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Nonlinear Retrieval of Atmospheric Ozone Profile from Solar Backscatter Ultraviolet Measurements: Theory and Simulation①

Li Jun (李　俊) and *Lu Daren* (吕达仁)
LAGEO, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100029
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ABSTRACT

The Solar Backscatter Ultraviolet and Total Ozone Mapping Spectrometer (SBUV / TOMS) instrument has provided useful data for deducing ozone vertical profiles and total ozone amounts. Although, data processing techniques for solving the inverse problem have been discussed, the retrieval accuracy still needs to be improved by developing new methodology. In this paper the Newtonian non-linear iteration method was applied to the Ultraviolet radiative transfer equation to retrieve the atmospheric ozone vertical distribution. In order to reduce the number of unknowns for retrieval and make the solution procedure more stable, the atmospheric ozone profile is represented by its Empirical Orthogonal Functions (EOFs) which can be derived from a set of global ozone profiles such as TIGR. Ozone retrievals based on simulated SBUV albedo measurements from 6 model atmospheres show the potential application of this method in operational processing of SBUV real observed measurements which will fly on the satellite such as NOAA-K.

Key words: Retrieval, SBUV

1. INTRODUCTION

There has been much interesting in atmospheric ozone in the last decades mainly due to its function in the complex middle atmospheric photochemistry and the critical ecological effect of ozone depletion induced by anthropogenic impacts and natural processes. The Nimbus-4 satellite was launched in 1970 with a Backscatter Ultraviolet spectrometer (BUV) to determine the atmospheric ozone, then the Solar Backscatter Ultraviolet (SBUV) was launched aboard the Nimbus-7 and NOAA's TIROS-N satellite. The instrument description may be found elsewhere (Heath et al., 1975; 1978). The instrument measures the ultraviolet radiances backscattered by the earth and its atmosphere at 12 wavelengths from 2555 to 3399°A. Up to 8 shorter wavelengths (2555, 2735, 2830, 2876, 2922, 2975, 3019 and 3085°A) are used to infer the atmospheric ozone profile, while the other 4 longer wavelengths (3126, 3176, 3313 and 3399°A) are used to determine the total ozone amount.

Vertical ozone distribution can be retrieved by the mathematical inversion of the radiative transfer equation. The inversion problem here is ill-posed and needs additional information for conditioning (Li et al., 1994). The traditional way is so called "Pressure Increment Method" (Mateer, 1976) which needs to know the vertical distribution of air density. Also, there are several discussions on the ozone profile retrieval (Mateer, 1972; Rogers, 1976; McPeters, 1980), in almost all the processing techniques, the linear approach was adopted to solve the UV radiative transfer equation.

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Recently, the one dimension variational method was applied successfully to the inversion of infrared remote sensed radiance measurements (Li, 1996), this method was illustrated to be a good way for solving the inversion problems. In this paper, the same way was used to retrieve the atmospheric ozone profile from SBUV albedo measurements. Also, the ozone profile is represented by the linear combination of its Empirical Orthogonal Functions (EOFs) from TOVS Initial Guess Retrieval (TIGR) (Chedin et al., 1985) in order to reduce the number of unknowns and make the solution more stable. Retrievals from simulated SBUV albedo radiances based on 6 model atmospheres of tropical, mid–latitude summer, mid–latitude winter, subarctic summer, subarctic winter, and the U.S. standard atmosphere show that the ozone vertical distribution can be achieved with high accuracy from satellite based UV remote sensing.

II. FORWARD MODEL OF SBUV REMOTE SENSING

The solar UV radiance backscattered by the earth and its atmosphere depends on:

(1) absorption by atmospheric ozone;

(2) scattering by the atmosphere;

(3) scattering and absorption of atmospheric aerosols and clouds;

(4) reflectivity of the surface.

In addition, trace gases in the atmosphere have also absorption bands in UV. In the forward model consideration, the single–scattering case is assumed. In the earth's atmosphere, ozone is present at sufficiently high altitude that the solar UV at certain wavelengths can be totally absorbed within the atmosphere. Ozone absorption cross–sections, as shown in Fig. 1, reach maximum near 250 nm, then decrease roughly exponentially at longer wavelength. The normal amounts of ozone in the atmosphere are sufficient to absorb essentially all of the sunlight in the path to the ground at wavelengths less than 300 nm. Contribution functions of the SBUV are shown in Fig. 2, the altitude of the peak contribution decreases with wavelength, under some conditions only single scatter light is returned to space. For detail physical consideration of atmospheric UV remote sensing, refer to Krueger (1995).

