

1 Article

## 2 Trace gas retrieval from AIUS: Algorithm description 3 and O<sub>3</sub> retrieval assessment

4 Xiaoying Li<sup>1</sup>, Tianhai Cheng<sup>1,\*</sup>, Jian Xu<sup>2,\*</sup>, Hailiang Shi<sup>3</sup>, Xingying Zhang<sup>4</sup>, Shule Ge<sup>5</sup>,  
5 Mingmin Zou<sup>1</sup>, Hongmei Wang<sup>1</sup>, Yapeng Wang<sup>1</sup>, Songyan Zhu<sup>1</sup> and Jing Miao<sup>1</sup>

6 1. State Key Laboratory of Remote Sensing Science, Institute of Remote Sensing and Digital Earth, Chinese  
7 Academy of Sciences, Beijing 100101, China; lixy01@radi.ac.cn (X.L.)

8 2. Remote Sensing Technology Institute, German Aerospace Center (DLR), Oberpfaffenhofen, Germany

9 3. Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui, 230031, China

10 4. National Satellite Meteorological Center, China Meteorological Administration

11 5. China Center for Resources Satellite Data and Application, China

12 \* Correspondence: chength@radi.ac.cn (T.C.), jian.xu@dlr.de (J.X.)

13

14 **Abstract:** AIUS (Atmospheric Infrared Ultraspectral Sounder) is an infrared occultation  
15 spectrometer onboard the Chinese GaoFen-5 satellite, which covers a spectral range of 2.4--13.3  $\mu\text{m}$   
16 ( $750\text{--}4100\text{ cm}^{-1}$ ) with a spectral resolution of about  $0.02\text{ cm}^{-1}$ . AIUS is designed to measure and  
17 study chemical processes of ozone (O<sub>3</sub>) and other trace gases in the upper troposphere and  
18 stratosphere around Antarctic. In this study, the corresponding retrieval methodology is described.  
19 The retrieval simulations based on the simulated spectra of AIUS have been carried out, with a  
20 focus on O<sub>3</sub>. The relative difference between the retrieved and the true O<sub>3</sub> profiles is within 5% from  
21 the 15km to 70km and about 10% below 15km. The corresponding averaging kernels illustrate that  
22 the overall retrieval information mainly come from the spectra, not the a priori. The retrieval  
23 experiments also demonstrate that the shape of the retrieved profiles resembles the shape of the  
24 true profile even if the shape of the a priori profile is different from that of the true profile. Further,  
25 we perform the O<sub>3</sub> retrieval from the real ACE-FTS (Atmospheric Chemistry Experiment-Fourier  
26 Transform Spectrometer) measurements and compare the results with the official ACE-FTS Level-2  
27 products. Overall, both profiles agree well in the stratosphere where the retrieval sensitivity is  
28 high. The relative difference between both profiles is about 15% below 70km, which may due to the  
29 measurement errors and different forward model parameters.

30 **Keywords:** AIUS; Occultation; Retrieval algorithm; Microwindows; Ozone

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### 32 1. Introduction

33 The annual occurrence of the Antarctic ozone hole has been well documented. For studying  
34 ozone recovery, many efforts have been made to understand the chemical and dynamical processes  
35 around Antarctic [1-3]. Occultation and limb sounding techniques have provided an important way  
36 for remotely observing Earth's middle atmosphere. These measurements have greatly promoted our  
37 understanding of the chemical process of atmospheric composition in the upper troposphere and  
38 stratosphere by providing profiles measurements with different altitudes. As compared to  
39 nadir-viewing measurements, occultation/limb sounding measurements have higher vertical  
40 resolution, which can be used to derive vertical information of atmospheric components.  
41 Furthermore, high-resolution atmospheric mid-infrared spectra are suitable for detection of many  
42 trace species, since a wide variety of vibrational-rotational bands with molecular absorption lines are  
43 found within this spectral range. Recently, many occultation observation/limb sounding sensors  
44 have been developed and provided abundant profiles of trace gases, such as O<sub>3</sub>, CO, H<sub>2</sub>O, NO, etc  
45 [4-9].

46 AIUS is one of six payloads onboard the Chinese GaoFen-5 satellite that is expected to launch in  
47 May, 2018. AIUS is the first occultation spectrometer developed in China, which is designed to  
48 detect the trace gases over the Antarctic. AIUS will operate in a solar synchronous orbit, with a  
49 nominal height of 700 km. The instrument is a Fourier transform infrared spectrometer and its main  
50 objective is to measure the O<sub>3</sub> and other species in the stratosphere and upper troposphere in order  
51 to study the ozone change over the Antarctic.

52 The aim of this study is to introduce the trace gas retrieval algorithm developed for AIUS and to  
53 assess its performance based on ozone retrievals. In Section 2, the instrument parameters and level 1  
54 processing of AIUS are introduced briefly. Section 3 describes the retrieval algorithm in detail.  
55 Integrated atmosphere profiles dataset is presented and a sensitivity analysis of atmosphere profiles  
56 is showed in Section 4. In Section 5, the simulated spectra and the ACE-FTS observation spectra are  
57 adopted to retrieve O<sub>3</sub> profiles and to assess the retrieval performance.

