Simulation and analysis of radiant intensity for critical

Shaoze Li[1,a*],Fuqi Si[2,b]

[1]College of Biofood, Environment and Biology, Hefei University, Economic Development Zone, Hefei, China
[2]Key Laboratory of Environmental Optics and Technology, Anhui Institute of Optics and Fine Mechanics, Hefei Academy of Physical Sciences, Chinese Academy of Sciences, Shushan District, Hefei, China

Abstract: Atmospheric oxygen A-band (759-767nm) airglow has strong radiation intensity in the visible band, and the global atmospheric temperature field can be obtained based on the oxygen A-spectrum line. In order to realize the marginal observation of oxygen A-airglow, the intensity distribution and change at different heights need to be simulated. Firstly, the body emissivity at different heights and solar zenith angles is obtained based on the photochemical model of oxygen A-band airglow. Secondly, the oxygen airglow radiation transmission process is established based on the observation geometry of the edge. Then, the airglow radiation intensity is simulated based on the detection geometry path of the edge to obtain the airglow spectrum lines at different observation heights of the edge.

1 Preface

The near-space atmosphere (60~110km) will affect the accuracy of weather forecasting and the safety assessment of spacecraft launch and orbit[1][2], and the observation and study of near-space atmosphere has important military value and scientific signific-ance[3][4]. Oxygen A-band gas glow is one of the brightest spectra in the visible spectrum, and the distribution and change of gas glow spectral lines can be used to study the problems of atmospheric composition and temperature distribution. The wavelength region of oxygen A-band gas glow spectrum is 759~767nm, and it has strong self-absorption below 70 km[5].Spaceborne detection can achieve global observation in a short time, provide global temperature distribution data, and have a large spatial coverage. The Space Physics Laboratory of the United States uses the high-resolution Doppler imager (HRDI) to measure the temperature of the emission spectral lines in the oxygen A-band[6].The optimal estimation method based on the perturbation theory was used to invert the atmosphere at an altitude of 80~100km, and the temperature profile with an error of about 7K was obtained by using the coordinated inversion of three spectral lines. The Odin satellite is a Swedish and Canadian satellite that carries OSIRIS instruments, which include spectrometers and infrared imaging systems. These instruments are designed to make observations of atmospheric composition and structure. OSIRIS obtains information near a certain altitude in the atmosphere by observing the emission spectrum of oxygen in the A-band, which is the radiation of oxygen molecules in the A-band. The accuracy of the temperature inversion is about ±2K for the MLT region, but about ± 6K for the higher-level atmospheric temperature inversion, which indicates that the accuracy is relatively low in the higher-level temperature measurement. This discrepancy can stem from a number of factors, including instrument resolution, observation techniques, inversion algorithms, data processing methods, and different understandings of atmospheric properties.

In this paper, a radiative transmission model for the critical observation of oxygen A-band gas glow is established, and the emission spectrum intensities at different tangent point heights are obtained, which are used for the selection of detection schemes and inversion algorithms for the detection scheme and inversion algorithm of oxygen glow in the marginal atmosphere. The first part introduces three mechanisms of photochemical reaction mechanism of oxygen A-band gas glow. The second part is the calculation of bulk emissivity at different altitudes and at different solar zenith angles according to three mechanisms. In the third part, the critical observation gas light transport model is established, and the gas light radiation intensity at different heights is obtained.

2 Photochemical model of atmospheric oxygen A gas

A photochemical model is a mathematical model used to describe photochemical processes in the atmosphere, which combines the theory of photochemistry, the principle of photochemical reactions, and the theory of atmospheric dynamics. Its main purpose is to reveal how the concentration of atmospheric components affects the radiative properties of the atmosphere, especially the emissivity. Photochemical models typically employ differential equations to describe the evolution of

* Corresponding author: [a]994482658@qq.com
[b]sifuqi@aiofm.ac.cn

photochemical reactions and component concentrations in the atmosphere.

In the photochemical model, oxygen A-band gas glow refers to the spectrum produced by the radiation of oxygen molecules in the excited state, which usually includes spectral lines with a wavelength of 763.84 nm. This gas glow is mainly related to the excited state of oxygen molecules $O_2(b^1\Sigma_g^+)$. This excited state is usually formed through the following three processes:

1. Resonance scattering: When the energy of the photon is close to the energy of the excited state of the oxygen molecule, the photon and the oxygen molecule are resonantly scattered, so that the oxygen molecule enters the excited state.

