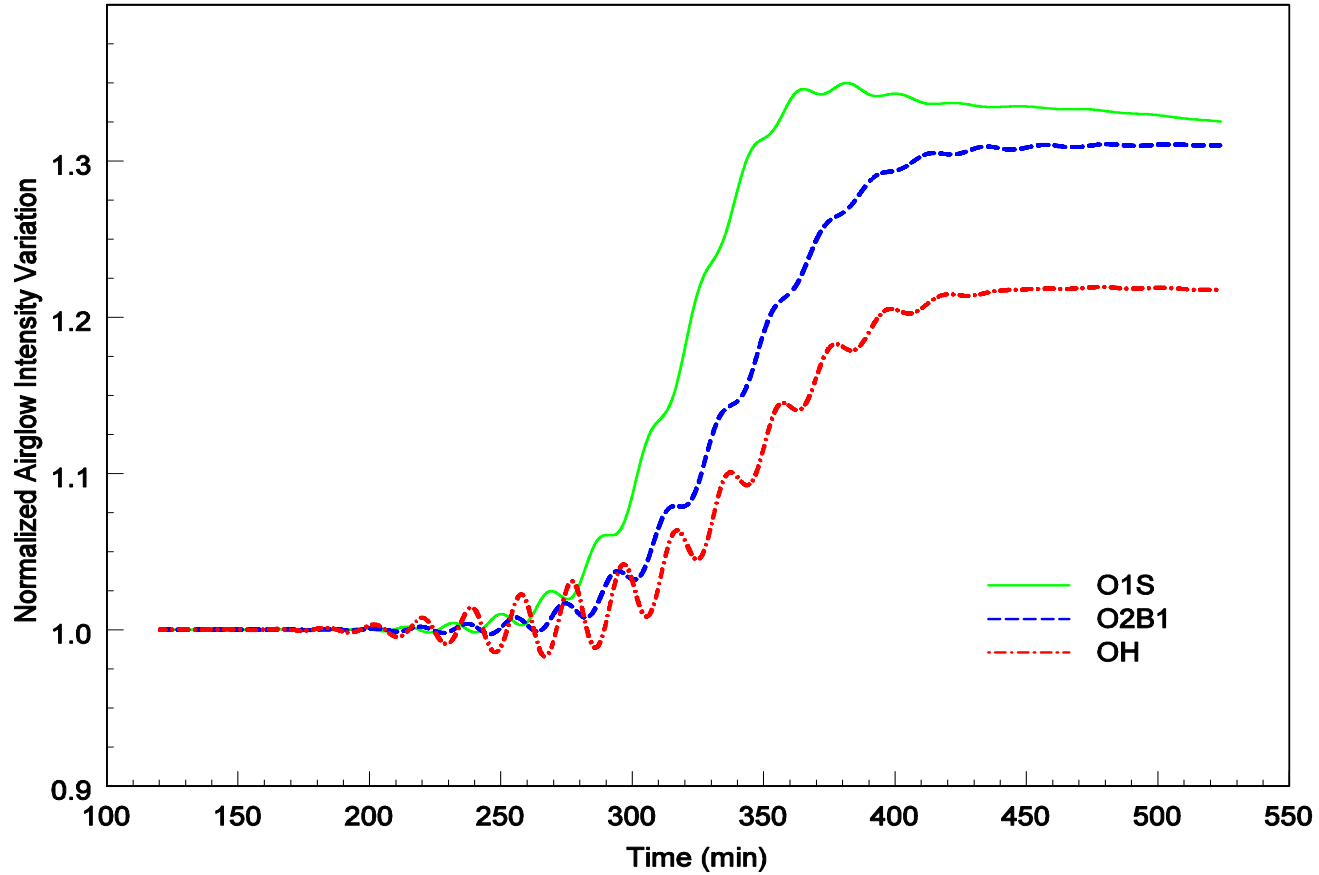**Secular variations of minor species**
T=20 min, Lx=30 km, z=90 km