## 58 2. AIUS instrument

59 AIUS is a Fourier transform infrared spectrometer for the detection of occultation transmittance  
60 spectra in the middle and upper atmosphere, which has similar characteristics to ACE-FTS. Both  
61 instruments have a spectral resolution of 0.02 cm<sup>-1</sup>. AIUS covers the spectral range from 750 cm<sup>-1</sup> to  
62 4100 cm<sup>-1</sup>, while ACE-FTS covers 750--4400 cm<sup>-1</sup>. It is a dual-band system composed of MCT  
63 (mercury cadmium telluride, 750--1850 cm<sup>-1</sup>) and InSb (1850--4160 cm<sup>-1</sup>). AIUS covers an altitude  
64 range from 8 to 100 km and has a field of view of 1.25 mrad. The latitude coverage of AIUS  
65 measurements is about 55° S to 90° S, which is mostly over Antarctica.

66 GF5-AIUS level 0 is original auxiliary and interferogram data in binary format and level 1 is  
67 HDF5 format file includes reconstructed spectra and processed auxiliary data. GF5-AIUS level 0 to  
68 level 1 processing includes three steps. The first step is the acquisition and processing of auxiliary  
69 data. By unpacketing the auxiliary data package, the information of observation, such as  
70 acquisition time, sun position and satellite position, is acquired. The geometric parameters, the  
71 height and the latitude and longitude coordinates, are calculated from the information of the sun  
72 and satellite. The second step is to reconstruct the spectra from the original interferogram. However,  
73 since the AIUS is an interferometer, the interferogram will contain some spikes produced by the  
74 effect of energetic particles due to space electromagnetic environment on orbit, which will  
75 contaminate the complete spectra. Thus, some processes have to be involved to correct these errors.  
76 The nonlinear behavior of the detectors is expected and characterized on-ground, which requires an  
77 additional correction. This nonlinearity correction will be consolidated in-flight using  
78 commissioning phase data. After that, the FFT is performed to compute the spectra. The last step is  
79 to evaluate the spectra's quality by standard deviation or mean value of imaginary part of the  
80 calculated spectra and then make the mark to show if the spectra is well reconstructed. "0" is for  
81 good quality and "1" for bad quality.

82 Level 1 data is the spectra data which are the relative intensities of each tangent heights using  
83 DN (digital number) values. Our inversion takes the transmittance converted from the Level 1 data.  
84 In addition to the observation of the Sun outside and inside the atmosphere, GF5-AIUS also observes  
85 the deep space to remove the instrumental emission. Commonly, the transmittance  $\tau(h, \lambda)$  at  
86 tangent point  $h$  of wave number  $\lambda$  can be calculated by the following equation:

$$87 \quad \tau(h, \lambda) = \frac{D(h, \lambda) - B(\lambda)}{S(\lambda) - B(\lambda)}, \quad (1)$$

88 Where  $D(h, \lambda)$ ,  $S(\lambda)$  and  $B(\lambda)$  are the digital counts of the observation of signal at tangent point  $h$ ,  
89 the solar radiation outside atmosphere and the deep space signal.

## 90 3. Retrieval methodology of AIUS

91 Accurate knowledge of pointing and  $p/T$  information is important to high-precision  
92 quantitative retrieval of abundances of atmospheric species from occultation observed  
93 transmittances. The tangent height correction for AIUS is carried out by employing the triangular

94 iteration with tangential strides technique in a microwindow of N<sub>2</sub> continuum absorption, whereas  
 95 the scheme of  $p/T$  retrieval is by introducing the hydrostatic equation into the iterative process of  
 96 optimal algorithm. Details of the design and development of these two algorithms are introduced in  
 97 our other two papers in preparation.

### 98 3.1. Inversion model

99 The inversion algorithm employed in this study is based on OEM (Optimal Estimation  
 100 Method) proposed by Rodgers [10]. Since OEM is generally applicable and facilitates a theoretical  
 101 error analysis, this method has been widely used in the inversion of atmospheric state parameters  
 102 using infrared and microwave remote sensing measurements, with nadir, occultation or limb  
 103 viewing [11-16]. OEM stabilizes the inversion process by taking into account the statistical  
 104 information about the atmospheric variability, which has been investigated by many studies  
 105 [17-23].

106 Our inversion scheme is adapted from the retrieval software Qpack 2.0 [23] that uses LM  
 107 (Levenberg–Marquardt) approach for a nonlinear least squares fitting. The LM iteration method  
 108 adopted in the Qpack is the same as the LM iteration method modified by Rodgers [17]. By  
 109 introducing a constraint factor  $\gamma$ , the next iterate is yielded by:

$$110 \quad \mathbf{X}_{i+1} = \mathbf{X}_i + [(1 + \gamma)\mathbf{S}_a^{-1} + \mathbf{K}_i^T \cdot \mathbf{S}_e^{-1} \cdot \mathbf{K}_i]^{-1} \cdot \{\mathbf{K}_i^T \mathbf{S}_e^{-1} [\mathbf{Y} - \mathbf{F}(\mathbf{X})] - \mathbf{S}_a^{-1} [\mathbf{X}_i - \mathbf{X}_a]\}. \quad (2)$$

111 The inverse of the solution covariance in equation (2) is given by:

$$112 \quad \mathbf{S}_x^{-1} = \mathbf{K}^T \cdot \mathbf{S}_e^{-1} \cdot \mathbf{K} \quad . \quad (3)$$

113

114 And the cost function  $C(X)$  is given by:

$$115 \quad C(X) = [(\mathbf{Y} - \mathbf{F}(X))^T \cdot \mathbf{S}_e^{-1} \cdot (\mathbf{Y} - \mathbf{F}(X)) + (\mathbf{X} - \mathbf{X}_a)^T \cdot \mathbf{S}_a^{-1} \cdot (\mathbf{X} - \mathbf{X}_a)]/n_y \quad , \quad (4)$$

116 where  $\mathbf{F}$  is the forward model,  $\mathbf{Y}$  is a series of observations value,  $\mathbf{X}$  is the state of the  
 117 atmosphere,  $\mathbf{S}_e$  is the covariance matrix of the observation error and  $\mathbf{K}$  is the matrix of weighting  
 118 function. The a priori state vector is denoted by  $\mathbf{X}_a$ , with its covariance matrix  $\mathbf{S}_a$ . And  $n_y$  is the  
 119 number of  $\mathbf{Y}$  vector.