2. Collision annihilation of ground state oxygen and atomic oxygen: Ground state oxygen $O(^3P)$ collides $O(^1D)$ with atomic oxygen produced by photolysis，This causes the annihilation of excited oxygen. This process occurs mainly in the higher atmosphere, where the concentration of ground state oxygen and atomic oxygen is higher.

3. Barth chemical reaction[7][8]: This reaction is a chemical reaction between an oxygen atom and an oxygen molecule. It is caused by the transfer of energy when an oxygen molecule encounters other oxygen molecules in the atmosphere, causing some oxygen molecules to enter an excited state.

These mechanisms work together to cause oxygen molecules to radiate out of the A-band spectrum when excited. As shown in Figure 1[9]in the photochemical model, J, k, and g represent the reaction coefficients of these generating mechanisms, which are used to describe the rates of various reactions.

By establishing photochemical models, combined with atmospheric dynamics theory and known reaction mechanisms, it is possible to simulate the phenomenon of atmospheric glow in order to study the changes in atmospheric chemical and optical processes and their effects on the atmospheric radiation balance and the environment.

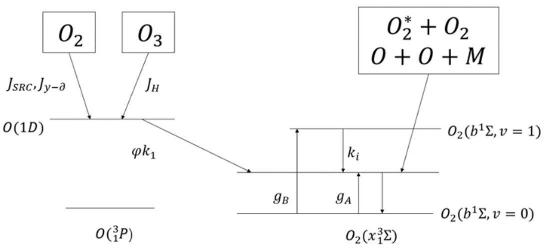

Fig. 1. Processes that oxygen A-band airglow production.

Oxygen molecules are resonantly excited by photons that absorb solar radiation at a wavelength of 763.84 nm, transitioning from the ground state to the excited state $O_2(b^1\Sigma_g^+)$. This process involves a resonant matching between the energy of the photon and the energy level of the excited state of oxygen. The reaction equation is as follows:

$$O_2 + hv \rightarrow O_2(b^1\Sigma_g^+)g \quad (1)$$

where g represents the transition of oxygen molecules to the excited state, and hv represents the photons of solar radiation, representing the $O_2(b^1\Sigma_g^+)$ oxygen molecules in the excited state.

Collision annihilation is a photochemical reaction process in which the excited state of oxygen molecules $O_2(b^1\Sigma_g^+)$ undergoes a quenching reaction with the excited state of oxygen atoms through collision $O(^1D)$ to form non-excited state oxygen molecules $O(^3P)$. This process can usually be represented by the following reaction equation:

$$O(^1D) + O_2 \rightarrow O_2(b^1\Sigma_g^+) + O(^3P)k_{D,O_2} \quad (2)$$

where k_{D,O_2} is the response rate.

The Barth chemical reaction is a two-step mechanism in photochemistry involving the generation of gas glows in the oxygen A-band (763.84 nm). The following is a description of the two steps:

The first step describes the collision of an oxygen atom and a quenched molecule, resulting in the production of an excited state of an oxygen molecule O_2^* :

$$O + O + M \xrightarrow{k_{14}} O_2^* + V \quad (3)$$

$$V = O_{2,}N_{2,}k_{14} = 4.7\times10^{-33}(300/T)^2\partial cm^6 s^{-1} .$$

The second step describes the O_2^* collision annihilation reaction between the excited state oxygen molecule and the oxygen molecule, and finally produces the excited state $O_2(b^1\Sigma_g^+)$:

$$O_2^* + O_2 \rightarrow O_2(b^1\Sigma_g^+) + O_2 \quad k_{15} \quad (4)$$

Efficiency factor in the $k_{15} = 5\times10^{-13}\beta cm^{-1}s^{-1}$, quenching rate $\alpha\beta = 0.8$ reaction.

In the two-step Barth reaction, an intermediate product is obtained, and the intermediate product O_2^* is quenched with the oxygen atom to produce a non-excited state of the oxygen molecule and the oxygen atom The reaction equation is as follows:

$$O_2^* + O \rightarrow O_2 + O \quad k_{16} \quad (5)$$

Quenching rate $k_{16} = 3\times10^{-11}cm^3 s^{-1}$.

