ESMOSII/NDSC - IR SPECTRAL FITTING ALGORITHMS INTERCOMPARISON EXERCISE

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INTRODUCTION

Since 1990, a number of European groups with remote sensing observational and related analytical capabilities have been financed by national and international organizations within the frame of ESMOS (European Stratospheric MOnitoring Stations), to conduct a series of activities as a precursor/complementary effort in support of the maturing global Network for the Detection of Stratospheric Change (NDSC). Key tasks which ESMOS participants resolved to investigate dealt with the performances of available instruments for atmospheric remote measurements from the ground and the validation of codes needed to convert such measurements into geophysical parameters.

In the following pages, we report the main results and conclusions from a first phase intercomparison exercise of infrared spectral fitting algorithms (also called "codes" hereafter) conducted as part of the above mentioned effort and coordinated by the Liège group. Non-european colleagues involved in the NDSC activities who manifested their interest to participate in the exercise were provided with the related input data.

PARTICIPATING INSTITUTIONS

TABLE 1 lists the Institutions (with their abbreviations given between parentheses) and the contact persons which manifested their interest to participate in the exercise. Notice that UW and MPIC returned results derived jointly; ULG and LaRC used different versions of the same code. Three groups not listed in Table 1 failed to report any results.

INPUT DATA FOR THE EXERCISE

Two sample spectra for each of the target molecules HF, HCl, HNO$_3$ and N$_2$O, excerpted from wideband infrared solar spectra recorded in October 1992 at the International Scientific Station of the Jungfraujoch (ISSJ, Switzerland) by one of us (Ph.D.) were distributed for analysis. The first three molecules were selected because of their relevance to the overall objective of ESMOS (investigation of stratospheric gases), while N$_2$O was included to test the algorithms performances for a constituent having a vertical distribution quite different from the others. Also supplied were the following ancillary data and recommendations :

TABLE 1.-

Institution Name, Abbreviation and Representative(s)

National Physical Laboratory (NPL), Teddington, U.K.
W. Bell, P. Woods
Alfred Wegener Institut (AWI), Potsdam, Germany
J. Notholt
Institut für Meteorologie und Klimaforschung (IMK),
KFK, Karlsruhe, Germany
G. Adrian, T. von Clarmann
University of Wollongong (UW), Australia,
D. Griffith
Max Plank Institut für Chemie (MPIC), Mainz, Germany
D.W. Arlander
Institute of Astrophysics - Univ. of Liège (ULG), Belgium
Ph. Demoulin, E. Mahieu, R. Zander
Langley Research Center (LaRC), Hampton, VA, USA
C.P. Rinsland
University of Denver (UDe), Denver, CO, USA A. Goldman, D.G. Murcray University of Reims (URe),
Reims, France
A. Barbe, H. Hamid
Belgian Institute for Space Aeronomy (IASB),Brussels, Belgium
M. De Mazière, P.C. Simon
Jet Propulsion Laboratory (JPL), Pasadena, CA, USA
G.C. Toon

(a).- the observational and instrumental parameters pertinent to the distributed sample spectra (see TABLE 2)

(b).- a pressure-temperature model atmosphere given at successive 1-km altitudes above the ISSJ station, out to 90 km

(c).- a set of "initial best guess" volume mixing ratio (VMR) profiles provided on the same vertical grid as the physical model, for both the target molecules and for significantly interfering gases identified as H_2O, CH_4, O_3, OCS and NO_2

(d).- the limits of the spectral intervals over which to perform the analysis

(e).- adoption of the HITRAN-1992 spectroscopic line parameters compilation throughout the exercise.

The purpose of the exercise was primarily to fit the distributed sample spectra, taking into account the above points (a) to (e), and to derive vertical column abundances above ISSJ for the target molecules by solely scaling the distributed VMR profiles. If justified and documented, the groups could further improve their fits by tuning some input parameters (i.e., modifying the shape of the VMR profile; adjusting the instrumental line shape function;...).

The results were collected at Liège and kept anonymous until the convening of a workshop where each participating group would briefly describe his code and present details about his findings.