120 In our retrieval scheme, retrieval experiments are made based on many simulated spectra and  
 121 ACE-FTS observation data to decide an optimal choice of  $\gamma$ . After statistical analysis, the factor of  $\gamma$   
 122 is defined as a linear scaled function to the cost function. It will be updated at each iteration, which  
 123 is given by the following equation. Here,  $a$  is a constant and it is different for different  
 124 atmospheric species.

$$125 \quad \gamma_i = a \cdot C(\mathbf{X}_i) \quad . \quad (5)$$

126 The definition of the a priori covariance matrix  $\mathbf{S}_a$  follows Gaussian statistics and  
 127 considers the correlation between different components of the state vector and the forward  
 128 model vector. Different types of the correlation function [24] for computing the correlation  
 129 have been tested based on the retrievals from simulated and observed ACE-FTS data. In  
 130 this study, we employ the linear correlation function:

$$131 \quad \mathbf{S}_a(i, j) = \max \{0, \sigma(i)\sigma(j) \left[ 1 - (1 - e^{-1}) \frac{2|z(i)-z(j)|}{lc(i)-lc(j)} \right] \} \quad , \quad (6)$$

132 where  $i$  and  $j$  are position indexes,  $z$  is the position,  $lc$  is the correlation length and  $|*|$  signifies the  
 133 absolute value.  $\sigma$  is the standard deviation calculated from the a priori.

134 In the retrieval scheme of AIUS, we adopt the “ $dx$ ” in the Qpack 2.0 as the threshold of  
 135 convergence. The iteration is considered converged in the condition that the value of  $dx$  is smaller  
 136 than 0.01. The definition of  $dx$  is that:

$$137 \quad dx = [(\mathbf{X}_{i+1} - \mathbf{X}_i)^T \cdot \mathbf{S}_x^{-1} \cdot (\mathbf{X}_{i+1} - \mathbf{X}_i)]/n_x \quad , \quad (7)$$

138 where  $n_x$  is the length of the state vector.

### 139 3.2 Adopted forward model

140 An accurate modeling of the radiative transfer through the atmosphere plays an important role  
141 in the inversion. The forward model adopted in the retrieval algorithm of AIUS is the RFM  
142 (Reference Forward Model) with the latest release version v4.36 [25]. RFM is a GENLN2-based  
143 line-by-line radiative transfer model originally developed at AOPP, Oxford University, under an  
144 ESA contract to provide reference spectral calculations for the MIPAS (The Michelson Interferometer  
145 for Passive Atmospheric Sounding) instrument launched on the ENVISAT (Environmental Satellite)  
146 in 2002. It has been subsequently developed into a general purpose code suitable for a variety of  
147 different spectroscopic calculations. Von Clarmann [26] has compared five forward models  
148 including the RFM. The inter-comparison experiment showed that the overall inter-consistency of  
149 spectra for all participants is good, which also can demonstrate that the RFM works fine and reliable.

150 RFM can deal with various measurement conditions including nadir viewing, limb sounding,  
151 occultation observation from different platforms (satellite /balloon /aircraft). Its main features are  
152 listed below:

- 153 1. It has high flexibility when defining observation geometry (including scanning features) and  
154 sensor characteristics.
- 155 2. It can provide Jacobians for  $p$ ,  $T$ , VMR, line-of-sight pointing and surface temperature and  
156 emissivity.
- 157 3. Cross sections can be computed from HITRAN (High-resolution Transmission) spectroscopic  
158 database or read from external files.
- 159 4. Continua for  $H_2O$ ,  $O_2$ ,  $N_2$  and  $CO_2$  are included [27-31].

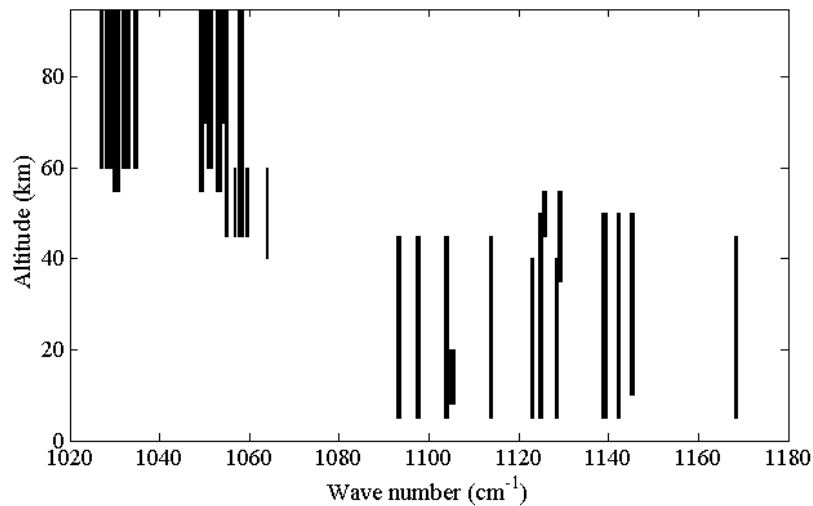
160 For all considered microwindows, scattering can be negligible and is not taken into account in our  
161 retrieval scheme.