The 763.84 nm radiation emitted by the reaction of the three mechanisms is the A-band gas glow, which A_Σ is the spontaneous emissivity coefficient and F_C the Frank-Condon factor of the A-band[10] The A-band volume emissivity is:

$$\eta_{O_2(b^1\Sigma_g^+)}(z) = F_C A_\Sigma n_{O_2(b^1\Sigma_g^+)}(z) \quad (6)$$

3. Bulk emissivity simulation calculations

As can be seen from Figure 2, the bulk emissivity of the solar glow is stronger than that of other altitude ranges in the altitude range of 40-100 km. In this altitude range, the bulk emissivity of the air glow is affected by a variety of factors. First of all, resonance scattering is an important mechanism, contributing to bulk emissivity in the altitude range of 30-120km. Resonance scattering refers to the resonance scattering of photons and oxygen molecules when the energy of photons is close to the energy of the excited state of oxygen, so that the oxygen molecules enter the excited state. This process works in the higher layers of the atmosphere, bringing the range of bulk emissivity to 30-120 km. Secondly, the photolysis of oxygen and ozone also plays an important role in the bulk emissivity of solar light. The photolysis of oxygen mainly occurs at an altitude of about 100 km, whereas the photolysis of ozone mainly occurs at an altitude of about 40 km. Taken together, the photolysis process of oxygen and ozone plays a key role in the generation of solar glow, by excitation of gas molecules and resulting in the emission of light at specific wavelengths. These processes also reflect the chemical and photophysical properties of the atmosphere at different altitudes. The photons produced by these photolysis excite oxygen molecules, resulting in the bulk emission of solar light. In addition, the figure shows that the contribution of the Barth effect to solar energy is relatively small. The Barth effect refers to a chemical reaction between oxygen molecules, which causes some oxygen molecules to enter an excited state. However, in the overall emissivity, the contribution of the Barth effect is relatively low, and it has not become the main mechanism for generating solar glow.

The bulk emissivity of the low-altitude atmosphere may be affected by the optical thickness, which reduces the intensity of solar radiation. In addition, the low solar photolysis coefficient at low altitude may lead to a decrease in body emissivity at low altitudes. At altitudes above 120 km, the optical thickness is smaller in this altitude range, but the bulk emissivity may also decrease due to a sharp decrease in reactant concentration. This is because bulk emissivity is related to the concentration of reactants, and within this altitude range, a decrease in reactant concentration can be a major factor. The optical thickness and sunlight photolysis coefficient at low altitude are larger, which may lead to a decrease in body emissivity in the low altitude range. At altitudes over 120 km, the optical thickness is small, but a decrease in reactant concentration may also lead to a decrease in bulk emissivity. Together, these factors influence atmospheric optical and chemical processes in different altitude ranges.

In general, resonance scattering and photolysis of oxygen and ozone are the main generating mechanisms, while the contribution of the Barth effect is small. Together, these mechanisms form the bulk emissivity intensity of solar glow in the altitude range of 30-100 km. Atmospheric conditions and chemical processes in this altitude range make solar glow radiation relatively strong. The optical thickness and sunlight photolysis coefficient at low altitude are larger, which may lead to a decrease in body emissivity in the low altitude range. At altitudes over 120 km, the optical thickness is small, but a decrease in reactant concentration may also lead to a decrease in bulk emissivity.

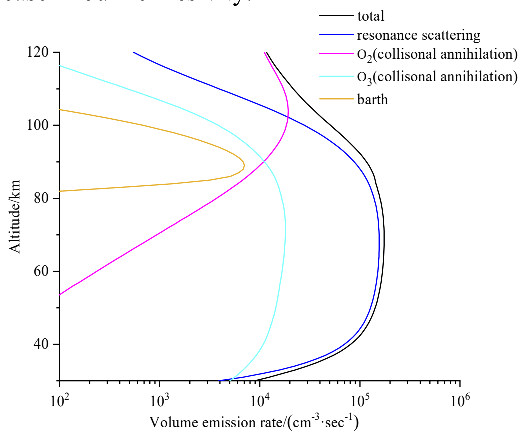

Fig.2. Simulated profile of the emissivity of oxygen in the A-band of solar gas glow.