Legend:
- O, 18S
- O3, 18S
- OH*, 18S
- O, 18N
- O3, 18N
- OH*, 18N

From OHCD

Wave-induced variations of airglow intensity
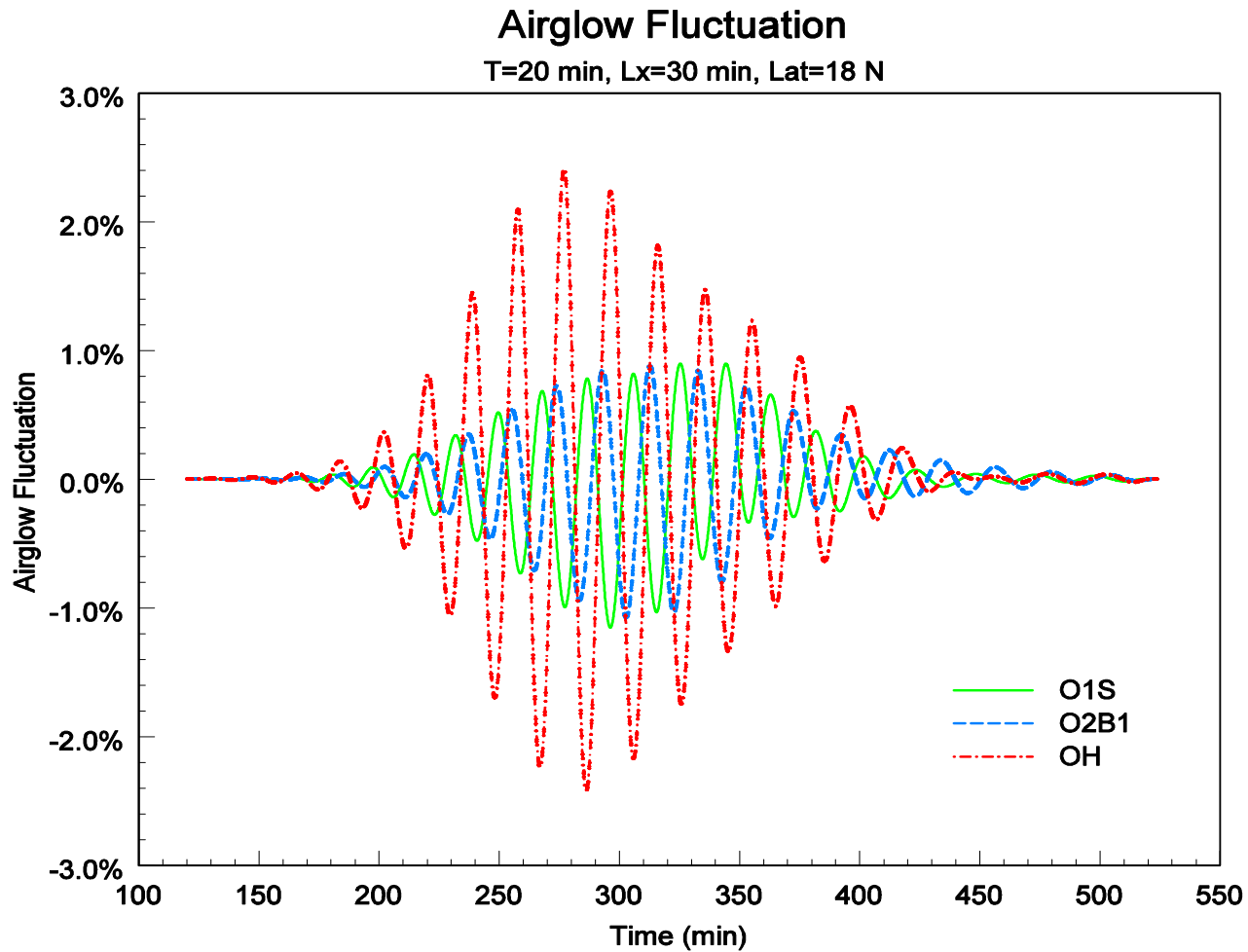