### 162 3.3 Microwindows

163 The spectral resolution of AIUS is about  $0.02\text{ cm}^{-1}$ . Because of this, the number of data points  
164 from each absorption band becomes unrealistic for an efficient inversion process. Furthermore, one  
165 should avoid the effect of interfering species on the retrieval of the target species and have the best  
166 information on the retrieval. Thus, the retrieval is performed using a set of narrow spectral interval  
167 (called "microwindow") instead of an entire spectral band.

168 To select an appropriate set of microwindows, a sensitivity analysis with Jacobians is required.  
169 First of all, we select the spectral points which are sensitive to the target gas on each cutting height  
170 and are not sensitive to the interference gas according to the Jacobians of target and the interference  
171 species. Then, the selected spectral points are grown on the basis of information entropy to generate  
172 a series of continuous window. Finally, all the selected microwindows at different tangent height are  
173 combined.

174 The absorption lines of  $O_3$  in the infrared band are mainly located near  $9.6\ \mu\text{m}$  and the main  
175 interfering gases of  $O_3$  in this spectral band include  $CO_2$ ,  $H_2O$  and  $N_2O$ . The chosen microwindows  
176 for  $O_3$  retrieval are shown in Figure 1. For  $O_3$  retrieval, about 20 microwindows are selected, covering  
177 from 5 km to 95 km. Microwindows in the range of  $1000\text{--}1070\text{ cm}^{-1}$  are sensitive at higher altitudes,  
178 while others are sensitive at lower altitudes.



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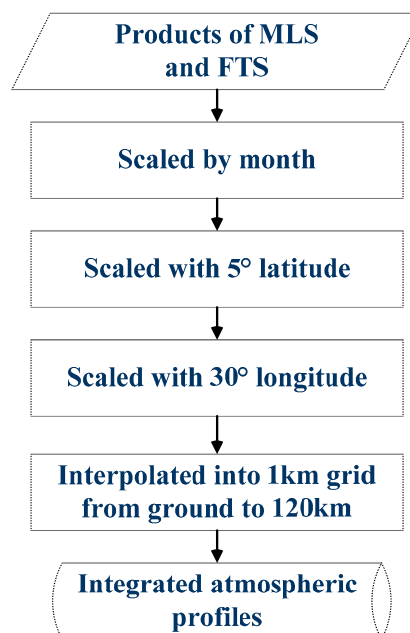
Figure 1 The microwindows selected for O<sub>3</sub> retrieval.

#### 181 4. Sensitivity analysis of atmospheric profiles in forward model

##### 182 4.1 Integrated Atmospheric profiles

183 The forward model generates a numerical simulation of measurements based on the given  
 184 atmospheric state. In other words, the accuracy of the simulated measurements depends on the  
 185 reliability of the atmospheric parameters used in the forward model. In our retrieval scheme, we  
 186 compute a dataset of integrated atmospheric profiles based on MLS (Microwave Limb Sounder)  
 187 level 2 products, ACE-FTS level 2 products and the profiles from AFGL(Air Force Geophysics  
 188 Laboratory) atmospheric models.

189 The ACE-FTS level 2 v3.6 and the MLS level 2 (v4.2) products between 2014 and 2016 are  
 190 considered. We classify and store the species profiles month by month for each set of products. Then,  
 191 the monthly mean profiles are acquired and classified into different coordinate grids, which is  
 192 discretized with a 5° latitude and 30° longitude spacing.. That is, both of two set of dataset are  
 193 classified by month and coordinate grid. A diagram of constructing the integrated atmospheric  
 194 profiles is shown in Figure 2.



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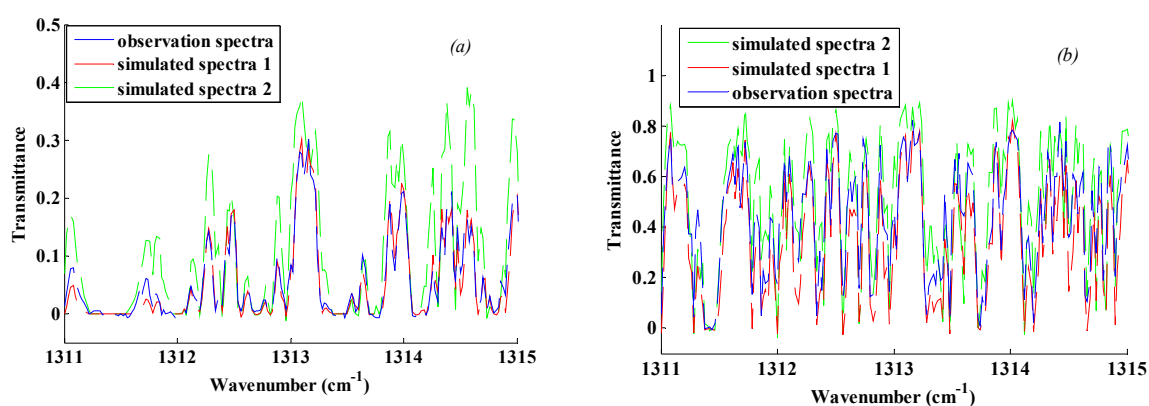
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Figure 2 The technological process of constructing the integrated atmospheric profiles.