Changes in the sun's zenith angle have a direct impact on atmospheric radiation, especially in the emission of solar globes. Changes in the sun's zenith angle directly affect the intensity of sunlight hitting the atmosphere. When the sun's zenith angle is smaller, the gaseous glow of sunlight directly into the atmosphere undergoes a more intense photochemical reaction, resulting in a relatively high bulk emissivity. This is because a smaller solar zenith angle means that the path of sunlight passes through a longer layer of the atmosphere and interacts more with atmospheric molecules, resulting in more photochemical reactions. As the zenith angle of the sun increases, the sunlight path is shorter and the radiation angle is more sloping, and the gas glow of sunlight into the atmosphere is less, so the bulk emissivity decreases. At an altitude of around 90 km, the change in the solar zenith angle has the least effect on the bulk emissivity, because the solar glow in this altitude range is mainly produced by the Barth effect and has less to do with solar radiation. When the solar zenith angle is 0°, that is, when the solar height is at its highest at noon, the gaseous glow directly from the sunlight into the atmosphere undergoes the most intense photochemical reaction, resulting in a stronger bulk emissivity relative to other altitudes. This phenomenon can be observed in Figure 3.

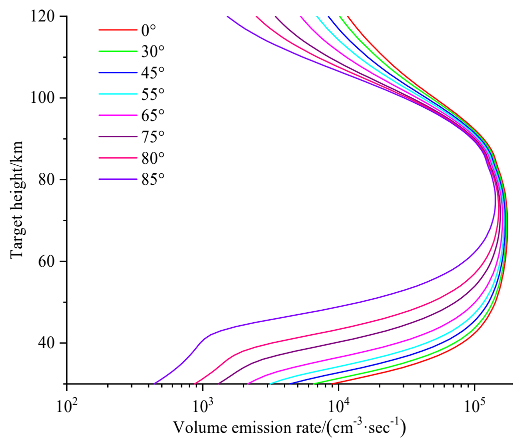

Fig.3. Changes in the emissivity profile of solar airglow at different angles.

4 Simulation results of critical radiant intensity

4.1 Radiative Transfer Mode

When describing the emission of photons in the oxygen A band, the radiant intensity of a particular rotational line is usually taken into account. This can be represented by the following relationship:

$$S_u(T_0)=\frac{T_S S_u(T_S)}{T_0}\times\exp\left(\frac{1.439E^{"}(T_0-T_S)}{T_0T_S}\right) \tag{7}$$

where the $T_S = 296K$ intensity of the spectral line at the reference temperature is denoted as $S_u(T_0)$ and the vibrational energy level of the $O_2(b^1\sum_g^+)$ excited oxygen molecule $E^{"}$ is denoted as . The formula (8) is a v_1 Doppler line with the center of the spectral line:

$$D(V)=\frac{1}{\partial_D\sqrt{\pi}}\exp\left(-\left(\frac{v-v_1}{\partial_D}\right)^2\right) \tag{8}$$

$$\partial_D=\frac{V_0}{C}\sqrt{\frac{2KT}{m}} \tag{9}$$

where C is the speed of light, Boltzmann's constant is expressed as K, and m is the mass of the oxygen molecule.

Because there is self-absorption in the oxygen A-band, it is necessary to consider the calculation of transmittance. The expression can be written as:

$$\tau(v,s)=\exp\left[-\sec\theta\int_z n_{o_2}(z)\sum_J S_J(T)D(V,T)dz\right] \tag{10}$$

In the above equation, the line-of-sight path of the satellite scan is expressed as s, the $n_{o_2}(z)$ density of oxygen number at a certain height z, and σ the v absorption cross section at the wavenumber. The formula for the absorption section is:

$$\sigma=\sigma_{ref}\frac{T_{ref}}{T}\exp\left(\frac{1.439E"(T-T_S)}{TT_S}\right) \tag{11}$$

In the above equation is $E"$ the vibrational energy level of the $O_2(b^1\sum_g^+)$ excited oxygen molecule, σ_{ref} which is the absorption cross section at the reference temperature. The absorption section is sensitive to temperature changes in the line-of-sight path, so changes in temperature across the integration path need to be considered.