TABLE 2. – SPECTRA FOR ESMOS II / NDSC ALGORITHMS INTERCOMPARAISON EXERCISE – Phase 1

Infrared solar absorption spectra recorded with the ULg FTS instrument at ISSJ and used in the algorithms intercomparison exercise.

molec.	interval distributed (cm^{-1})	interval to be fitted (cm^{-1})	spectra identif.	date	mean ZPD time (UT+1)	apparent zenith angle	entrance diameter (mm)	S/N	max. path difference (cm)
HF	4033–4043	4038.80–4039.10	SSH961	07 oct 1992	9.168	66.44°	2.3	2290	62.42
			SSI152	15 oct 1992	11.625	55.85°	2.3	2760	62.42
HCl	2920–2930	2925.74–2926.06	SSH958	07 oct 1992	8.757	69.90°	2.3	1260	101.2
			SSH970	07 oct 1992	10.828	55.64°	2.3	1560	101.2
N_2O	2435–2445	2439.20–2440.00	SSH966	07 oct 1992	9.998	60.31°	2.3	1680	100.8
			SSI149	15 oct 1992	11.077	57.38°	2.3	2810	100.8
HNO_3	865–875	868.75–869.75	SSI031	13 oct 1992	7.766	80.55°	4.0	570	81.93
			SSI054	13 oct 1992	10.118	61.67°	4.0	860	81.93

Entrance focal length : 700 mm

TABLE 3. – RESULTS OF ESMOS II / NDSC ALGORITHMS INTERCOMPARAISON EXERCISE – Phase 1

Molecule	HF		HCl		N_2O		HNO_3		Remarks : scaling, plus
Spectrum Zen. angle (°)	SSH961 66.44	SSI152 55.85	SSH958 69.90	SSH970 55.64	SSH966 60.31	SSI149 57.38	SSI031 80.55	SSI054 61.67	
Institution									
	(E15)		(E15)		(E18)		(E16)		
A (NPL)	1.03	0.94	3.69	3.61	3.79	3.89	1.47	1.45	adjust apodization
B (AWI)	1.08	1.03	3.87	3.95	3.58	3.90	1.41	1.44	apparat. funct. approx.
C (IMK)	1.18	1.07	4.06	4.10	3.84	4.00	1.42	1.44	vertical shifting
D (UW+MPIC)	1.11	0.98	3.94	3.98	3.86	4.00	1.40	1.41	adjust apodization
E (ULg)	1.14	1.00	4.12	4.07	3.91	3.97	1.48	1.49	adjust apodization
F (LaRC)		1.01	4.22	4.19			1.48	1.47	adjust apodization
G (UDe)			3.96	3.96			1.45	1.45	adjust apodization
H (URe)	1.22	1.15	3.94	3.98	3.75	3.90	1.49	1.52	adjust apodization
I (IASB)	1.07	0.94	3.96	3.93	3.82	4.04	1.43	1.41	adjust apodization
J (JPL)	1.07	0.99	3.73	3.76	3.81	3.94	1.43	1.46	vertical shifting
Mean :	1.11	1.01	3.95	3.95	3.80	3.96	1.45	1.45	
St.dev. :	0.06	0.06	0.15	0.16	0.09	0.05	0.03	0.03	
St.dev. (%) :	5.4	6.2	3.9	4.0	2.4	1.3	2.1	2.2	
Extreme diff. (%)	16.9	20.1	13.4	14.9	8.8	3.8	6.2	7.5	

MAIN FINDINGS FROM THE EXERCISE

The results from the exercise have been intercompared and discussed during a workshop organized by one of us (G.P.A.) at the IMK, Karlsruhe, Germany, on June 17-18, 1993. With the exception of AWI and LaRC (see Table 1 for the abbreviations), all groups having produced results were represented. **TABLE 3** summarizes the vertical column abundances obtained by each group for the various spectra (LaRC and UDe, were unable to provide results for all spectra). The four bottom lines of Table 3 give, successively, the means of the reported columns (expressed in number molecules per cm^2), their standard deviations expressed both in molec./cm^2 and in % of the mean columns, and the extreme percent differences among the retrieved columns.