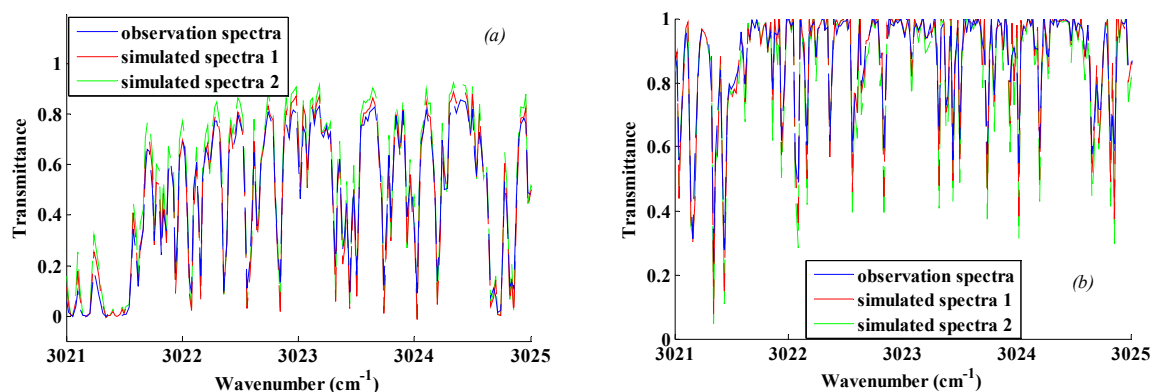
197 The next step is to combine the two sets of profiles. Since ACE-FTS and AIUS have similar  
 198 instrument characteristics, the ACE-FTS product is chosen in case that the profile of a particular  
 199 species at the same geolocation and time can be found in both ACE-FTS and MLS datasets. Finally,  
 200 profiles of the missing species are read from the AFGL dataset. The species profiles imported from  
 201 AFGL dataset include NH<sub>3</sub>, HBr, HI, PH<sub>3</sub>, H<sub>2</sub>S, F11, F12, F13, F21, F22, F114, F115 and HNO<sub>4</sub>. These  
 202 species profiles from FASCOD (Fast Atmospheric Signature Code) Model 1-6 are resampled and  
 203 packed into the monthly geographic grids. In the end, the integrated atmospheric species profiles  
 204 dataset is produced.

#### 205 4.2 Data simulation and sensitivity analysis

206 A comparison between the integrated atmospheric and AFGL profiles is carried out by  
 207 simulating the ACE-FTS spectra. The simulation is made with the geolocation and geometry  
 208 parameters of the ACE-FTS instrument. Figures 3 and 4 compare the simulated ACE-FTS using the  
 209 two atmospheric profiles database to the observed spectra in two spectra ranges.



210 Figure 3 Comparison experiment between the integrated atmospheric and AFGL profiles (67.5°S,  
 211 72.5°W, August 5, 2012). (a) Tangent height=10.71 km; (b) Tangent height=20.48 km.



212 Figure 4 Comparison experiment between the integrated atmospheric and AFGL profiles (77°S, 86°E,  
 213 March 25, 2012). (a) Tangent height=16.16 km; (b) Tangent height=30.4 km.

215 The simulated spectra 1 and 2 stand for the ones using the integrated atmospheric and AFGL  
 216 profiles, respectively. Figures 3 and 4 show that in both spectral ranges, the simulated spectra using  
 217 the integrated atmospheric profiles are obviously more close to the ACE-FTS observed spectra than  
 218 those using the AFGL atmospheric profiles. The two comparison experiments demonstrate that the  
 219 simulated spectra are very sensitive to the atmospheric profiles and that the simulated spectra using  
 220 the dataset of integrated atmospheric profiles agree well to the actual measurements.

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223 5. O<sub>3</sub> retrieval and assessment

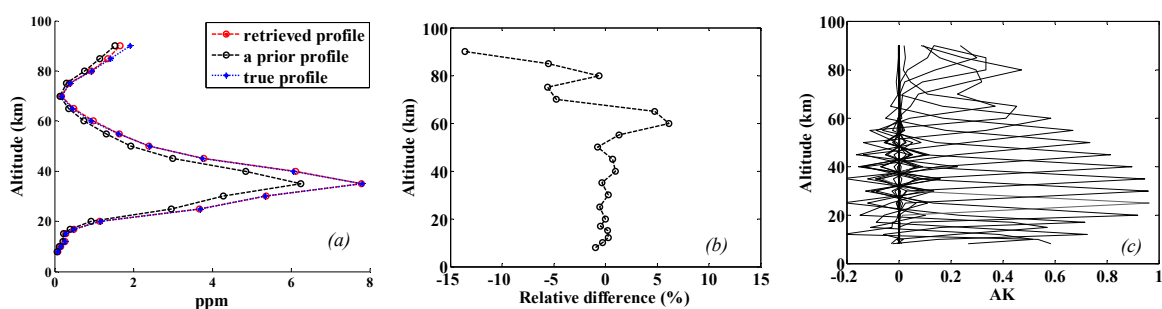
## 224 5.1 Assessment of retrieval algorithm based on simulated spectra

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Table 1 Retrieval configuration	
Parameters	Retrieval configuration
spectroscopic database	Hitran 2012 [32]
continua used	O <sub>2</sub> , H <sub>2</sub> O, N <sub>2</sub>
Retrieval altitude grids /km	8 10 12 15 17 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90
altitude grids in the forward model	0-100 km with 1 km resolution
O <sub>3</sub> true profiles ( $X_{true}$ )	Taken from integrated atmospheric database
$X_a$	$0.8 \cdot X_{true}$