The oxygen number density is calculated from the oxygen number density at temperature and reference height using the following formula:

$$n(z)=\frac{n(z_0)T(z_0)}{T(z)}\exp\left[-\int_{z_0}^{\infty}\frac{mg}{kT(z')}dz'\right] \tag{12}$$

where g is the gravitational force and the integral term represents the z_0 hydrostatic effects in the range of heights from the reference height to infinity.

In summary, the integral term takes into account the effects of oxygen absorption over the entire altitude range from the current gaze path position to infinity. The entire formula can be expressed as:

$$B(v,z_t)=\int_{-\infty}^{+\infty}\eta(s)S(s)D(v,s)\exp\left[-\int_s^{\infty}n(s')\sigma(s')D(v,s)ds'\right]ds \tag{13}$$

Among them, $S(s)$ is the intensity of the rotating spectral line in the line-of-sight path, the $n(s')$ oxygen number density in the line-of-sight path, and $\sigma(s')$ the absorption cross-section. Figure 4 is a critical line-of-sight path model.

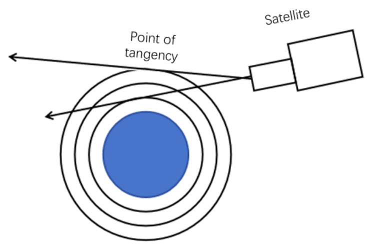

Fig.4. Limb line of sight path model.

4.2 Radiation intensity simulation results

Obtaining the optical thickness requires the calculation of the absorption coefficient, and in the atmosphere, the widening around the transition wavenumber v_{ij} , the expansion of which is expressed by the normalized linear function $f_L(v,v_{ij},p,T)$. In the lower atmosphere, the pressure broadening of the spectral lines predominates, and the Lorentz distribution can be assumed:

$$f_L(v,v_{ij},p,T)=\frac{1}{\pi}\frac{\gamma(p,T)}{\gamma(p,T)^2+\left[v-\left(v_{ij}+\delta(p_{ref})p\right)\right]^2} \tag{14}$$

In the low-pressure environment of the upper atmosphere, the Doppler broadening dominates in the linear and can be assumed to be a Gaussian distribution:

$$f_G(v,v_{ij},T)=\sqrt{\frac{\ln 2}{\pi\alpha_D^2}}\exp\left(-\frac{(v-v_{ij})^2\ln 2}{\alpha_D^2}\right) \tag{15}$$

Absorption coefficient $k_{ij}(v,T,p)=S_{ij}(T)f_L(v,v_{ij},p,T)$

Figure 5 shows the normalized absorption coefficient of the A-band of oxygen from 30 to 80 km. Table 1 shows the data of the MISI database data for different heights of data density, temperature, and pressure.

Table 1. Number density, temperature, and pressure at 30-80km.

height(km)	Oxygen number density (g/cm3)	Temperature（K)	pressure (Pa)
30	6.727E+16	214.3	0.199
40	1.35E+16	244.8	0.0456
50	3.43E+15	255.1	0.012
60	9.40E+14	239.9	0.0031
70	2.37E+14	223.7	0.0007
80	5.34E+13	215.3	0.0001

The HITRAN database sample line strengths selected at different heights are shown in the figure below.

