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### **Operational trace gas retrieval algorithm for the Infrared Atmospheric Sounding Interferometer**

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[1] The Infrared Atmospheric Sounding Interferometer (IASI) is a nadir-viewing remote sensor due for launch on board the European Metop satellites (to be launched in 2005, 2010, and 2015). It is dedicated to the study of the troposphere and the lower stratosphere to support operational meteorology as well as atmospheric chemistry and climate studies. For this purpose, it will record high resolution atmospheric spectra in the thermal infrared, allowing the measurement of several infrared absorbing species. This paper describes the clear-sky retrieval scheme developed in the framework of the preparation of the IASI mission for the operational, near real time, retrieval of  $O_3$ ,  $CH_4$ , and COconcentrations. It includes the inversion module, based on a neural network approach, as well as an error analysis module. The studies undertaken on test simulations have shown that a performance of the order of 1.5%, 2%, and 5% for the retrieval of total columns of O<sub>3</sub>, CH<sub>4</sub>, and CO, respectively, can be achieved, and of the order of 28%, 15%, and 9% for the retrieval of partial columns of  $O_3$  between the surface and 6, 12, and 16 km high, respectively. The efficiency of the algorithm is demonstrated on the atmospheric measurements provided by the Interferometric Monitor for Greenhouse Gases (IMG)/ADEOS, allowing to obtain the first remote-sensing simultaneous distributions of ozone and its two precursors, CO and CH<sub>4</sub>. INDEX TERMS: 0325 Atmospheric Composition and Structure: Evolution of the atmosphere; 0365 Atmospheric Composition and Structure: Tropospherecomposition and chemistry; 0394 Atmospheric Composition and Structure: Instruments and techniques; 1640 Global Change: Remote sensing; KEYWORDS: atmospheric chemistry, trace gases, remote sensing

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### 1. Introduction

[2] The Infrared Atmospheric Sounding Interferometer (IASI) [*Phulpin et al.*, 2002], is a new tropospheric remote sensor to be carried for a period of 15 years on the Metop-1, 2, and 3 weather satellites deployed as part of the future EUMETSAT Polar System (EPS) starting from 2005. The instrument consists of a Fourier transform spectrometer associated with an imaging system, designed to measure passively the spectrum of the Earth-atmosphere system in

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the thermal infrared (IR) using a nadir geometry. It is a joint undertaking of the French spatial agency CNES (Centre National d'Etudes Spatiales) and EUMETSAT, the European Organisation for the Exploitation of Meteorological Satellites, with CNES managing the instrumental development part and EUMETSAT operating the instrument in orbit. Other space-borne instruments using the IR spectral range to probe the troposphere (e.g., AIRS [Pagano et al., 2001] on AQUA; MOPITT [Drummond and Mand, 1996] on TERRA, and TES [Beer et al., 2001] on AURA) should be flying during the IASI lifetime. The Interferometric Monitor for Greenhouse Gases (IMG) [Kobayashi et al., 1999], which operated in 1996–1997 on the Japanese ADEOS platform (until the failure of ADEOS due to the destruction of the solar paddle), was a forerunner of these missions, measuring a valuable set of infrared atmospheric spectra.

[3] The IASI mission will provide accurate measurements of the temperature profiles in the troposphere and lower stratosphere, as well as moisture profiles in the troposphere in order to improve the quality of numerical weather forecasts. It will also allow the probing of some of the chemical components playing a key role in the climate monitoring, the global change issues, and the atmospheric

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	Characteristics
Spectral range	$645-2760 \text{ cm}^{-1}$ (in 3 spectral bands)
Spectral resolution	$0.35 \text{ to } 0.5 \text{ cm}^{-1}$
Instrumental noise	0.2 to 0.35 K (NEDT at 280 K)
Pixel size	diameter of 12 km, 4 pixels matrix,
	across track scanning
Data rate	1.5 megabits per second
Lifetime	5 years
Power/Mass	200 watts/210 kg

 Table 1. IASI Instrumental Characteristics

chemistry. A summary of the main instrumental characteristics is provided in Table 1 (http://smsc.cnes.fr/IASI/ GP\_instrument.htm) and the requirements in terms of geophysical products and accuracy are detailed in Table 2 [*IASI Sounding Science Working Group (ISSWG)*, 1998].

[4] The scientific activities undertaken to prepare the IASI mission are coordinated through the ISSWG activities, under the auspice of CNES and EUMETSAT. It includes, among others, research work to improve spectroscopic databases [*Jacquinet-Husson et al.*, 2004], the development of fast radiative transfer codes [*Matricardi and Saunders*, 1999; *Matricardi*, 2003] and efficient inversion algorithm for the target species [*Prunet et al.*, 1998; *Hadji-Lazaro et al.*, 1999; *Lubrano et al.*, 2000; *Turquety et al.*, 2002; *Aires et al.*, 2002a; *Chédin et al.*, 2003; *Clerbaux et al.*, 2003], intercomparison exercises [*Tjemkes et al.*, 2002; *Clerbaux et al.*, 2002; *Newman and Taylor*, 2002; *Taylor et al.*, 2003], and data assimilation [*Clerbaux et al.*, 2001; *Rabier et al.*, 2002].

[5] IASI and all the instruments cited previously are passive remote sensors. One major difficulty of passive remote sensing comes from the fact that the satellite measurement is indirect, i.e. the information on the atmospheric state is provided through the analysis of spectral radiances. Inference of trace gas concentration from radiance measurements requires the development of a retrieval algorithm adapted to each instrument, which is a continuing effort for several research teams around the world [e.g., *Clerbaux et al.*, 1999; *Hadji-Lazaro et al.*, 1999; *Prunet et al.*, 2001; *Turquety et al.*, 2002; *Luo et al.*, 2002; *Aires et al.*, 2002b; *Coheur et al.*, 2003; *Deeter et al.*, 2003]. A strong constraint for IASI is associated with its near real-time delivery of data, requiring a very fast inversion procedure.

[6] This paper describes the Level 2 trace gas retrieval algorithm currently implemented in the EPS core ground segment for the operational analysis of carbon monoxide (CO), ozone (O<sub>3</sub>), and methane (CH<sub>4</sub>). After some general description of the inverse problem (section 2), the inversion scheme based on a neural network is presented (section 3). The sensitivity is accessed in terms of vertical resolution and accuracy, and the performance of the algorithm is evaluated (section 4). Synthetic IASI data were produced using radiance measurements from the IMG instrument to test the inversion algorithm (section 5), and conclusions for the achievable performance of IASI are provided (section 6).

### 2. Trace Gas Concentration Retrieval

### 2.1. General Description

[7] The IASI instrument is a nadir-looking remote sensing instrument which uses the Earth surface and its atmosphere as radiation source. While crossing the atmosphere, the IR radiation emitted is modified by the absorption, emission, and scattering properties of the atmosphere. The atmospheric spectrum recorded by the instrument in space is the result of the radiative interaction of the IR radiation with the atmosphere and is composed of thousands of absorption/ emission features organized in bands. The relationship between profile abundance for a target gas and the absorption lines is a complex non-linear function of the emitting surface features, the temperature distribution, the atmospheric elements contributing to the radiative budget in the same spectral range (other gases, clouds, aerosols), and also of the instrumental characteristics as spectral response function, spectral resolution, and radiometric noise. Atmospheric state variables such as temperature or trace gas concentration may be retrieved from the measured IR upwelling radiances using the so-called inversion algorithm.