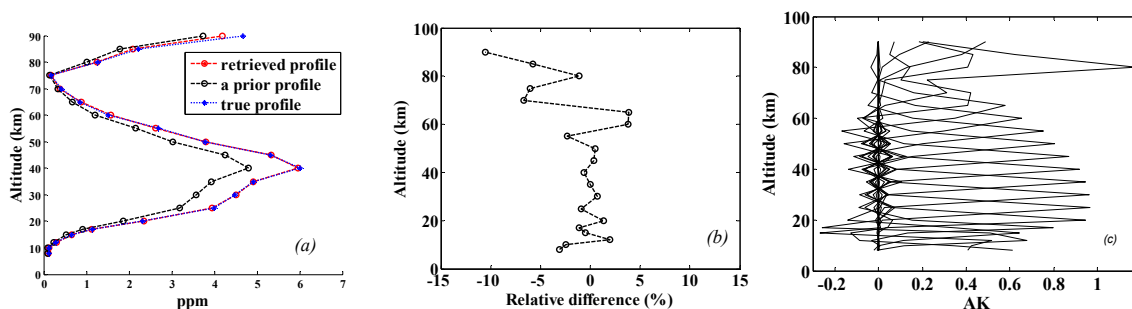
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227 The O<sub>3</sub> retrieval performance is first assessed by using simulated measurements. The  
 228 microwindows selected in section 3.3 are adopted. Two O<sub>3</sub> profiles picked from two grids of the  
 229 integrated atmospheric dataset (75°S, 150°W in October and 65°S, 90°E in March) are taken as the  
 230 true profiles to simulate spectra of AIUS. Then, the artificial noise with SNR = 300 is added to the  
 231 simulated spectra. Details of retrieval configuration are specified in Table 1. The retrieved profiles  
 232 are shown in Figure 5 and 6.



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234 Figure 5 O<sub>3</sub> retrieval experiment based on simulated spectra at 75°S, 150°W in October. (a) Retrieved  
 235 profile; (b) Relative difference between retrieved and true profiles; (c) Averaging kernel.



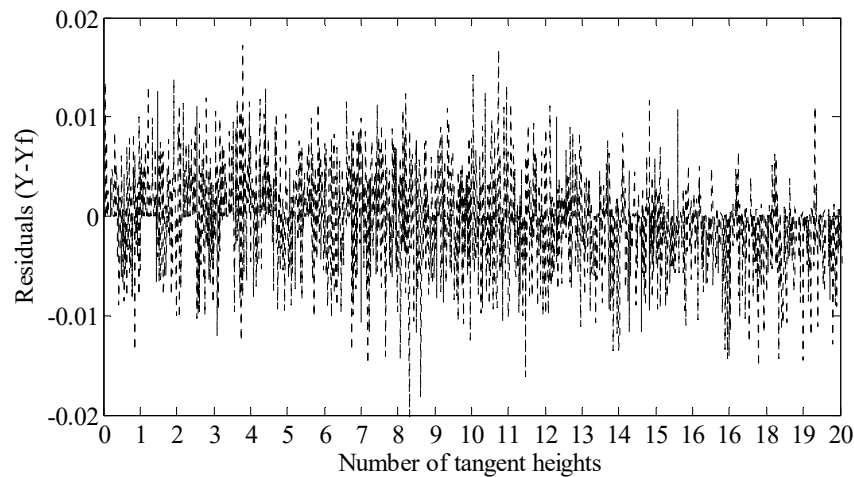
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237 Figure 6 O<sub>3</sub> retrieval experiment based on simulated spectra at 65°S, 90°E in March. (a) Retrieved  
 238 profile; (b) Relative difference between retrieved and true profile; (c) Averaging kernel.

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240 The a priori, true profile and retrieval profile of O<sub>3</sub> are shown in figure 5(a) and 6(a). The shape  
 241 and the values of retrieval profiles are consistent with the true profiles. The relative difference  
 242 between the retrieval and true profiles presented in figure 5(b) and 6(b) shows that it is within ±5%  
 243 below 60 km, within ±7% from 60 km to 80 km. The averaging kernels in figure 5(c) and 6(c) illustrate  
 244 that the retrieval information mainly comes from the measurements.

245 As the residual in both experiments seems nearly identical, only the one in the first experiment  
 246 is shown in Figure 7. The lowest to the highest tangent heights is from left to right. The residuals at  
 247 each tangent height are within  $\pm 0.02$ , which are very small.



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Figure 7 The residuals of the first retrieval experiment.

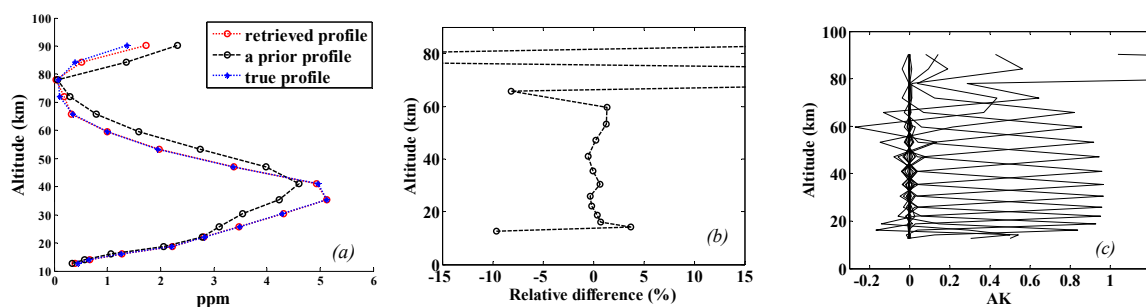
250 In the above retrieval experiments,  $X_a = 0.8 \cdot X_{true}$ , but the shape is the same. Thus, more  
 251 retrieval experiments are made to assessment the dependence of the AIUS algorithm on the shape of  
 252 the a prior profile. In this experiment, the ACE-FTS O<sub>3</sub> level 2 products are taken as the true profiles.  
 253 The information of five products selected is shown in table 2. The a prior profiles are from the mean  
 254 monthly profiles of MLS O<sub>3</sub> level 2 products, which indicates that the shape of the a prior profiles  
 255 can be different from that of the true profiles.