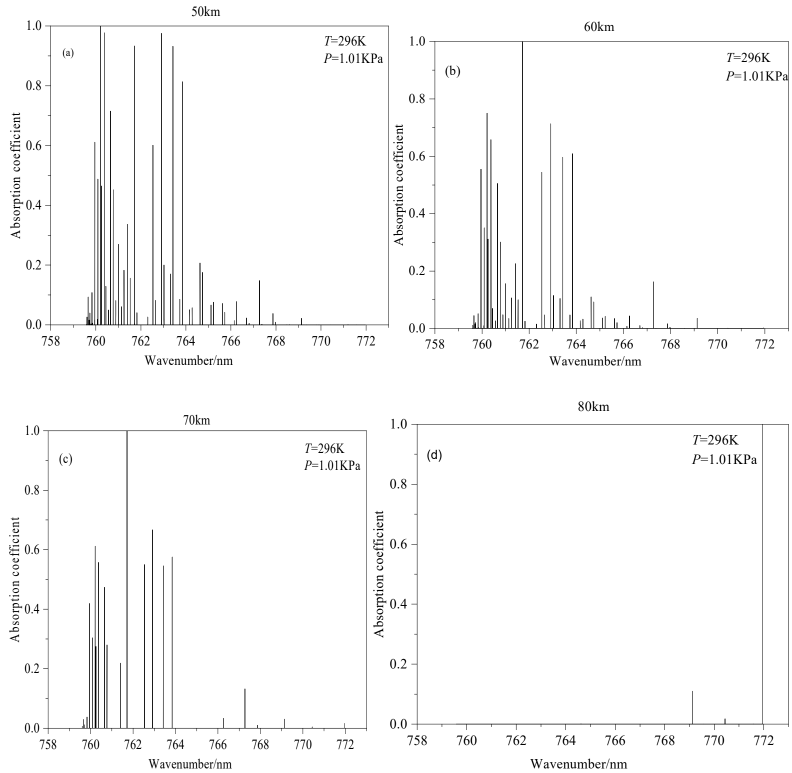

Fig.5. Schematic diagram of absorption coefficient spectral lines in the A-band of oxygen.

According to the schematic diagram of the absorption coefficient spectral line of oxygen A-band, it can be seen that the absorption coefficient is negligible after reaching 80 km, and the influence of the absorption coefficient needs to be considered when calculating the optical thickness of oxygen below 80 km, and the influence of the absorption coefficient can be ignored above 80 km.

Based on the calculated bulk emissivity of the oxygen A band, the HITRAN database, and the established radiative transfer model, the oxygen A emission lines at different heights were obtained, as shown in Figure 6.

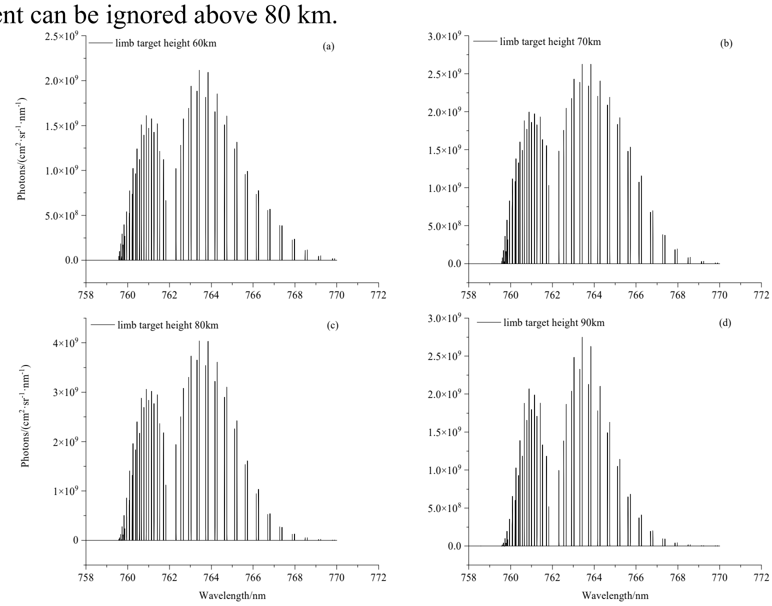

Fig.6. Emission Spectral Intensity of Oxygen A-band.

Figure 6 is the emission line under the simulated high resolution, in the actual observation, the spectral resolution of different instruments is different, the spectral response function of the instrument and the high-resolution spectrum line are convoluted, and the emission spectrum line at different resolutions can be obtained:

$$C = \int_{-\infty}^{+\infty} I(\lambda)B(\lambda)d(\lambda) \tag{16}$$

For the grating spectrometer, the spectral response function is usually of the Gaussian type, and the half-height and width of the cm^{-1} Gaussian function are selected to obtain the simulated values of the critical radiant intensity at different tangent point heights, as shown in Figure 7.

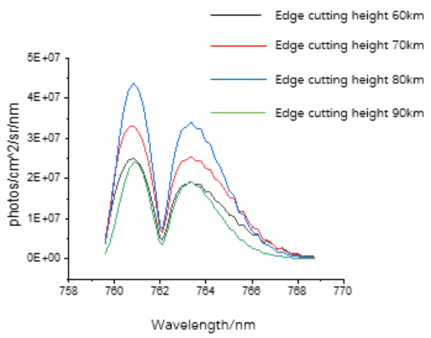

Fig.7. Convolutional Results of Oxygen A Spectral Lines.