[8] Let y be the measurement vector containing the measured radiances, and x be the concentration of a given constituent, then the general remote sensing equation can be written as follows [*Rodgers*, 2000]:

$$\mathbf{y} = \mathbf{f}(\mathbf{x}, \mathbf{b}) + \boldsymbol{\epsilon} \tag{1}$$

where f represents the forward radiative transfer function, **b** the other parameters having an impact on the measurement, and  $\boldsymbol{\epsilon}$  the measurement noise. In the case of a nadir sounding instrument measuring the IR radiation, the vector **b** includes the Earth surface radiative features (emissivity and temperature), variables describing the state of the atmosphere (vertical profiles of atmospheric temperature, water vapor and other atmospheric constituents, clouds, aerosols, etc.), and some characteristics of the instrument (spectral response function and resolution). The inverse problem consists in retrieving  $\hat{\mathbf{x}}$ , an estimate of the true state **x**, from the measurement **y**, and can be written:

$$\hat{\mathbf{x}} = \mathbf{R}(\mathbf{y}, \hat{\mathbf{b}})$$

$$= \mathbf{R}(\mathbf{f}(\mathbf{x}, \mathbf{b}) + \boldsymbol{\epsilon}, \hat{\mathbf{b}})$$
(2)

where  $\hat{\mathbf{b}}$  corresponds to an estimate of the non-retrieved parameters  $\mathbf{b}$ , and R is the inverse transfer function. The inversion of geophysical parameters from remotely sensed observations is well-known to be an ill-posed problem, which can not be entirely defined by the measurement. A priori knowledge of the state vector is required in order to

 Table 2. Scientific Products That Will Be Measured From the IASI Mission<sup>a</sup>

Geophysical Variable	Required Accuracy
Temperature profile	1K/1 km troposphere
Sea Surface Temperature	<0.5 K
Land surface temperature	1 K
Humidity profile	10%/1-2 km troposphere
Ozone total column	5%
Ozone profile <sup>b</sup>	10%
CO total column	10%
CH <sub>4</sub> total column	10%
N <sub>2</sub> O total column	10%

<sup>a</sup>The accuracy are provided for a 25 km horizontal resolution (averaged of 4 pixels) and for cloud-free conditions.

<sup>b</sup>Two to three pieces of independent information.



**Figure 1.** Schematic representation of the IASI trace gas inversion algorithm, providing total and partial (for  $O_3$  only) columns, and the associated error, for  $O_3$ , CH<sub>4</sub>, and CO.

determine the most probable solution, with a probabilistic Bayesian approach. This a priori information consists of an a priori state vector  $\mathbf{x}_a$  and its covariance matrix  $\mathbf{S}_a$ , which may be provided by a climatology or by model simulations. The inverse problem can then be rewritten:

$$\hat{\mathbf{x}} = \mathbf{R}(\mathbf{y}, \hat{\mathbf{b}}, \mathbf{x}_a) \tag{3}$$

### 2.2. IASI Trace Gas Retrieval Algorithm

[9] In the framework of the preparation of the IASI mission, a trace gas inversion algorithm is being developed to retrieve  $O_3$ , CH<sub>4</sub>, and CO concentrations from the IASI IR measurements, using several additional physical and geographical parameters. The structure of this algorithm is summarized by the diagram in Figure 1. It is divided into three steps: the first step consists in isolating the measurements (apodized IASI radiances, or Level 1C products, and additional geophysical products context from IASI measurements, or Level 2 products: note that the Level 1A data

correspond to the nonapodized calibrated spectra, and the Level 1B correspond to the Level 1A data resampled to nominal interval) which will be used as inputs to the inversion algorithm, an inversion module based on neural network (NN) techniques then estimates the trace gas concentrations using this input data, and an error analysis module finally provides information on the inversion characteristics as well as an estimate of the error associated with the inversion results, determined using auxiliary parameters.

[10] The input and output parameters of the inversion algorithm are detailed in the following paragraphs, and a description of the development of the inversion and error analysis modules is provided in the following sections.

### 2.2.1. Input Parameters

[11] Figure 2 represents an example of a partial IASI-like spectrum, which was obtained by adapting a spectrum recorded by the IMG instrument to the IASI characteristics following the method described in section 5.

[12] It exhibits strong  $O_3$ ,  $CH_4$ , and CO absorption features, enabling the global monitoring of these trace



**Figure 2.** Location on a IASI-like spectrum of the channels selected for the retrieval of  $O_3$ , CH<sub>4</sub>, and CO (in dark gray). The channels used for the calculation of the surface temperature are also indicated (in light gray).

gases. For each retrieved gas, m spectral channels corresponding to strong absorption features and minimizing the interferences due to other absorbing species have been selected [*Clerbaux et al.*, 1998]. They are indicated in Figure 2, and are provided in Table 3.

[13] The radiances measured by the instrument at these channels constitute the measurement vector y of equation (1). All the selected channels are used in the input vector, the information redundancy resulting in an increased signal to noise ratio. In order to minimize the unwanted contributions from the surface emissivity, aerosols, and, to a lesser extent, clouds (all these parameters being fixed during the development of the algorithm) a differential signal is used. The IASI radiances are subtracted from radiances referenced to a blackbody baseline, calculated using the Planck's law with mean emissivity values provided by Wilber et al. [1999] (these values could be replaced by IASI Level 2 emissivity data during the operational phase) and the surface temperature extracted from IASI radiances [Hadji-Lazaro et al., 2001]. The channel selection and this pre-processing imply that the inversion algorithm mainly uses absorption features of the studied species for the retrieval, even if some information in the wings of absorption lines may be lost in the process.

[14] In addition to the measurement vector  $\mathbf{y}$ , the inputs of the NN module include the skin surface temperature and the atmospheric temperatures on l selected pressure levels. These temperatures constitute the vector  $\hat{\mathbf{b}}$ , corresponding to an estimate of the most important parameters among the non-retrieved parameters  $\mathbf{b}$ . The pressure levels, indicated

in Table 4, have been chosen among the levels operationally retrieved during the IASI mission (RTIASI pressure levels [*Matricardi and Saunders*, 1999]). For  $O_3$ , a greater number of levels is required in order to provide information about the location of the tropopause.

[15] Hence, for each species, an input is composed of *m* differential Level 1C radiances (**y**), and *l* Level 2 temperatures ( $\hat{\mathbf{b}}$ ), with *m* and *l* being specific to each constituent. Some of the other parameters **b**, not used for the input to the NN, may have an impact on the retrievals and are used for the calculation of the error budget (as shown in Figure 1). They could be added as input parameters in forthcoming versions of the NN module. It currently includes the emissivity, the cloud content (derived from 5 AVHRR - Advanced Very High Resolution Radiometer [*Saunders and Kriebel*, 1988] - channels and the IASI imager), the H<sub>2</sub>O content, and geographical parameters like the surface altitude (or surface pressure), the longitude, and the latitude.