The radiance of a sunlit, single–scattering, ozone–absorbing atmosphere viewed in the nadir Field of View (FOV) from a satellite at wavelength λ is given by

$$I(\lambda,\theta) = F_0(\lambda)\beta(\lambda)P(\theta)\int_0^{p_s} \exp[-(1+\sec\theta)(\alpha(\lambda)X(p)+\beta(\lambda)p]dp \quad (1)$$

where F_0 is the solar irradiance, β is the Rayleigh scattering coefficient, $P(\theta)$ is the Rayleigh phase function for solar zenith angle θ as follows

$$P(\theta) = \frac{1}{4\pi}[\frac{3}{4}(1+\cos^2\theta)], \quad (2)$$

α is the ozone absorption coefficient, and $X(p)$ is the integrated atmospheric ozone amount from the top of the atmosphere to pressure p. This expression is valid for the Earth's atmosphere for wavelengths shorter than 300 nm where essentially no UV light penetrates below the ozone maximum in the lower stratosphere. The ratio of $A_\lambda = I(\lambda) / F_0(\lambda)$ is called "albedo". Fig. 3 illustrates the simulated variations of Earth's albedo in the middle–ultraviolet spectral range of the tropical atmosphere.

The atmosphere are divided into 66 levels from 1 to 1050 hPa as follows:

1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140, 150,

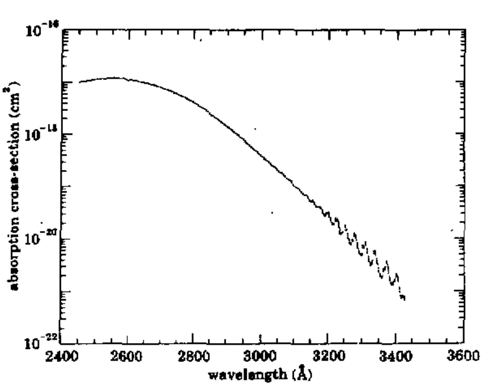

Fig. 1. The absorption cross-section of ozone at UV wavelengths (taken from Krueger, 1995).

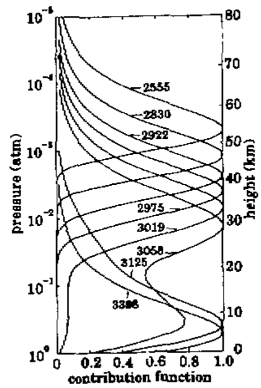

Fig. 2. Relative contribution functions for backscattered UV radiation at a solar zenith angle of 60° for several wavelengths (in °A units) used in nadir sounding (taken from Krueger, 1995).

160, 170, 180, 190, 200, 220, 240, 260, 280, 300, 320, 340, 360, 380, 400, 425, 450, 475, 500, 525, 550, 575, 600, 625, 650, 675, 700, 725, 750, 775, 800, 825, 850, 875, 900, 925, 950, 975, 1000, 1025, 1050.

All the calculations are based on the above 66-level coordinate.

III. NONLINEAR ITERATIVE METHOD FOR RETRIEVAL OF ATMOSPHERIC OZONE PROFILE

LAGEO ozone physical retrieval algorithm is based on the Newton nonlinear iteration method of solution of SBUV radiative transfer equation (RTE). Briefly, the physical retrieval algorithm begins with a first guess field of atmospheric ozone according to the difference between the observed albedo radiances and those computed from the first guess through RTE. The process is repeated until the residuals between the measured and calculated albedo radiances approach to a given small value. The first guess can be obtained from a climate mean or an empirical regression equation. In general, a good first guess reduces the number of iterations required and minimizes the impact of instrument noise and other uncertainties on the final solution.

Assuming that there are K wavelengths (channels) to observe the earth-atmosphere simultaneously at nadir, define $Y=(y_1, y_2, \cdots, y_K)^T$, where $y_i (i=1,2,\cdots,K)$ is the albedo radiance of the ith channels, thus, retrieval of the atmospheric ozone profile from the SBUV albedo radiances means to solve the following equation

$$J(X) = \| Y^m - Y(X) \| = \text{Minimum}, \quad (3)$$

where the Y^m is the vector of satellite observations; $Y(X)$ is the vector of computed albedo radiances from the ozone state X; $X=(x_1, x_2, \cdots, x_L)^T, x_j (j=1,2,\cdots,L)$ is the integrated ozone amount from the top of atmosphere to pressure level p_j. Since the problem is ill-posed, additional condition is required to stabilize the solution, here the first guess is used as a constraint in the solution, therefore the $J(X)$ becomes

$$J(X) = \| Y^m - Y(X) \|^2 + \gamma \| X - X^0 \|^2, \quad (4)$$

where X^0 is the first guess of X, γ is the Lagrange factor.