Normalized Airglow Intensity Variations
T=20 min, Lx=30 km, Lat=18 N

From MACD & OHCD
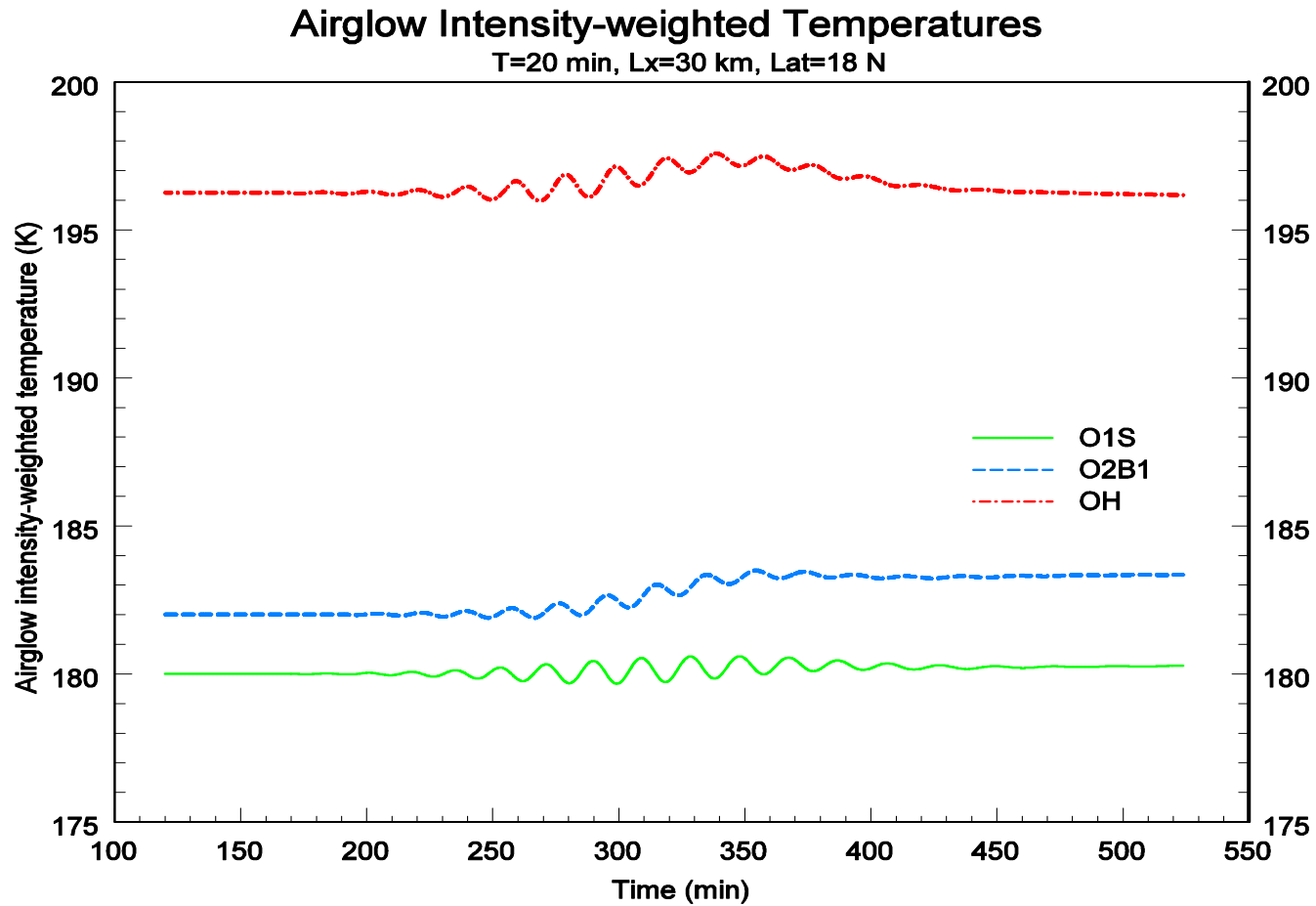
Wave-induced airglow fluctuation

Airglow Fluctuation
T=20 min, Lx=30 min, Lat=18 N

From MACD & OHCD

Wave-induced variations of airglow temperature

Airglow Intensity-weighted Temperatures
T=20 min, Lx=30 km, Lat=18 N

From MACD & OHCD

Phase relationship reveals wave information

- The phase relationship of airglow intensity or airglow temperature in multiple airglow layers can provide information of the gravity wave propagating through the airglow layers.

- If the airglow intensity (or airglow temperature) located at a higher altitude leads the airglow intensity (airglow temperature) located at a lower altitude, it indicates downward phase propagation, i.e., upward energy propagation of the gravity wave.