### 2.2.2. Output Parameters

[16] In order to evaluate the information content for  $O_3$ , CH<sub>4</sub>, and CO, we have undertaken preliminary sensitivity studies on simulated IASI spectra. The number of independent elements in the signal, the degrees of freedom for signal (DOFS) [*Rodgers*, 2000], has therefore been estimated. This study has shown that around 3.5 DOFS on the O<sub>3</sub> vertical distribution, 1.5 DOFS on the CO vertical distribution, and 1 DOFS on the CH<sub>4</sub> vertical distribution are available from the radiance signal. The vertical resolution for the retrieval of an O<sub>3</sub> concentration profile

Table 3. Radiances Selected for Each Trace Gas

		Spectral Interval,	IASI Channel	Number of	
Molecule		$cm^{-1}$	Number	IASI Channels	Total
$O_3$	1	1001.50-1003.00	1427-1433	7	
-	2	1005.00-1009.25	1441 - 1458	18	
	3	1011.50-1013.75	1467 - 1476	10	
	4	1015.25-1017.00	1482 - 1489	8	
	5	1018.50-1027.75	1495 - 1532	38	
	6	1033.75 - 1035.00	1556 - 1561	6	
	7	1035.75 - 1037.25	1564 - 1570	7	
	8	1037.75-1039.25	1572 - 1578	7	
	9	1039.75-1040.75	1580 - 1584	5	
	10	1041.75-1042.00	1588 - 1589	2	
	11	1043.75-1044.50	1596 - 1599	4	
	12	1045.50-1046.25	1603 - 1606	4	
	13	1047.50-1048.00	1611-1613	3	
	14	1049.75-1050.00	1620-1621	2	
	15	1052.50-1053.50	1631-1635	5	
	16	1054.25-1055.00	1638-1641	4	
	17	1056.25-1057.00	1646-1649	4	
	18	1057.50-1058.50	1651-1655	5	
	19	1061.00-1061.75	1665-1668	4	
	20	1063.25-1064.25	16/4-16/8	5	149
CH₄	1	1230.00-1230.25	2341-2342	2	140
4	2	1235.75-1236.00	2364-2365	2	
	3	1241.00	2385	1	
	4	1245.75	2404	1	
	5	1246.50	2407	1	
	6	1247.50-1248.00	2411-2413	3	
	7	1249.75-1250.00	2420-2421	2	
	8	1253.25-1253.75	2434-2436	3	
	9	1263.25-1263.50	2474 - 2475	2	
	10	1275.00-1275.25	2521 - 2522	2	
	11	1282.75-1283.50	2552 - 2555	4	
	12	1302.75-1306.50	2632 - 2647	16	
	13	1327.00-1327.50	2729-2731	3	
	14	1332.00-1332.75	2749 - 2752	4	
	15	1341.75-1342.00	2788 - 2789	2	
	16	1342.75-1343.00	2792-2793	2	
	17	1346.50-1347.00	2807 - 2809	3	52
CO	1	2111 25-2112 00	5866-5869	4	33
00	2	$2150\ 25-2150\ 75$	6022 - 6024	3	
	3	2154.00-2154.50	6037-6039	3	
	4	2157.75-2158.75	6052-6056	5	
	5	2165.00-2166.00	6081-6085	5	
	6	2168.75-2169.50	6096-6099	4	
	7	2172.50-2173.25	6111-6114	4	
	8	2176.25-2176.50	6126-6127	2	
					30

has been estimated to be 8 km in the free troposphere and 10 km in the lower stratosphere.

[17] For CH<sub>4</sub> and CO, the retrieval of a total column amount gives a good outline of their tropospheric distributions since their vertical concentration distributions are characterized by maximum concentration values in the lower layers of the atmosphere, as shown in Figure 3. For  $O_3$ , 90% of the total amount is located in the stratosphere, and the total column amount is therefore mostly influenced by its stratospheric concentration. Information on its vertical distribution is required in order to get access to its tropospheric concentration.

[18] The parameters calculated by the inversion algorithm, summarized in Table 5, are the total column for each species, as well as several partial columns for  $O_3$ , corresponding to integrated concentration amounts between the surface and (1) 6 km (*C*6): partial column

almost always located in the troposphere, whatever the latitude may be; (2) 12 km (C12): good approximation of the tropospheric column in the mid-latitudes; (3) 16 km (C16): good approximation of the tropospheric column in the tropics.

[19] In order to assess the performance that should be achieved for their retrieval, the variabilities of the columns have been evaluated by calculating the standard deviations of their global distributions over one year (represented by one day per month). This estimation is based on simulated atmospheric profiles used in the development of the NN module (see section 3.2 for a description of these profiles). Over the year, the total column O<sub>3</sub> varies by 2 to 5% in the tropics and by 5 to 10% at mid latitudes. The partial columns of  $O_3$  vary by 10 to 30% depending on the area: the variability is lower than 10% above clean areas and larger than 40% above polluted areas and above high latitude regions for C12 and C16. The temporal variability associated with the total column CH<sub>4</sub> is globally comprised between 2 and 5%, and that of the total column CO between 5 and 20%, depending on the location, with variabilities larger than 20% for CO above highly polluted areas. The calculated overall spatio-temporal variability is equal to 18, 9, and 34% for the total columns O<sub>3</sub>, CH<sub>4</sub>, and CO, respectively, and to 42, 57, and 87% for the C6, C12, and C16 partial column O3, respectively. The target

**Table 4.** RTIASI Pressure Levels for Which the Temperatures Are

 Entered to the NN Module<sup>a</sup>

RTIASI Pressure Levels, hPa	O <sub>3</sub>	CH <sub>4</sub> , CO
0.222227827		×
0.872158587	×	
1.3611629		×
3.1094799	×	
6.94999981	×	
10.3699999		×
14.8100004	×	
27.2600002	×	
56.730011	×	
77.2013168	×	
93.2342148	×	×
102.050011	×	
111.598289	×	
132.492386	×	
155.428146	×	×
180.673065	×	
222.940018	×	×
253.710022	×	
286.600067	×	
321.499939	×	×
377.053253	×	
436.949982	×	×
499.539154	×	×
543.052979		×
587.638245	×	×
610.599976		×
667.708179	×	×
727.435579		×
759.155699	×	
792.183940		×
826.576006		×
899.686381	×	×
978.981728	×	×
Total number of levels selected $(I - 1)$	25	18

 $^{a}$ Crosses indicate the (l - 1) pressure levels selected for each trace gas retrieval.



**Figure 3.** O<sub>3</sub>, CH<sub>4</sub>, and CO concentration profiles for the US 1976 standard atmosphere [*Anderson et al.*, 1986].

accuracy for the trace gas retrievals, required for a good representation of their spatio-temporal variabilities is set to 5%, 2%, and 10% for total  $O_3$ ,  $CH_4$ , and CO, respectively, 30% for the *C*6 partial column  $O_3$ , and 20% for the *C*12 and *C*16 partial columns  $O_3$ .

