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An evaluation of infrared microwindows for ozone retrievals using the Eureka Bruker 125HR Fourier transform spectrometer

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ABSTRACT

A Bruker 125HR Fourier transform spectrometer was installed at the Polar Environment Atmospheric Research Laboratory (PEARL) at Eureka, Nunavut, Canada in the summer of 2006 to study atmospheric composition. Using the optimal estimation method, typically over a limited spectral region called a microwindow, information about the vertical distribution of trace gas species that have absorption bands in the mid-infrared spectral range can be retrieved. Total and partial columns can also be determined to show the temporal evolution of the target gas. For ozone in particular, retrievals have been performed using several of its many mid-infrared absorption features, resulting in a lack of consistency in the literature in the microwindows chosen for retrievals. This work focuses on the optimization of the ozone retrieval, assessing a set of 22 microwindows between 780 and 3052 cm^{-1} to determine which is best suited to conditions at Eureka. The 1000–1004.5 cm^{-1} spectral interval is shown to be the most sensitive to both the stratosphere and troposphere. This microwindow gives the highest number of degrees of freedom for signal ($\sim$7 for total column), and the smallest total error (4.3%) compared with 21 other spectral regions. Retrievals performed with this microwindow agree well with results obtained from other instruments on-site. Total column ozone measured by the Bruker 125HR in this microwindow agreed to 2% with two other Fourier transform spectrometers, to 0.7% with a Brewer spectrophotometer, to 8% with a SAOZ UV–VIS spectrometer, and to 7% with ozone sondes.

1. Introduction

Ozone is a naturally occurring substance which was first made in the laboratory in 1839 by Schönbein [1,2]. It is well known as an important component of our atmosphere, as it strongly absorbs solar ultraviolet (UV) radiation.

Total ozone column measurements in the first half of the twentieth century were mostly based on photometry in the UV wavelength range from 300 to 340 nm. Fabry and Buisson were the first to measure the atmospheric ozone column using a double spectrograph [3–5]. In the mid 1920s, Dobson designed the Fery spectrograph [6], which led to the development of the Dobson spectrophotometer which, in combination with its successor, the Brewer spectrophotometer [7], remains the backbone of the global ground-based ozone monitoring network today.

Many other techniques and instruments have since been developed to measure ozone concentrations. The

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Table 1
Infrared microwindows previously used for ozone retrievals.

Reference	Spectral range (cm^{-1})	Interfering species (if available)
Vigouroux et al. [37], Senten et al. [38]	1000–1005	H_2O, CO_2, C_2H_4, O_3(668), O_3(686)
Wunch et al. [39], Taylor et al. [40]	3039.90–3040.60	H_2O, CH_4
	2775.68–2776.30	CH_4, CO_2, HCl, N_2O
	2778.85–2779.20	CH_4, HDO, N_2O
	2781.57–2782.06	CH_4, HDO, N_2O, CO_2
Yamamori et al. [41], Kagawa et al. [42]	3051.29–3051.90	H_2O, CH_4, HDO, CH_3D
Sung et al. [43], Fu et al. [30]	2775.78–2775.88	HCl, N_2O, CH_4
	2775.68–2776.30	
	2778.90–2779.50	CH_4, CO_2, HCl, N_2O, HDO, solar lines
	2781.54–2782.09	
	1104.78–1105.08	CH_3D, CHF_2Cl, CCl_2F_2, H_2CO_2, HDO, O_3(668)
	1119.73–1119.95	CHF_2Cl, N_2O, O_3(668)
	1121.67–1122.03	O_3(668), H_2CO_2, CHF_2Cl, N_2O, H_2O
	1122.84–1123.06	O_3(668), H_2CO_2, CHF_2Cl, CH_3D, CH_4, H_2O
	3039.80–3041.70	CH_4, H_2O, CH_3D
Griesfeller et al. [44]	782.561–782.861	Not available
	788.850–789.369	
	1000.0–1005.0	
Hase et al. [45], Schneider et al. [35,18]	782.56–782.86	H_2O, CO_2, solar lines
	788.85–789.37	H_2O, CO_2, solar lines
	993.3–993.9	H_2O, CO_2, O_3(668), O_3(686)
	1000.0–1005.0	
	1007.3–1009.0	H_2O, CO_2, O_3—all isotopologs
	1011.1–1013.6	
Meier et al. [46]	3039.75–3040.55	CH_4, H_2O
	3045.08–3045.38	CH_4
Barret et al. [17]	1002.567–1003.2	O_3(668), O_3(686)
	1000.0–1005.0	O_3(668), O_3(686), H_2O
Notholt et al. [47]	1002.58–1003.50	H_2O
	1003.90–1004.38	H_2O
	1004.58–1005.00	H_2O
Goldman et al. [48]	3045.08–3045.38	
	3027.42–3027.60	
Hamdouni et al. [16]	2107.80–2107.86	not available
	2780.81–2780.96	
	3037.32–3037.80	
Pougatchev et al. [20,15]	1002.567–1003.203	
Rinsland et al. [49]	764.03–764.43	
	773.20–773.38	
	781.08–781.25	CO_2
	1127.60–1129.50	HDO, CH_4
	1146.40–1146.56	
	1146.55–1147.40	N_2O, H_2O, HDO
	1155.39–1155.56	
	1162.85–1163.50	
	1163.34–1163.48	
	1167.50–1167.75	
	2083.50–2084.72	H_2O, CO_2
	2754.55–2755.45	HDO, CH_4, solar lines
	2778.90–2779.20	
	2781.60–2781.86	HDO
	2792.65–2793.28	N_2O, HDO, solar
	3040.00–3040.90	H_2O, CH_4
Adrian et al. [50], Wegner et al. [51]	996.5–998.5	H_2O, CO_2
	2768.0–2773.0	HDO, H_2O, N_2O, CH_4
	2773.0–2776.0	CH_4, N_2O, HDO, HCl

References are specified along with the spectral range used and the interfering species when they were available. The numbers in brackets for O_3 define its isotopes, with 6,7, and 8 indicating ^{16}O, ^{17}O, and ^{18}O, respectively.