- The amplitude ratio of airglow intensity fluctuations and that of airglow temperature fluctuations from multiple airglow layers also reveal whether the gravity wave's amplitude is increasing, decreasing, or constant.
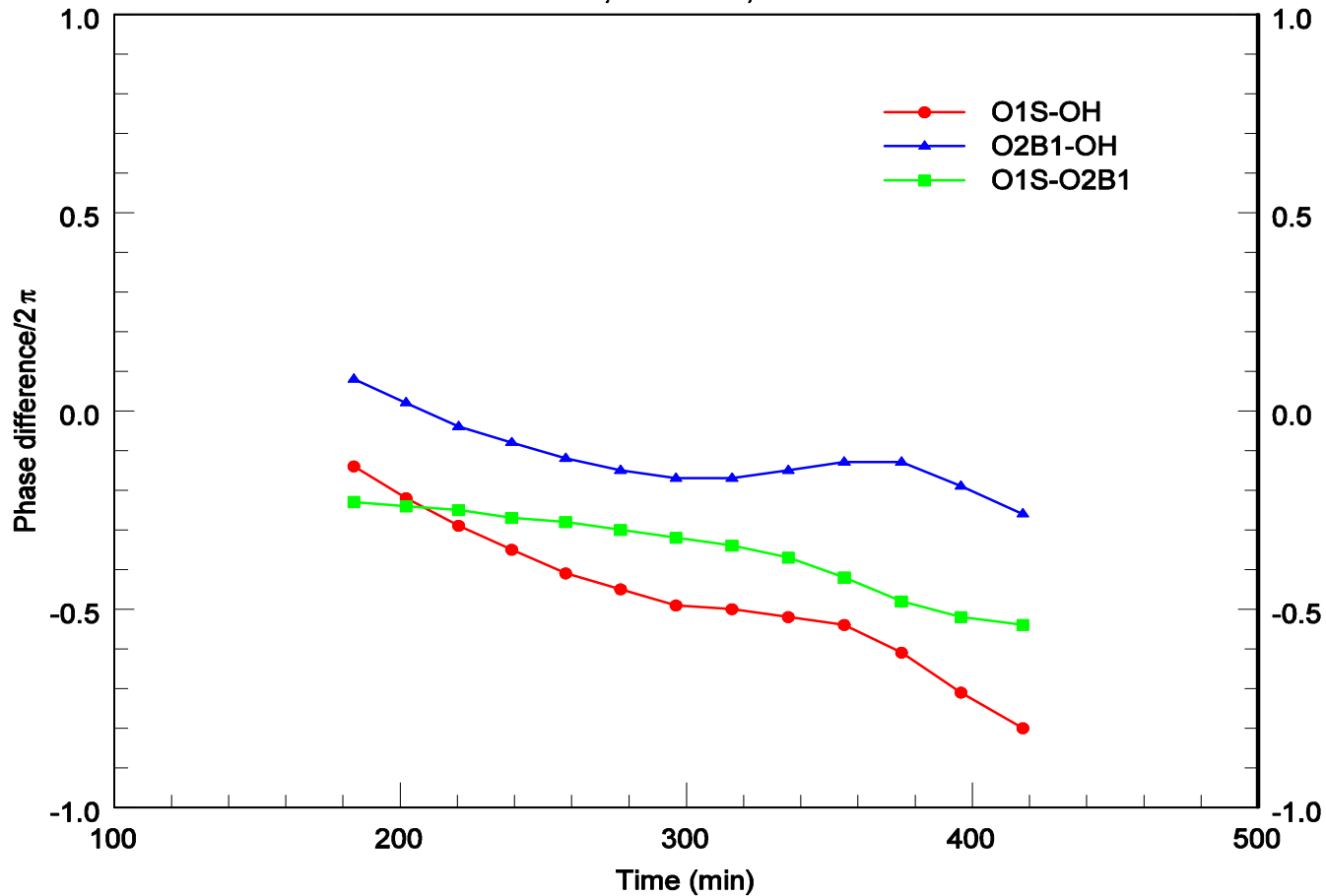
From MACD & OHCD

O(^{1}S) intensity leads both the O$_2$(0,1) and OH(8,3) airglow intensity, indicating downward phase propagation.

The Krassovsky ratio

The Krassovsky ratio, η, is a measure of the airglow response to a passage of wave trains and is defined as