[20] In addition to the trace gas concentrations, two selected radiances are retrieved in order to check the internal consistency of the algorithm and support the error diagnostic. Currently, this consistency test is implemented for  $O_3$  only. These radiances correspond to channels at 976.75 cm<sup>-1</sup>, an atmospheric window, and at 1034.75 cm<sup>-1</sup>, in the  $O_3$  absorption band, which were excluded from the input measurement vector.

### 3. NN Module Development

[21] The inversion algorithm uses neural network techniques, which present several properties required for the real-time processing of satellite data. These techniques allow the statistical modeling of complex, non-linear, transfer functions using a probabilistic Bayesian approach, are easily adaptable, and very efficient in the operational phase. Since the late 1980s, several mathematic publica-

tions have demonstrated that standard multilayer feedforward NN (also called multi-layer perceptrons) with one or two hidden layers of Heaviside step function neurons can be considered as a class of universal approximators: they can approximate any continuous function uniformly on any compact set (they can estimate values of these functions at any point, to any desired degree of accuracy) provided sufficient degrees of freedom (neurons) are available in the NN [Hornik et al., 1989; Blum and Li, 1991]. In practice, the function modeled by the NN needs to be differentiable (at least for the NN training) and the step function neurons are replaced by sigmoid function neurons (hyperbolic tangent for example) as we will see in the application presented in this paper. Various studies have shown that multilayer perceptrons with hidden sigmoid function neurons allow the solution of non-linear inverse problems in geophysics [e.g., *Thiria et al.*, 1993; Hadji-Lazaro et al., 1999; Chevallier et al., 2000; Richaume et al., 2000; Aires et al., 2001; Müller et al., 2003; Jimènez et al., 2003]. An intercomparison exercise, comparing different methods developed to retrieve CO from IR measurements, has further demonstrated the good performance of the neural network approach [Clerbaux et al., 2002].

[22] The NN developed allows the modeling of the transfer function R which links the inputs, including the measurements **y** and the estimators  $\hat{\mathbf{b}}$  of some parameters **b** (the surface and atmospheric temperatures here, the other parameters **b** being fixed during the development), to the output quantities calculated: the  $n_c$  trace gas columns  $\hat{\mathbf{c}}$  and the  $n_r$  test radiances  $\hat{\mathbf{r}}$ . The inverse problem described by equation (3) may be rewritten

$$\{\hat{\mathbf{c}}, \hat{\mathbf{r}}\} = F(\mathbf{y}, \hat{\mathbf{b}}, \mathbf{W}) \tag{4}$$

where the matrix **W** includes the parameters of the NN global function F. The size of this matrix depends on the architecture chosen for the NN, and determines the number of degrees of freedom available for the solution of the inverse problem. The parameters of **W** are adjusted during a calibration phase, which uses a training database comprising the a priori knowledge of the atmospheric state to be retrieved as well as the physics of the problem to be solved (i.e. the forward model). This information is provided implicitly through the so-called training phase. The

	(m + l) Inputs	$S_1$	$S_2$	Outputs	Symbol	Unit
O <sub>3</sub>	173	16	16	Total column	$\hat{c}(1) = CT$	Dobson unit (DU)
	m = 147			Partial column [surface - 6 km]	$\hat{c}(2) = C6$	DU
	1 = 25 + 1			Partial column [surface - 12 km]	$\hat{c}(3) = C12$	DU
				Partial column [surface - 16 km]	$\hat{c}(4) = C16$	DU
				Test radiance 1 (976.75 $\text{cm}^{-1}$ )	$\hat{r}(1)$	$\times 10^8$ W/(cm <sup>2</sup> cm <sup>-1</sup> sr)
				Test radiance 2 (1034.75 $\text{cm}^{-1}$ )	$\hat{r}(2)$	$\times 10^8$ W/(cm <sup>2</sup> cm <sup>-1</sup> sr)
$CH_4$	72 m = 53	8	8	Total column	$\hat{c} = CT$	molecule/cm <sup>2</sup>
	1 = 18 + 1					
CO	49 $m = 30$	8	8	Total column	$\hat{c} = CT$	molecule/cm <sup>2</sup>

Table 5. NN Module Architecture and Outputs Description for Each Studied Constituent



**Figure 4.** Schematic representation of a neural network with 2 hidden layers of  $S_1 = S_2 = 8$  neurons, providing for one constituent  $n_c$  columns **c**, and  $n_r = 2$  test radiances  $\hat{r}(1)$  and  $\hat{r}(2)$  from *m* radiance channels (**y**), l - 1 atmospheric temperatures associated to fixed pressure levels, and the surface temperature ( $\hat{\mathbf{b}}$ ).

hypotheses made on several non-retrieved forward problem parameters **b** which are not considered in the input vector (the spectroscopic parameters and the instrumental characteristics in particular), are also implicitly included in the retrieval process through this **W** matrix. A detailed description of the development steps is provided in the following paragraphs.

### 3.1. Neural Network Architecture

[23] The first step to build an efficient neural network is to find the optimal architecture, which has enough degrees of freedom to solve the problem. The architecture of a multilayer feed-forward NN is defined by the number of layers, the number of neurons on each layer, the topology of their connections, and the elementary transition functions associated with each neuron. An efficient architecture is chosen on the basis of empirical considerations depending on the complexity of the problem to be solved [*Bishop*, 1995].

[24] In our case, successive performance testing has shown that a well-suited architecture is a multilayer perceptron with two hidden layers, as schematically represented in Figure 4. The network is composed of an input layer, comprising m + l neurons (*m* radiances y and *l* temperatures  $\hat{\mathbf{b}}$ ), which reads the inputs of the algorithm, two hidden layers of  $S_1$  and  $S_2$  neurons, and an output layer of  $n_c + n_r$  neurons. The neurons of the hidden and output layers estimate the outputs using their attributed elementary transition functions. The connections between the different layers are weighted and biases can be added to the neurons inputs. As the transfer function F to be modeled is strongly non-linear, non-linear sigmoid transition functions *f* have been chosen for the neurons of the hidden layers:

$$f(x) = \tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$
(5)

The output layer is composed of  $n_c + n_r$  neurons with linear transition functions *g*:

$$g(x) = x \tag{6}$$

[25] For each quantity retrieved, the global transfer function modeled may be written:

$$\hat{c}(p) = g \left[ \sum_{k=1}^{S_2} w_{pk}^3 f \left[ \sum_{j=1}^{S_1} w_{kj}^2 f \left( \sum_{i=1}^m w_{ji}^1 y(i) + \sum_{i=m+1}^{m+l} w_{ji}^1 \hat{b}(i-m) + \beta_j^1 \right) + \beta_k^2 \right] + \beta_p^3 \right],$$

$$p = 1, ..., n_c$$
(7)

and

$$\hat{r}(p - n_c) = g \left[ \sum_{k=1}^{S_2} w_{pk}^3 f \left[ \sum_{j=1}^{S_1} w_{kj}^2 f \left( \sum_{i=1}^m w_{ji}^1 y(i) + \sum_{i=m+1}^{m+l} w_{ji}^{l} \hat{b}(i-m) + \beta_j^1 \right) + \beta_k^2 \right] + \beta_p^3 \right],$$

$$p = n_c + 1, \dots, n_c + n_r$$
(8)

where  $w_{ji}^1$ ,  $w_{kj}^2$  and  $w_{pk}^3$  represent the matrices of connection weights with i = 1, ..., (m + l) the elements of the input layer,  $j = 1, ..., S_1$  the neurons of the first hidden layer,  $k = 1, ..., S_2$  the neurons of the second hidden layer and  $p = 1, ..., (n_c + n_r)$  the neurons of the output layer. The biases associated with the neurons correspond to the vectors  $\beta_j^1, \beta_k^2$ and  $\beta_p^3$ . The weights and biases of the NN are included in the W matrix.