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Table 2 Information of O<sub>3</sub> L2 products from ACE-FTS.

Scene ID	latitude	longitude	date
40993	-78	87	2012-3-25
39926	-68	131	2011-1-11
38154	63	-73	2010-9-13
43544	63	75	2011-9-14
43611	70	-119	2011-9-18

257 Similarly, the artificial noise with same SNR is added randomly to the simulated spectra. O<sub>3</sub>  
 258 retrieval is performed and the results for these five retrieval experiments are similar. Thus, only  
 259 results of two retrieval experiments using the O<sub>3</sub> products from scenes of 40993 and 38154 are  
 260 presented in Figures 8 and 9, respectively. The two scenes are located in Antarctica and Arctic,  
 261 respectively.



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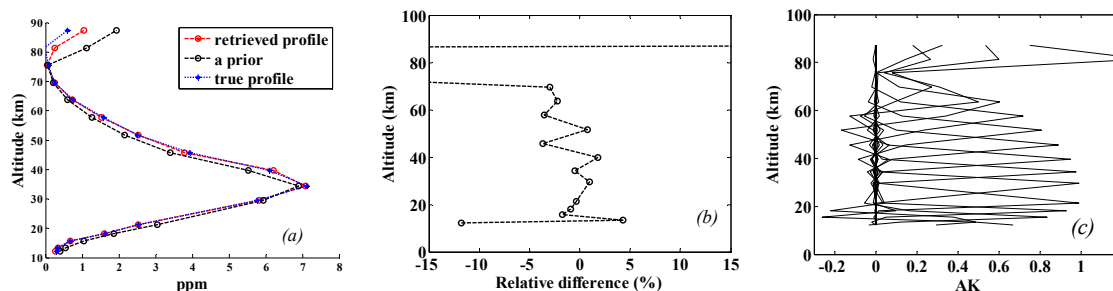
Figure 8 O<sub>3</sub> retrieval experiment based on O<sub>3</sub> product from scene 40993 of ACE-FTS. (a) Retrieved profile;

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(b) Relative difference between retrieved and true profile; (c) Averaging kernel.





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Figure 9 O<sub>3</sub> retrieval experiment based on O<sub>3</sub> product from scene 38154 of ACE-FTS. (a) Retrieved profile; (b) Relative difference between retrieved and true profile; (c) Averaging kernel.

Figures 8(a) and 9(a) show that the shape of the retrieval profiles is almost the same with the true profiles even that the shape of the a priori profiles is different from that of the true profiles. Figures 8(b) and 9(b) illustrate that the relative difference between the retrieval O<sub>3</sub> profiles and the true O<sub>3</sub> profiles is almost within 5% from 10 km to 70 km, about 10% near 10 km. However, the relative difference will reach beyond 30%. The reasons may be due to the low concentration of O<sub>3</sub> profiles and the retrieval above 70 km is dominated by the a priori information. The averaging kernels in Figures 8(c) and 9(c) are similar as those in Figures 5(c) and 6(c), which indicate that the retrieval information mainly comes from the measurement in the troposphere and stratosphere. We also check the residuals of these five retrieval experiments, which are consistent with the residuals in Figure 7. All residuals of these five retrieval experiments are within  $\pm 0.02$ .

The retrieval experiments using synthetic AIUS spectra demonstrate that the algorithm produces reasonable results and sufficient retrieval sensitivity.

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### 5.2 O<sub>3</sub> retrieval based on ACE-FTS measurements

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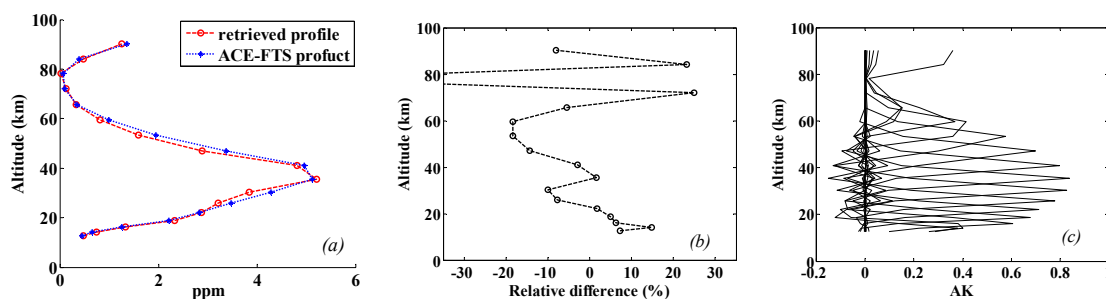
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Under real-world conditions, in addition to the thermal noise of the instrument, the actual measurements are influenced by more factors. To evaluate the influence of various uncertainties on the retrieval algorithm of AIUS, we adopt the level 1 products of ACE-FTS to perform the O<sub>3</sub> retrieval experiments, as AIUS expects to perform measurements with similar characteristics. All the a priori profiles of O<sub>3</sub> and other species are taken from the dataset of integrated atmospheric profiles. The level 1 products used are those five scenes of ACE-FTS observation data in table 2. Since the results for these five retrieval experiments are similar, only results of two retrieval experiments from scene 40993 and 38154 are presented.



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Figure 10 O<sub>3</sub> retrieval experiment based on FTS observation spectra from scene 40993. (a) Retrieved profile; (b) Relative difference between retrieved and FTS level 2 product; (c) Averaging kernel.