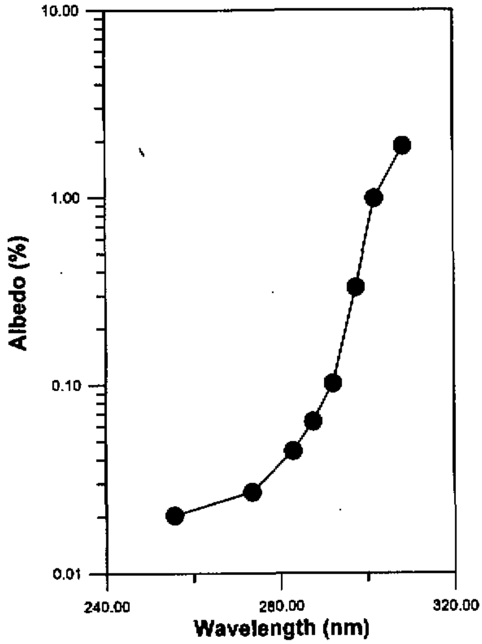

Fig. 3. The simulated variations of Earth's albedo in the middle–ultraviolet spectral range of the tropical atmosphere.

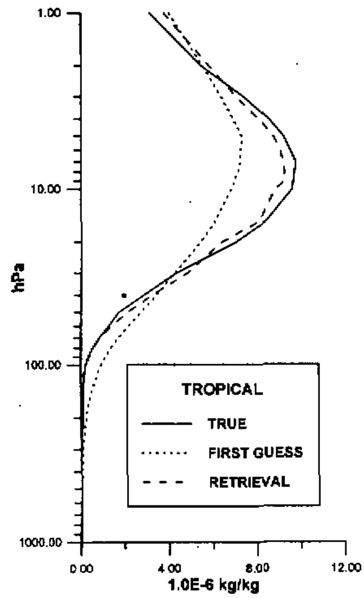

Fig. 4. The atmospheric ozone profile retrieval for tropical atmosphere.

The definition of norm $\| \cdot \|$ has influence on the final solution, the norm is a kind of "distance", the Mahalanobian distance is more suitable to the satellite data application (Li et al., 1990), therefore define

$$\| Y^m - Y(X) \|^2 = [Y^m - Y(X)]^T E^{-1} [Y^m - Y(X)], \tag{5}$$

$$\| X - X^0 \|^2 = (X - X^0)^T B^{-1} (X - X^0), \tag{6}$$

where E is the error covariance matrix of satellite observations which includes the instrument noise and the forward model error, B is the error covariance matrix of X^0.

The purpose of retrieval is to solve X from Eq. (4), the traditional linear approach is just set $J'(X) = 0$, that means

$$0.5J'(X) = \gamma B^{-1}(X - X^0) - F^T \cdot E^{-1} \cdot [Y^m - Y(X)] = 0, \tag{7}$$

where F is the first derivatives of $Y(X)$ with respect to X, or the weighting function matrix. With the expansion of the first order

$$Y(X) = Y(X^0) + F \cdot (X - X^0). \tag{8}$$

Substituting Eq.(8) into Eq.(7), we have the solution form

$$X = X^0 + (F^T \cdot E^{-1} \cdot F + \gamma\beta^{-1}) \cdot F^T \cdot E^{-1} \cdot [Y^m - Y(X^0)], \tag{9}$$

Eq.(9) is the traditional linear iterative form.

Since the high nonlinearity of SBUV albedo radiance with respect to ozone profile, the Newtonian nonlinear iteration method is applied here to solve the RTE as follows:

$$X_{n+1} = X_n - J''(X_n)^{-1} \cdot J'(X_n), \tag{10}$$

from Eq.(7), we have

$$0.5J''(X) = \gamma B^{-1} + F^T \cdot E^{-1} \cdot F - F^T \cdot E \cdot [Y^m - Y(X)], \tag{11}$$

if we consider $[Y^m - Y(X)]$ is small at the minimum, Eq.(11) becomes

$$0.5J''(X) = \gamma B^{-1} + F^T \cdot E^{-1} \cdot F. \tag{12}$$

By matrix manipulation based on Eqs.(7), (10), (12), we arrive at the Newtonian quasi–nonlinear iterative form