[26] The NN architectures chosen for the inversion of CO,  $O_3$ , and CH<sub>4</sub> are detailed in Table 5. The number of parameters to be adjusted (in the W matrix), corresponding

to the number of degrees of freedom available for the solution of the inverse problem, is equal to 3158 for  $O_3$ , 665 for  $CH_4$ , and 481 for CO.

### **3.2.** Constitution of a Comprehensive Database

[27] NN techniques allow an approximation of the transfer function F which links the inputs to the outputs of the problem. This approximation, based on statistical theory, requires a comprehensive dataset of known examples, representative of the behavior of the function to be estimated. This dataset includes the physics of the problem to be solved, with the forward model, and the a priori known realistic variation range of the state to be retrieved. A part of this dataset, called the training set, is used for the fitting of the NN parameters  $\mathbf{W}$  (weights and biases), during the training phase. The examples which are not included in the training set are divided into two additional data sets: a validation set, used to check the generalization capacities of the NN during the training phase, and a test set, used to evaluate the performance of the inversion.

[28] In order to build a comprehensive and realistic dataset, IASI spectra have been simulated using threedimensional chemistry-transport model (CTM) trace gas simulations with temperatures extracted from the European Center for Medium-Range Weather Forecasts (ECMWF) analysis — defining the state of the atmosphere —, coupled to a high resolution radiative transfer code.

[29] The atmospheric mixing ratio profiles of  $O_3$ ,  $CH_4$ and CO provided by the Model for OZone And Related chemical Tracers MOZART version 1.0 [Brasseur et al., 1998; Hauglustaine et al., 1998] have been used for that purpose. MOZART simulates the evolution of 56 chemical species with a 20 minutes time step, an horizontal resolution of  $2.8^{\circ} \times 2.8^{\circ}$ , and on 25 levels from the Earth's surface up to 3 hPa. The model is driven by dynamical and physical input fields generated by the NCAR CCM2 general circulation model, updated every 3 hours. Since the MOZART photochemical scheme is representative of the troposphere, the O<sub>3</sub> profiles have been connected above the tropopause height to the monthly satellite based 4D ozone climatology from Li and Shine [1995], interpolated to the MOZART grid, in order to get full atmospheric profiles. The CH<sub>4</sub> profiles have been connected to a latitudinal dependant satellite based climatology (D. Diebel, personal communication) between 19 km and 60 km, and to the US 1976 standard atmosphere [Anderson et al., 1986] above 60 km. The latitudinal dependant model profiles from Anderson et al. [1986] have been used to complete the CO profiles above 24 km. The temperatures from the ECMWF analysis have been colocated with MOZART grid points, and cloud-free and aerosol free conditions have been considered, with a constant mean emissivity estimated from values provided by Wilber et al. [1999].

[30] Using these atmospheric state data, the IASI spectra have been simulated using the Line-By-Line Radiative Transfer Model (LBLRTM) [*Clough et al.*, 1995a, 1995b, 2004] version 5.10 with the HITRAN 1996 spectroscopic database [*Rothman et al.*, 1998]. The simulated spectra have then been convoluted with the instrument spectral response function for IASI Level 1C data [*Camy-Peyret et al.*, 2001]. The instrumental noise has been accounted for by adding a

random noise to the simulated spectra. A more detailed description of the simulations used for the construction of the training dataset is provided in *Clerbaux et al.* [1998].

[31] A dataset representative of a wide range of atmospheric situations (spanning all seasons and locations) has been constructed, in order to get only one general function F for all the situations to be processed.

[32] To improve the NN generalization capacity and avoid a forcing of the results by over-represented cases, the training, validation, and test sets must be homogeneously representative of the different situations that the algorithm will have to process in operational phase. A selection of representative examples has been carried out in the input space, using a principal component analysis to reduce the dimensionality. The number of examples included in the training datasets is at least equal to 10 times the number of parameters to be determined during the training (elements of the **W** matrix).

### **3.3.** NN Training Phase

[33] A supervised learning is used for the training of the neural network. The training phase consists in fitting the NN parameters so that the outputs  $\hat{\mathbf{c}}$  calculated by the NN agree with the desired outputs  $\mathbf{c}$  (real state) for the elements of the training set. A stochastic gradient descent algorithm has been used, based on the calculation of a cost function  $C(\mathbf{W})$  which evaluates the quadratic difference between the desired and the calculated outputs [*Bishop*, 1995].

[34] The training phase requires a long computation time because of the minimization process. Conversely, the operational phase only consists of algebraic computations (**W** fixed) and is therefore very fast (about 1/100 second per retrieval).

# 4. Characterization of the Retrievals and Inversion Error Analysis

[35] A comprehensive assessment of the characteristics and accuracy of the retrievals is required for an optimal use of the data by the scientific community. It allows the evaluation of the capabilities of the observing system, including the instrument and the retrieval algorithm developed, and to access the level of accuracy achieved for the trace gas concentration retrieval.

### 4.1. Sensitivity of the Observing System

[36] The sensitivity of the observing system (IASI instrument and NN inversion algorithm) may be studied by calculating the averaging kernel **A** characterizing the sensitivity of the columns retrieved to the trace gas vertical distribution, defined as

$$\mathbf{A} = \frac{\partial \hat{\mathbf{c}}}{\partial \mathbf{x}} \tag{9}$$

It can be estimated by applying the gain matrix associated with the input radiances  $G_y$ , characterizing the sensitivity of the retrieval to the input radiances, to the weighting functions or Jacobians **K**, characterizing the sensitivity of the instrument to the observed species:

$$\mathbf{A} = \mathbf{G}_{\mathbf{y}} \, \mathbf{K} \tag{10}$$



**Figure 5.** IASI Jacobians for  $O_4$ ,  $CH_4$ , and CO at three characteristic radiance channels, calculated for the US 1976 standard atmosphere.

with

$$\mathbf{G}_{\mathbf{y}} = \frac{\partial \hat{\mathbf{c}}}{\partial \mathbf{y}} \tag{11}$$

and

$$\mathbf{K} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \tag{12}$$

[37] The Jacobians have been calculated using forward model simulations of the measurements, which requires that the situation considered be fully known.  $\mathbf{K}$  is defined as the partial derivative of the measurement with respect to the variable observed, so here, as the partial derivative of the radiances with respect to the trace gas vertical concentration profile. For this study, a method of perturbation was used, so that

$$\mathbf{K} \simeq \frac{\Delta \mathbf{y}}{\Delta \mathbf{x}} \tag{13}$$

where  $\Delta \mathbf{x}$  is the perturbation applied to the concentration profile  $\mathbf{x}$  of the molecule studied. If  $\mathbf{x}$  is defined on *n* vertical levels, then **K** is a  $m \times n$  matrix. The rows of **K** correspond to the sensitivity of the radiance in a given channel to the vertical distribution of the trace gas concentration.