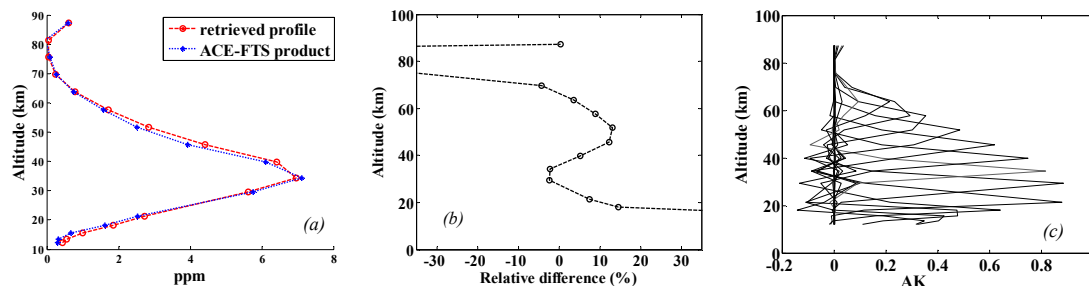


Figure 11 O<sub>3</sub> retrieval experiment based on FTS observation spectra from scene 38154. (a) Retrieved profile; (b) Relative difference between retrieved and FTS level 2 product; (c) Averaging kernel.

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The retrieval profiles, the relative difference and averaging kernels are shown in figure 10 and 11. The retrieval profiles presented in figure 10(a) and 11(a) show that the shape of the retrieval O<sub>3</sub> profiles agree well to those of ACE-FTS level 2 products. However, the relative difference in figure 10(b) and 11(b) is bigger than that in figure 8(b) and 9(b). The relative difference of these two retrieval experiment below 70 km is mainly within 10%, with some points reach 15%-20%. The relative difference here is larger mainly because of the uncertainties in the measurements and different forward model parameters. The bias of the ACE-FTS O<sub>3</sub> products is +1 to +8% in the stratosphere (16–44 km) and can be up to +40% (+20% on average) above 45 km (Jones A., et al., 2012; Dupuy E., et al., 2009). Although the averaging kernels in Figures 10(c) and 11(c) are somewhat broader than those in Figures 8(c) and 9(c), it still reveals that the retrieval information mainly comes from the measurement in the stratosphere. The statistical analysis of the residuals demonstrate that about 90% residuals are within  $\pm 0.02$ , with some points reaching  $\pm 0.06$ , demonstrating the retrieval fits very well. Our algorithm dedicated to AIUS performs stable and delivers comparable results using ACE-FTS real measurements.

## 313 6. Discussion and conclusions

314 In this study, we have introduced a retrieval algorithm developed for an infrared occultation  
315 spectrometer called AIUS. The retrieval algorithm comprises a forward model based on RFM and  
316 an OEM framework adapted from Qpack, which employs the LM iteration method. The retrieval  
317 experiments of ozone retrievals were carried out based on simulated spectra and ACE-FTS  
318 measurements.

319 In the condition of experiments on simulated spectra, there are some differences depending  
320 on the profile shape of the a prior. When the shape of the a prior is the same as the true profile, the  
321 relative difference between the retrieval profile and the true profile is within  $\pm 5\%$  below 60 km and  
322 within 7% in the range of 60-80 km. When the shape of the a prior is and the true profile is different,  
323 the retrieval profile shape still keep close to the true profile. The relative difference is a litter bigger.  
324 It is mainly within 5% below 60 km, but can reach 10% near 10 km and 10-15% from 60 km to 70 km.  
325 However, the relative difference is in a reasonable range. And the averaging kernels achieved  
326 illustrate that the retrieval information mainly comes from the simulated observation spectra. Thus  
327 the retrieval experiments based on simulated spectra indicate that the retrieval algorithm of AIUS  
328 work fine and successful.

329 When it comes to experiments based on ACE-FTS observation data, the retrieval algorithm of  
330 AIUS also behaves well. The retrieval experiments show that the relative differences between them  
331 are greater than those in the retrieval experiments using simulated spectra. The greater relative  
332 differences may be produced by the following reasons. Firstly, although the instrument parameters  
333 AIUS and FTS are similar, there must be different in some of the details. Thus, some errors will be  
334 brought by using ACE-FTS observation spectra as the AIUS observation spectra. Secondly, the  
335 ACE-FTS levels are not the true profiles. They also have uncertainties, which will make the relative  
336 difference greater. The last and the most important reason is the greater uncertainty of the observed  
337 spectra, which will generate some errors between the simulated spectra by the forward model and

338 the observation spectra in the retrieval process. Nevertheless, the retrieval profiles still agree well  
339 with the ACE-FTS level 2 products and the range of the relative differences is satisfactory.

340 All the retrieval experiments based on the simulated spectra and the measured spectra of  
341 ACE-FTS indicate that the retrieval algorithm of AIUS is reliable and robust. Overall, the retrieval  
342 profiles agree well with the true profiles or the ACE-FTS level 2 profiles. However, the uncertainties  
343 of the retrieval profiles at lower tangent height are still requiring further investigations. After the  
344 instrument is launched, we will improve the retrieval algorithm by fine-tuning the forward model  
345 parameters according to the characteristics of the AIUS observed spectra and the instrument  
346 performance. In addition, an extensive retrieval error characterization is on-going and will be  
347 consolidated during the operational phase.

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358 Mingmin Zou, Hongmei Wang, Yapeng Wang, Songyan Zhu and Jing Miao performed the experiments;  
359 Xiaoying Li, Tianhai Cheng, Jian Xu, Hailiang Shi, Xingying Zhang and Shule Ge analyzed the data; Xiaoying  
360 Li wrote the paper.  
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