While the magnitudes of the standard deviations of the mean columns appear satisfactory at this first stage of the exercise, ranging from about $\pm$ 4 to $\pm$ 6 % for HF and HCl, and being less than $\pm$ 2.5 % for N_2O and HNO_3, individual results differ, however, by as much as 20 % for HF, 15 % for HCl, 8.8 % for N_2O and 7.5 % for HNO_3 (the extreme values are underlined in Table 3) and their causes need to be assessed. It was further noticed in Table 3 that the columns of HCl reported by ULG and by LaRC differ by some 3 %, while their results for HF and for HNO_3 are in excellent agreement; this difference is substantial when realizing that both groups use the same code, but different versions. With this exception, it appears that the codes used by the other groups have little "commonality" with each other, although many refer to various sub- routines which may well have some FASCODE-related origin.

Along the detailed presentations of the results, it was realized that, while all groups had indeed scaled the initial VMR profiles over the entire altitude domain, some (but not all, nor in a consistent fashion; see the Remarks in Table 3) had further applied vertical shiftings to the profiles or/and modified somewhat arbitrarily the apodization function along the fitting process (i.e., changing the diameter of the apparatus diaphragm; adopting a Norton and Beer apodization function;...), in order to minimize the residuals (observed minus calculated signals) and have their fits "look good". In particular, most groups reported computing too narrow HF and HCl lines when only scaling the initial VMR profiles and making straight usage of the distributed instrumental and atmospheric characteristics.

FIGURE 1 reproduces three fitting cases to the HF line of spectrum Nr. SSI152 and their residuals (as produced by one of us, C.P.R.), visualizing the typical effect of either keeping the instrumental line shape consistent with the reported instrument's characteristics (frame A) or letting it be adjusted by the algorithm so that the residuals minimize (frame B); in both cases, the initial HF VMR profile was scaled over its entire altitude domain. Notice the increase of about 7 % in the HF column retrieved from the B fit. Frame C shows the fit when minimizing the residuals by both scaling and shifting the initial HF profile, the instrument function being const-rained by the parameters of Table 2. The "best" fits B and C return identical vertical column abundances of HF above ISSJ, yet resulting from quite different fitting options, instrument-related in case B, atmosphere-related in case C. Such alternatives are intolerable when aiming at algorithm performances allowing to derive precisely and unambiguously the vertical column abundance of a target molecule and information on its concentration versus altitude.This requires that the characteristics of the observation instruments be perfectly known, in particular their apparatus function.
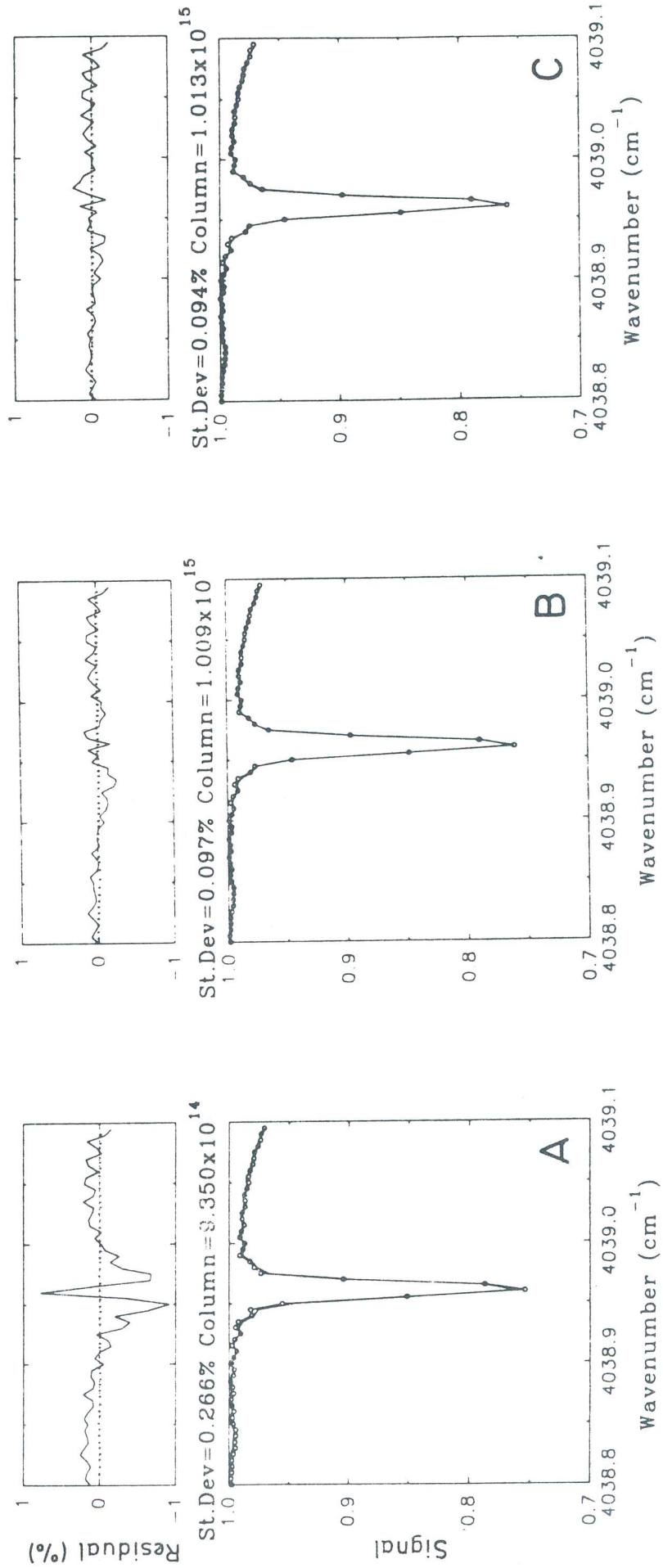
An attempt was made during the workshop to tabulate column abundances that had been obtained by the groups at an early stage of their retrieval process, i.e., when the initial VMR profiles were simply scaled and no allowance was made for adjusting the instrumental function