[38] Figure 5 shows, for one selected channel, the corresponding row of the IASI Jacobians for the three species, calculated for the example of the US 1976 standard atmosphere [*Anderson et al.*, 1986] using  $\Delta \mathbf{x} = 10\%$ . The magnitude of the sensitivity depends on the intensity of the radiance recorded at the corresponding channel, but the shape as a function of altitude is similar for all the selected channels. The sensitivity reaches a maximum in the free troposphere, at altitudes between 6 and 10 km, and rapidly

decreases below  $\sim 2$  km. The sensitivity rapidly increases at high altitudes (above  $\sim 45$  km for O<sub>3</sub>, and 35 km for CH<sub>4</sub> and CO) due to the extremely small concentrations at these levels. The reduced sensitivity to the lower layers of the atmosphere (atmospheric boundary layer) is a common problem to all nadir-viewing IR remote sensors, associated with the lack of thermal contrast between the surface and the boundary layer. The sensitivity also decreases at higher altitudes, due to the decrease in atmospheric pressure (inducing a decrease of the Lorentz collisional broadening of the spectral lines). For O<sub>3</sub>, there is more information above 25 km than for the other molecules due to its high stratospheric concentrations (ozone layer).

[39] The gain functions **G** are defined as the partial derivatives of the retrievals with respect to the input parameters, i.e., in our case, with respect to the input radiances **y** on one part,  $\mathbf{G}_{\mathbf{y}}$  (already defined in (equation (11)), and the input temperatures  $\hat{\mathbf{b}}$  on the other,  $\mathbf{G}_{\mathbf{b}}$ :

$$\mathbf{G}_{\mathbf{b}} = \frac{\partial \hat{\mathbf{c}}}{\partial \hat{\mathbf{b}}} \tag{14}$$

 $\mathbf{G}_{\mathbf{y}}$  is a  $n_c \times m$  matrix, where each element  $\mathbf{G}_{\mathbf{y}}^{p,i} = \partial \hat{c}_p / \partial y_i$ corresponds to the contribution of a given input  $y_i$  to the retrieval of the output variable  $\hat{c}_p$ , with i = 1, m and  $p = 1, n_c$ (similarly,  $\mathbf{G}_{\hat{\mathbf{b}}}$  is a  $n_c \times l$  matrix). They are computed analytically for each retrieval by differentiation of the NN global transfer function (equations (7) and (8)).

[40] The averaging kernel A ( $n_c \times n$  matrix) has been estimated using a combination of the two sensitivity functions K and G<sub>y</sub>. The general behavior of the averaging kernel profile is similar to that of the weighting functions K, with opposite signs (increased concentration implies decreased outgoing radiances, but increased columns): for all the variables retrieved, the sensitivity is maximum in the free troposphere.



**Figure 6.** Averaging kernels characterizing the retrieval of the  $O_3$  total (diamonds) and partial [0-6 km] (dots), [0-12 km] (plus), and [0-16 km] (x-mark) columns calculated for the standard atmosphere US 1976. The dashed lines correspond to the ideal sensitivity profiles.

[41] The kernels obtained for the  $O_3$  columns retrieved are plotted in Figure 6, together with the corresponding 'ideal' sensitivity profiles C. This figure highlights the strong sensitivity of the columns to the free troposphere, with a peak sensitivity around 6 to 8 km. For the total column O<sub>3</sub>, a secondary peak is obtained at altitudes near 15-20 km, and the sensitivity remains large throughout the stratosphere (up to 35-40 km), where the O<sub>3</sub> concentration is large enough to compensate the relatively small sensitivity of the instrument. The lower sensitivity to the boundary layer will induce an uncertainty on the O<sub>3</sub> retrievals, which should be taken into account while using the data. For the restitution of the O<sub>3</sub> total column, the lower sensitivity to the upper stratosphere may also induce uncertainties. This study also shows that the partial columns  $O_3$  are not fully independent from the adjacent atmospheric layers, the contribution of the atmospheric layers located above the limit altitude should be considered.

[42] For CO and  $CH_4$ , the kernels are single peaked functions with maximum sensitivities around 6 to 10 km for CO, and around 8 to 10 km for  $CH_4$ . The main source of uncertainty also comes from the lack of sensitivity to the boundary layer.

[43] In inverse problem solution, the sensitivity of the observing system and the a priori information used are provided with each retrieved product in order to allow for them in the comparison of the inversion results with other data or with model simulations [*Rodgers and Connor*, 2003]. Indeed, an observing system may be simulated by performing a forward radiative transfer simulation and by then applying the inversion process, or, more simply, by using the linear characterization formalized by *Rodgers* [2000] as follows:

$$\hat{\mathbf{c}} = \mathbf{C}\,\hat{\mathbf{x}} = \mathbf{C}\,\mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}_{\mathbf{y}}\boldsymbol{\epsilon}$$
$$= (\mathbf{C} - \mathbf{A})\mathbf{x}_a + \mathbf{A}\mathbf{x} + \mathbf{G}_{\mathbf{y}}\boldsymbol{\epsilon}$$
(15)

where C represents an integration operator allowing the calculation of integrated columns from vertical distributions (c = C.x). A is strongly dependent on the situation considered, and must be evaluated for each retrieval. Its evaluation requires forward model simulations (for calculation of **K**), for which the vertical distributions **x** must be known (or estimated). In the particular case of the NN inversion method, the retrieval is based on thousands of representative atmospheric situations (training database), and an a priori state in the statistical sense of the optimal estimation can not be provided. The classical linear characterization is therefore difficult to apply to the NN scheme, but a direct comparison with other data can be undertaken with good confidence provided that the training set be statistically representative of the real state. The linear representation may however be used for the error diagnosis (see paragraph 4.3).

### 4.2. Statistical Performance of the Retrieval

[44] A good insight into the performance that can reasonably be expected is given by a statistical approach: the global inversion error is estimated on test data sets composed of fully known examples. The inversion algorithm is calibrated during the training phase, which implies that the errors associated with the observing system are strongly dependent on the quality of the learning set used. Both the statistical representation of the examples chosen, and the quality of these examples will have an impact on the retrievals. Here, perfect forward model simulations are assumed (i.e. no uncertainty due to the synthetic atmospheres used — including the MOZART CTM, the climatologies and the standard profiles —, nor due to the spectroscopic parameters and radiative transfer model), and only the homogeneity of the training set is investigated. Therefore, test data sets with a statistical representation of the different situations similar to that of the training set are used.

[45] For each example of the data set, the retrieved variables ( $\hat{\mathbf{c}}$ ) have been compared to the corresponding desired values (real state  $\mathbf{c}$ ). Figure 7 represents the scatterplots of the test dataset for the different quantities retrieved. Globally the agreement is good, the clouds of points are well distributed around the first bisector, with no apparent bias, except for the extremely low column amount, which the NN seems to overestimate, and the very large ones, which seem, on the contrary, to be underestimated. The scatterplots also highlight that these "extreme" values (small or large) are less represented in the data sets (fewer examples).