$$\eta = \frac{I'/\overline{I}}{T'/\overline{T}} \qquad \text{or} \qquad \eta = \eta_{max}\,e^{-i\phi}$$
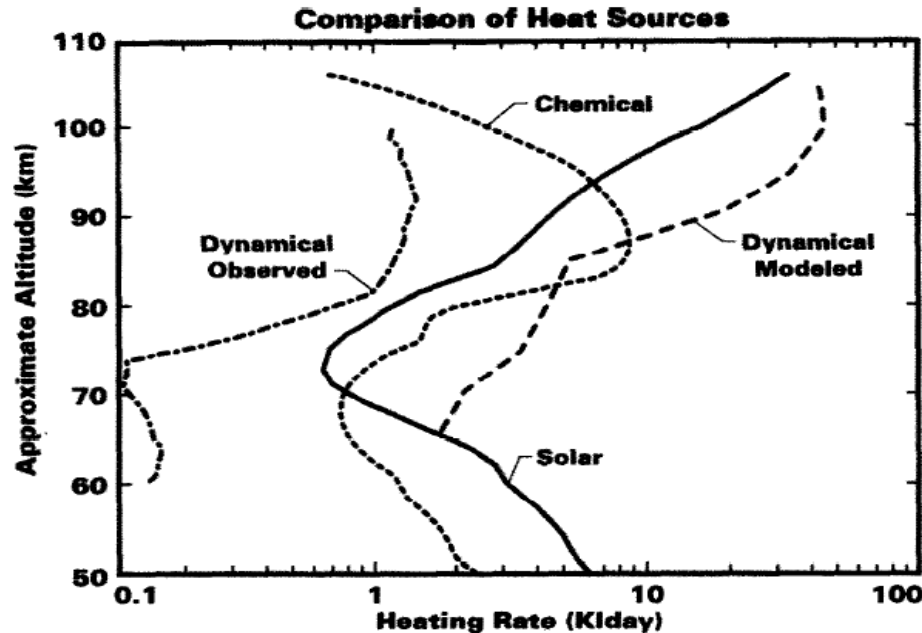
- The Krassovsky ratio can be used to deduce the chemical processes in the airglow chemistry responsible for its production

- It can also be used for tentative estimation of the long-term and seasonal variations of minor species involved in the airglow chemistry.

- The Krassovsky ratio depends on quite a few parameters: the wave periods, vibrational levels, quenching, horizontal wavelengths, wave dissipation rate, variations of local oxygen photochemistry, height variation of the emission layer, and temperature.

The amplitude and phase of Krassovsky ratio for the three airglow emissions in response to the 30-km wave packet.

	OH(8,3)	$O_2(0,1)$	$O(^1S)$
C	0.91	0.88	0.85
I_{max}	2.41E-2	1.08E-2	1.15E-2
T_{max}	2.27E-3	1.65E-3	2.40E-3
η_{max}	9.68	5.76	4.09
ϕ	-35.10^o	-33.30^o	-54.90^o

The amplitude of the Krassovsky ratio gets smaller with increasing altitude and the phase difference is larger for O(1S) greenline.

Exothermic Heating

Comparison of Heat Sources

Fig. 2. Comparison of heat sources in the mesosphere and lower thermosphere. The curve labeled "Chemical" is the heating due to exothermic chemical reactions as described in Mlynczak and Solomon [1993]. The curve labeled "Solar" is heating due directly to absorption of solar ultraviolet radiation as described in Mlynczak and Solomon [1993]. The "Dynamical" curve labeled "Observed" is from Lubken et al. [1993] and the curve labeled "Modeled" is from Fritts and Lu [1993].

Chemical heating serves as one largest leading heat source in that region [Mlynczak, 1996].

- For a chemical reaction A+B→C+D, the heating rate Q is εER[A][B] where ε is heating efficiency, E is enthalpy, R is the reaction rate, and [A] and [B] are concentrations of reactants A and B.
- Some of the reactions in the OH airglow chemistry are exothermic.
- The average wave-induced heating rate is $Q_{AVG} = \dfrac{1}{N}\sum_{i=0}^{N} Q(t_i) - Q(t_0)$