$$\delta X_{n+1} = (F_n^T \cdot E^{-1} \cdot F_n + \gamma B^{-1}) \cdot F_n^T \cdot E^{-1} \cdot (\delta Y_n + F_n \cdot \delta X_n), \tag{13}$$

where

$$\delta X_n = X_n - X^0, \tag{14}$$

$$\delta Y_n = Y^m - Y(X_n). \tag{15}$$

In the iteration procedure, the weighting function matrix $F = (f_{ij})$ is calculated through RTE by numerical perturbation as follows:

$$f_{ij} = \frac{\partial y_i}{\partial x_j} = \frac{y_i(x_j + \Delta x_j) - y_i(x_j)}{\Delta x_j}. \tag{16}$$

Since the effective information content of satellite observation is limited (Zeng, 1974), only a limited number of variables can be retrieved to explain the vertical variation of atmospheric ozone profile. The number of independent variables can be obtained from a set of global samples of atmospheric ozone profiles. Here the structure functions are defined from Empirical Orthogonal Functions (EOFs) analysis of the global TIGR data set, then the number of atmospheric variables for retrieval is significantly reduced. Table 1 is the cumulative percentage of variances explained by the first 10 EOFs, from Table 1 it can be seen that the first 5 EOFs explain almost all the variances. Therefore assume

$$\delta X = \Phi A, \tag{17}$$

Table 1. The Percentage of Variance Explained by the First 10 EOFs from TIGR

No.	%	Cumulative %
1	71.8135	71.8135
2	20.7155	92.5290
3	4.3845	96.9135
4	1.5914	98.5049
5	1.3171	99.8220
6	0.1210	99.9431
7	0.0269	99.9700
8	0.0135	99.9835
9	0.0004	99.9899
10	0.0001	99.9949

where $A = (\alpha_1, \alpha_2, \cdots, \alpha_{\tilde{N}})$, Φ is the matrix of the first $\tilde{N}(=5)$ EOFs of ozone profiles, it is obvious that

$$\Phi^T \Phi = I. \tag{18}$$

Then the cost function becomes:

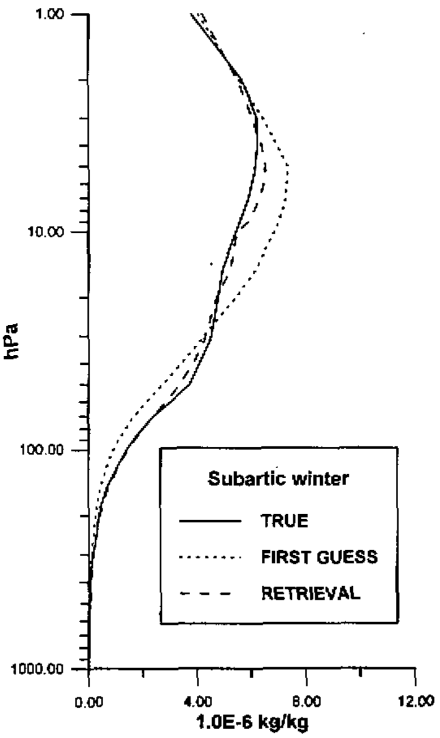

Fig. 5. The atmospheric ozone profile retrieval for subarctic winter atmosphere.

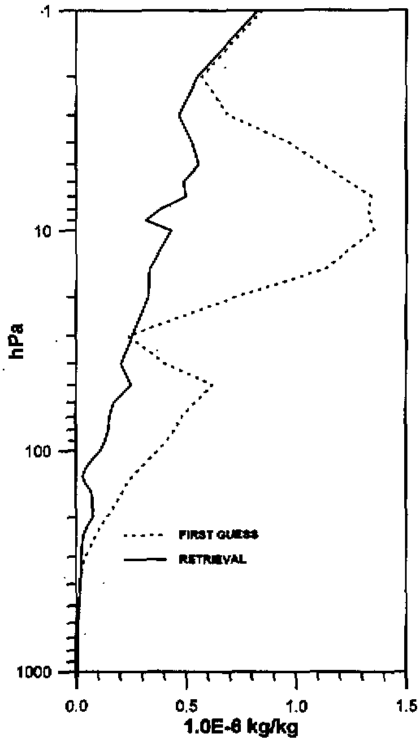

Fig. 6. RMSE distribution of total retrieval from 6 atmospheres of tropical, mid-latitude summer, mid-latitude winter, subarctic summer, subarctic winter and U.S. standard atmosphere.