[46] Our studies show that the retrievals will be biased for situations under-represented in the learning set, which is the case for the highest/lowest concentrations of the trace gases considered, as previously highlighted, but also for the very high/low surface temperatures. A large inversion error on the retrievals is also expected for input data that are not consistent with what the network has learned. However, the performance is very satisfactory considering the variability of the different column amounts to be retrieved. Globally, the RMS error between retrieved and desired values is estimated to less than 30% (3 DU) for the *C*6 column O<sub>3</sub>, 15% (4 DU) for the *C*12 column O<sub>3</sub>, 9% (4 DU) for the *C*16 column O<sub>3</sub>, 1.5% (5 DU) for the total column O<sub>3</sub>, 2% (5 × 10<sup>17</sup> molecules/cm<sup>2</sup>) for the total column CH<sub>4</sub>, and 6% (9 × 10<sup>16</sup> molecules/cm<sup>2</sup>) for the total column CO.

#### 4.3. Error Analysis

[47] Using equation (15) (simulated observation in a linear formalism), the difference between the retrieval and the true state is given by

$$\hat{\mathbf{c}} - \mathbf{c} = (\mathbf{A} - \mathbf{C})(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}\boldsymbol{\epsilon}$$
 (16)

This equation highlights the two principal sources of error that should be considered.

[48] The first term of the right-hand side of this equation corresponds to the error associated with the non-ideal sensitivity of the observing system to the real state, and is called the smoothing error. It depends on both the deviation between averaging kernel **A** and ideal sensitivity profile **C**, and the variability of the trace gas observed [*Rodgers*, 2000]. Its covariance matrix is a  $n_c \times n_c$  matrix defined as follows:

$$\mathbf{S}_{\mathbf{s}} = (\mathbf{A} - \mathbf{C}) \cdot \mathbf{S}_{a} \cdot (\mathbf{A} - \mathbf{C})^{T}$$
(17)

with  $S_a$  the covariance matrix of the vertical concentration profile.



**Figure 7.** Scatterplots between the concentration retrieved by the NN (retrieval) and obtained from the model (target) in DU for  $O_3$  and in molecules.cm<sup>-2</sup> for CH<sub>4</sub> and CO, to assess the performance of the retrieval for the test data set, composed of model simulations (17000 examples for  $O_3$ , 18760 for CH<sub>4</sub>, and 7392 for CO).



**Figure 8.** Expected radiometric instrumental noise for IASI, for a reference temperature of 280 K (left), and temperature error covariance matrix (right). For the highest pressure levels, the temperature error becomes relatively large, with values up to 10 to 25  $K^2$  above 2 hPa.

[49] In the case of a NN inversion method, the unique a priori information in the sense of the Rodgers linear characterization does not exist. To constrain an ill-posed inverse problem, the training database includes thousands of representative atmospheric situations based on our a priori knowledge. If we use the covariance of this dataset as covariance matrix  $S_a$ , we do not take into account the statistical character of the NN retrieval: the training data are not only used to mitigate the lack of information contained in the measurements (where the sensitivity is lower), but also to calibrate the global inversion transfer function. Furthermore, the NN is able to consider a reduced domain of possible solutions. Therefore, the smoothing error determined using the training set covariance matrix overestimates the associated uncertainty and gives an erroneous estimation of the NN capabilities. It can however provide information on the relative importance of the purely statistical contribution. For the standard atmosphere, the estimated smoothing error (corresponding to an upper limit value) is equal to 36% for the C6 column O<sub>3</sub>, 15% for the C12 column O<sub>3</sub>, 8% for the C16 column O<sub>3</sub>, 2% the total column  $O_3$ , 3% for the total column  $CH_4$ , and 8% for the total column CO.

[50] The second term on the right-hand side of equation (16) corresponds to the impact on the retrieval of the sensitivity of the algorithm to uncertainties on the input parameters. The resulting inversion errors may be deduced by applying the gain functions  $G_y$  and  $G_b$ , characterizing the sensitivity of the inversion algorithm, to the measurement errors on the input radiances  $\epsilon$  (radiometric noise) and on the input temperatures  $\epsilon_b$ , respectively:

$$\mathbf{e}_{\mathbf{n}} = \mathbf{G}_{\mathbf{y}} \cdot \boldsymbol{\epsilon} \quad , \quad \mathbf{S}_{\mathbf{n}} = \mathbf{G}_{\mathbf{y}} \cdot \mathbf{S}_{\boldsymbol{\epsilon}} \cdot \mathbf{G}_{\mathbf{y}}^{T}$$
(18)

$$\mathbf{e}_{\mathbf{b}} = \mathbf{G}_{\mathbf{b}} \cdot \boldsymbol{\epsilon}_{\mathbf{b}} \quad , \quad \mathbf{S}_{\mathbf{b}} = \mathbf{G}_{\mathbf{b}} \cdot \mathbf{S}_{\boldsymbol{\epsilon}_{\mathbf{b}}} \cdot \mathbf{G}_{\mathbf{b}}^{T}$$
(19)

where  $S_{\epsilon}$  is the covariance matrix of  $\epsilon$ , and  $S_{\epsilon_b}$  is the covariance matrix of the error associated with the retrieval

of the surface temperatures and atmospheric temperature profiles. For IASI, the expected radiometric noise — which includes all noise contributions (detectors, amplifiers, A/D converters, processing) and all errors sources which do not result in a bias (e.g., errors due to field-of-view motion, fluctuations of wavelength calibration, knowledge of the spectral response function, fluctuations of the radiometric calibration, http://smsc.cnes.fr/IASI/GP\_instrument.htm) — and temperature error covariance matrix (P. Prunet, personal communication) are represented in Figure 8.

[51] Their estimated contribution to the global inversion error is summarized in Table 6. The largest impact comes from uncertainty on the temperature profile, while the errors associated with noise on the input radiances and uncertainty on the surface temperature are relatively small. These results are largely explained by the magnitude of the input uncertainties, but also by the sensitivity of the inversion algorithm, and thus by the variability of the retrieved quantity. Compensations between the various contributions may also occur, we have therefore chosen to evaluate the global error using the quadratic sum of the different contributions.

**Table 6.** Inversion Error Associated With Errors on the Input Radiances ( $\mathbf{e}_n$ ), Temperature Profile ( $\mathbf{e}_{b=T}$ ), and Surface Temperature ( $\mathbf{e}_{b=T_s}$ ), Evaluated on a Test Data Set (17,000 Simulations for O<sub>3</sub>, 18,760 Simulations for CH<sub>4</sub>, and 7392 Simulations for CO)<sup>a</sup>

	$\sigma(\mathbf{e_n}), \%$	$\sigma(\mathbf{e_{b=T}}), \%$	$\sigma(\mathbf{e_{b=T_s}}), \%$	$\sigma(\mathbf{e}_{inputs}), \%$
$\hat{c}_{0}(1)$ (C6)	5.3	6.3	0.4	4.7
$\hat{c}_{0}(2)$ (C12)	7.5	8.6	0.5	6.4
$\hat{c}_{0}(3)$ (C16)	8.2	9.4	0.5	7.2
$\hat{c}_{0}(4)$ (CT)	1.5	2.4	0.2	1.7
$\hat{c}_{CH}(CT)$	0.3	0.6	0.01	0.4
$\hat{c}_{\rm CO}(CT)$	3	3.6	1.7	2.9

<sup>a</sup>For each retrieved variable, the standard deviation of the calculated errors are indicated in percent, as well as that of the total resulting uncertainty  $\mathbf{e}_{inputs} = \sqrt{\mathbf{e}_{n}^{2} + \mathbf{e}_{b=T}^{2}}, \mathbf{e}_{n}$ 



**Figure 9.** Global distributions of IMG CH<sub>4</sub> and CO total columns for the April 1–10, 1997 IMG period. The data are averaged over the time period and a  $5^{\circ} \times 5^{\circ}$  grid. The corresponding available NDSC measurements are represented by colored circles on each map.