ESMOS II/NDSC-SSII52 HF RETRIEVAL

FIGURE 1

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or shifting the VMR profiles (i.e., case A in Fig. 1). While only seven groups had these initial columns on hand, the agreement among them was much better than among the corresponding ones given in Table 3, with the extreme differences in the columns never exceeding 5.5 % of the mean for any of the four target molecules. This last evaluation indicates that the algorithms involved do not contain gross anomalies.

CONCLUSIONS AND RESOLUTIONS

The first phase of the IR-spectral fitting algorithms intercomparison exercise has allowed to validate satisfactorily a number of codes for their gross consistency. It has further revealed the need for more discipline to be imposed in the forthcoming steps of the intercomparison exercise whose objective is to evaluate qualitatively the algorithms and to assess their ultimate performances (the aim is to have them to agree to better than ± 2 %). While bringing together a dozen of groups making use of such codes, the exercise has provided a mechanism allowing to increase confidence in the quality of the geophysical parameters derived through least squares spectral fitting. Light has been shed on the need for precise characterization of instruments used to acquire transmission spectra of the atmosphere, in particular their apparatus function which is critical for deriving information on VMRs versus altitude.

The follow-on of the exercise described here will be based on :

a.- the spectra already distributed supplemented by a few additional ones containing N_2 and/or CO_2 lines observed at low and high solar zenith angles (the column abundances of these constituents are well known)

b.- a physical model atmosphere in hydrostatic equilibrium

c.- improved VMR profiles for those molecules to be considered in the various fittings

d.- a series of guidelines restricting the forward calculation and fitting options

e.- a common format in which the calculated spectra as well as the residuals ought to be provided, allowing for easy intercomparison.

The additional input for the exercise will be distributed not later than October 10, 1993 and a second workshop to review the progress of the intercomparison and evaluate the overall uncertainty of vertical column abundances is scheduled for January- February 1994. The important issues dealing with the influence of the apparatus function on column abundance- and VMR profile retrievals, and the best way to determine it accurately will further be addressed.

ACKNOWLEDGEMENTS