Wave-induced variations of exothermic heating

Initial and final total heating rates

T=20 min, Lx=30 km
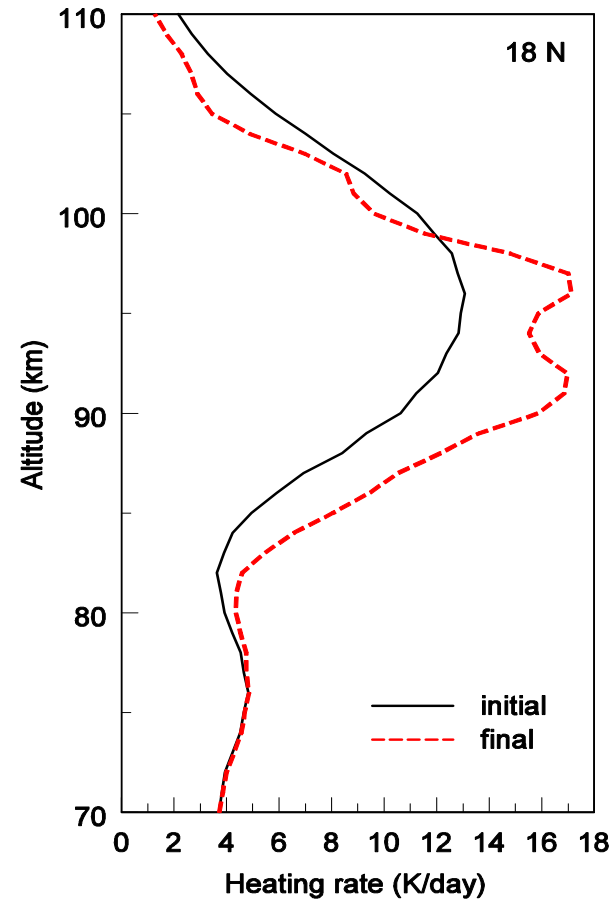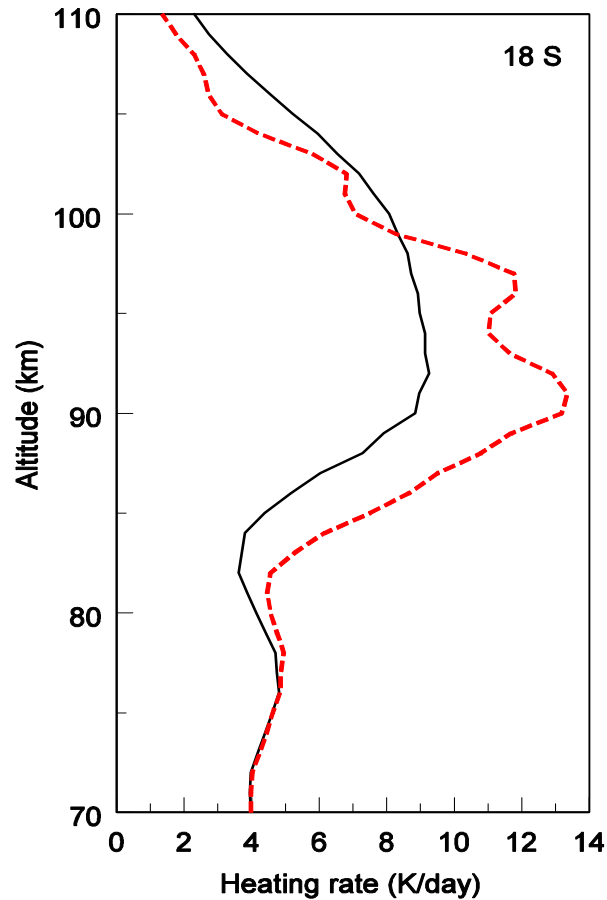
Summary

◆ Airglow intensity variation can be an indicator of wave activity; it is very sensitive to the local temperature and the change in the number densities of the species reacting in the airglow chemistry.

◆ Two 2D nonlinear, time-dependent numerical models (OHCD & MACD) were used to investigate gravity wave effects on minor species involving in the airglow chemistries, airglow, airglow temperature, exothermic heating, phase relationship and Krassovsky ratio.

◆ The OH(8,3), O2B1 and O(1S) greenline are the airglow emissions under study.

◆ We found that O(1S) has largest secular variation followed by O2B1 then OH. OH has largest fluctuation amplitude followed by O1S and O2B1.

◆ We found that the ultimate driver for the secular increases of minor species and airglow variations is the wave-driven downward transport of O.

Continued…

◆ The amplitude of the Krassovsky ratio gets smaller with increasing altitude and the phase difference is larger for O(1S) greenline.

◆ A ~22% secular increase in the OH(8,3) airglow intensity, a 30% increase in the O2B1 atmospheric band, and a 33% increase in the O(^{1}S) greenline.

◆ The largest wave-induced airglow intensity fluctuation amplitude is seen in the OH(8,3) emission (~2.4%), followed by the O2B1 atmospheric band and O(^{1}S) greenline with comparable maximum wave-induced airglow intensity fluctuation amplitudes of 1%.

◆ We found that the three-body recombination reaction (O+O+M) and the H+O3 reaction are the two major heating reactions below 100 km and two major cooling reactions above 100 km.

◆ The total heating rates have increased by 30.9% for 18 N. The peak value of the mean wave-induced total heating rates is 2.2 Kd^{-1} at 89 km for 18 N.