In the figure, the radiation intensity of gas glow is different at different altitudes, the radiation intensity is stronger at 80 km, and the radiation intensity is weaker below 70 km, mainly because the intensity of the gas glow spectral line decreases due to the strong oxygen self-absorption, and the weak radiation intensity of the gas glow above 90 km is mainly due to the thin atmosphere and the low concentration of participating in the photochemical reaction. At the same time, the influence of temperature on the shape of the spectral lines can be seen, for example, the lower temperature at 90 km weakens the radiation intensity on both sides of the spectral line, which indicates that different temperatures determine different spectral radiation shapes, because with the increase of temperature, the contribution of higher rotational energy levels to the spectrum increases, affecting the shape of the spectral bands. Therefore, by detecting the radiation intensity and distribution of oxygen A gas glow lines, the temperature field of the global atmosphere can be detected.

5. Conclusion

In this paper, the simulation method of atmospheric oxygen A emission line is studied. Firstly, the photochemical model of the gas glow of oxygen A band is established $O_2(b^1\Sigma_g^+)$, the bulk emissivity of the gas glow of the A band is calculated according to the photochemical model, and then the radiation transfer model of the gas glow of oxygen A band is established $O_2(b^1\Sigma_g^+)$ The radiative transmission model is carried out based on the critical edge detection geometric path to simulate the radiant intensity of the gas glow, and the factors affecting the emissivity and radiant intensity of the gas glow in the oxygen A-band are analyzed, and the following factors are verified, such as the solar zenith angle, when the solar zenith angle is 0°, that is, when the sun shines directly into the atmosphere, the bulk emissivity is the strongest. This is because the direct exposure of sunlight into the atmosphere causes strong photochemical reactions, including the photolysis of oxygen and ozone, resulting in a higher bulk emissivity, and the effect of temperature changes on the emission spectrum of oxygen in the A-band is symmetrical, with less radiation in the center and less radiation in both sides.

Acknowledgments

Natural Science Foundation of Anhui Province (1808085QD114)

References

1. Wang Ying Jian， SCIENCE IN CHINA(Scries A)，2000.30（S1）17.
2. LIU Zhenxing.Space Physics[M].Harbin:Harbin Institute of Techology Press,2005
3. CHRISTENSEN A B,YES J H,BISHOP R L,et al.Observations of molecular oxygen atmospheric band emission in the thermosphere using the near infrared spectrometer.on.the.ISS/RAIDS.experiment[J].j.Geophys.Res.SpacePhys,2012,117(A4):DOI:10.1029/2011ja016838
4. Hays P.B,Abreu V.J, Dobbs M.E, et al. High Resolution Doppler Imager on Upper Atmosphere Research Satellite, Geophysical Research: Atmospheres, 1993,98 (D6) : 10713-10723
5. Zarboo A,Bender S,Burrows J.P, et al. The volume emissivity of $O_2(1\Sigma)$ and $O_2(1\triangle)$ in the mesosphere and low thermosphere was retrieved using SCIAMACHY MLT edgewise scanning.Atmospheric Measurement Technology.2018, 11:473-487
6. Skinner W.R.,Hays P.B.,Grassl H.J.,et al. High resolution Doppler imager on the Upper Atmosphere Research Satellite. International Society of Optics and Photonics,1994
7. Bucholtz A, Skinner W. R, Abreu V.J., et al. O_2 Daily airglow of atmospheric band system. Planetary and Space Science, 1986,34 (11) : 1031-1035
8. WallaceL, HuntenD.M. Daylight in the oxygen A zone. J. Geophysical Research, 1968,73 (15) :4813-4834
9. Llewellyn E. J., Lloyd N.D., Degenstein D.A., et al. The OSIRIS instrument on the Odin spacecraft. Canadian Journal of Physics, 2004,82 (6) : 411-422

10. Nicholls R. W.Franck-Condon decomposed the high vibrational quantum number v-o for the O2 band system. National Bureau of Standards Research: Part A - Physics and Chemistry, 1965, 69A:369-373