$$J(A) = [Y^m - Y(A)]^T \cdot E^{-1} \cdot [Y^m - Y(A)] + \gamma A^T \cdot B_A^{-1} \cdot A, \tag{19}$$

following Eqs.(7), (10), (11), (12), we get another iteration form

$$A_{n+1} = (\tilde{F}_n^T \cdot E^{-1} \cdot \tilde{F}_n + \gamma B_A^{-1})^{-1} \cdot \tilde{F}_n^T \cdot E^{-1} \cdot (\delta Y_n + \tilde{F}_n \cdot A_n), \tag{20a}$$

$$X_{n+1} = X^0 + \Phi A_{n+1}. \tag{20b}$$

where $B_A^{-1} = \Phi^T B^{-1} \Phi, \tilde{F} = F \cdot \Phi$.

V. RETRIEVAL OF ATMOSPHERIC OZONE PROFILE FROM SIMULATED SBUV OBSERVATIONS

In this paper, the simulation is performed to test the retrieval algorithm described above. Six model atmospheres of tropical, mid-latitude summer, mid-latitude winter, subarctic summer, subarctic winter, and U.S. standard atmosphere are used to simulate the observed SBUV albedo radiances, assumed $\sqrt{2}$ observation error which includes the instrument noise and surface uncertainties is added to albedo radiances constant for each SBUV channel, and the solar zenith angle is set to be zero for simplicity. Channel 1 is not used in the retrieval due to the absorption of NO_x at this wavelength, also Channels 7 and 8 are not used since the multiscattering and surface uncertainties at these two wavelengths. The mean atmospheric

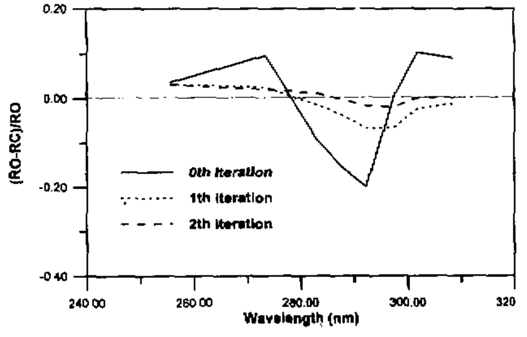

Fig. 7. Residual albedo spectra of the first two iterations of the tropical retrieval.

ozone profile of TIGR was used as the first guess in the retrieval procedure, the error covariance matrix E is set diagonal, constant for each channel as mentioned. The variance matrix of TIGR is used instead of the error covariance matrix of the first guess. The first 5 EOFs from TIGR as indicated in Table 1 are used to represent the vertical variation of atmospheric ozone profile. Fig. 4 is the retrieval of ozone mixing ratio profile for tropical atmosphere. It can be seen from Fig. 4 that the first guess (TIGR mean ozone profile) has less ozone concentration at the stratosphere, while the retrieval adjusted from such relatively poor first guess is very close to the true vertical distribution. Fig. 5 is the same as Fig. 4 but for retrieval of subarctic winter, it is interesting to see that the structure of the first guess is reverse to that of the true distribution with more ozone concentration at the upper stratosphere but less at the low stratosphere, while the retrieval makes the vertical structure of the first guess be adjusted very close to the true distribution. Fig. 6 is the Root Mean Square Error (RMSE) distribution of total 6 retrievals, the RMSE of retrievals is reduced significantly in comparison with that of the first guess.

Since the Newtonian nonlinear iteration is a kind of deepest descent iterative solution method, the iterative converge is very fast during the iteration, Fig. 7 is the residual spectra of the first two iterations of the ozone profile retrieval for the tropical atmosphere, the RO and RC are the observed and calculated albedos respectively. In general, two iterations will make the residual be the observation error level.

IV. CONCLUSIONS

Following conclusions are remarkable:

(1) The Newtonian iteration is suitable for solving the SBUV radiative transfer equation for the ozone profile retrieval.

(2) In order to reduce the number of unknowns and make the solution more stable, the ozone vertical structure can be represented by the linear combination of its EOFs which can be derived from a set of global sample data such as TIGR.

(3) Retrievals from simulated SBUV albedo radiances show that high accuracy ozone profile is achievable by use of the algorithm described in this paper.

Further works on SBUV real data processing based on this method will be carried out in the near future at LAGEO, IAP / CAS.

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