[52] Since  $G_y$  and  $G_b$  are determined analytically, the covariance matrices  $S_n$  and  $S_b$  can be evaluated for each retrieval, provided  $S_{\epsilon}$  and  $S_{\epsilon_b}$  are known or can be estimated.

### 4.4. Internal Consistency Checks

[53] The previous paragraphs were focused on the error estimation for the trace gas retrieval. The same considerations can be applied to the retrieval of the two radiances  $\hat{\mathbf{r}}$  retrieved in addition to the trace gas columns  $\hat{\mathbf{c}}$ (equation (3)). For  $\hat{\mathbf{r}}$ , low accuracy was found for situations with a small representation in the training set, and low precision was found for low signal to noise ratio measurements or poor quality input temperatures (large uncertainties). In practice, the algorithm may come across situations that are not consistent with what the network has learned. This will be the case, in particular, if the error on the surface emissivities is too important, if the surface emissivities are too far from the mean value used for the simulations of the training set, or for bad quality measurements (with calibration problems for instance). When different instruments are used for radiance measurements and temperature estimates, inconsistencies may also occur. The comparison of the retrieved and measured values for these test radiances provides an inversion error of these variables which may be used to highlight (and if required, eventually filter) less reliable or non-reliable retrievals. It should be kept in mind,

however, that the error of the output radiances is not always directly correlated to that of the trace gas columns.

### 5. Application of the Trace Gas Retrieval Algorithm to the Analysis of the IMG/ADEOS Measurements

[54] Although simulated observations are essential to the development of the inversion method and to the characterization of the retrievals, the algorithm should be tested on real data in order to evaluate the validity of the different approximations made, by the use of CTM simulations in particular.

[55] For this purpose, the infrared high-resolution spectra recorded by the Interferometric Monitor for Greenhouse Gases (IMG) on board ADEOS between August 1996 and June 1997 provide very valuable test data. IMG/ADEOS is indeed a precursor of IASI, which used similar observations techniques (nadir-looking Fourier transform spectrometer), optimized for the monitoring of trace gases. It therefore had a slightly wider spectral range (600 to 3030 cm<sup>-1</sup>) and an higher spectral resolution (lower or approximately equal to  $0.12 \text{ cm}^{-1}$ ).

[56] In order to enable the application of the IASI trace gas retrieval algorithm to the IMG data, the IMG spectra have been converted into IASI-like spectra by convolution with the IASI instrument spectral response function [*Camy-Peyret et al.*, 2001]. The temperatures associated with the IMG measurements were not available, and had to be estimated. The surface temperatures have been derived directly from the spectra, and the collocated ECMWF temperature profiles have been used. The uncertainties associated with the different input parameters were not known so that a complete error analysis could not be undertaken.

[57] The retrieved test radiances have been used to filter the data that could not be correctly processed by the algorithm, which comprises the low quality measurements (low signal/noise) and the situation that were not correctly represented in the training data set, corresponding, in particular, to extreme surface emissivities and/or surface temperatures, including clouds, deserts, shrub land and/or snow/ice covered areas. An additional filtering has been applied [*Hadji-Lazaro et al.*, 2001] to totally remove the cloudy pixels. These quality filters remove around 60-70%of the cases, with 40-50% of the cases removed by the cloud filter.

[58] This section presents the global distributions obtained for the April 1–10, 1997 IMG period (highest quality measurement period available) filtered and averaged over a constant  $5^{\circ} \times 5^{\circ}$  grid. The global distributions of CH<sub>4</sub> and CO retrieved from the IMG measurements for April 1–10, 1997 are shown in Figure 9, including correlative measurements at different sites of the National Oceanic and Atmospheric Administration (NOAA) Network for the Detection of Stratospheric Change (NDSC), providing a preliminary validation. The distributions of total and partial column O<sub>3</sub> are shown in Figure 10. A direct comparison of the IMG distributions with the available independent measurements is undertaken, which provides a first idea of the performance that can be expected.



**Figure 10.** Global distributions of IMG O<sub>3</sub> total and partial columns for the April 1–10, 1997 IMG period, filtered and averaged over a  $5^{\circ} \times 5^{\circ}$  grid and the time period.

[59] As already mentioned, the sensitivity of the different instruments should be considered in order to make accurate comparisons [*Rodgers and Connor*, 2003]. Work is currently in progress to supplement this direct validation with a validation taking into account the different characteristics of the observing systems (instrumental and retrieval characteristics).

### 5.1. Total Column CH<sub>4</sub>

[60] The largest concentrations of  $CH_4$  (Figure 9) are observed in the Northern Hemisphere and in the midlatitudes of the Southern Hemisphere. Its global distribution is representative of the major source regions. However, the precise emission areas are difficult to locate due to its long lifetime, of the order of 8 years [*Intergovernmental Panel on Climate Change (IPCC)*, 2001], which allows a transport and mixing on hemispheric to global scales.

[61] The total columns measured by ground-based instruments (solar tracking Fourier transform spectrometers) at different sites of the NDSC network have been used (http:// www.ndsc.ncep.noaa.gov). The precision of these measurements is estimated to 2%. The different sites which provided measurements during the period studied are summarized in Table 7, and the corresponding total columns are represented in Figure 9, together with the IMG distribution. In order to increase the number of coincident points, NDSC data were averaged over each measurement station and the ten days period considered. However, only stations located at the high latitude of the Northern Hemisphere provided measurements. A good agreement is reached at Ny Ålesund and Eureka but IMG seems to underestimate the column at Fairbanks.

[62] A quantitative comparison of the collocated measurements is limited since the only station for which collocated IMG measurements are available (within a  $2.5^{\circ} \times 2.5^{\circ}$  area) is Fairbanks. At this station, the bias between the two measurements is equal to 5.6%, which is large compared to the small variability of CH<sub>4</sub>. Further validation is needed in order to conclude on the quality of the retrievals. The good spatio-temporal coverage that will be achieved during the IASI mission will facilitate such comparison.

### 5.2. Total Column CO

[63] The distribution of CO (Figure 9) is more correlated to the emission areas than that of CH<sub>4</sub>. The highest columns are retrieved above the polluted industrialized areas of the

 Table 7. NDSC Stations Which Provided Measurements During

 April 1–10, 1997<sup>a</sup>

Station	Latitude	Longitude	Measurement
Lauder	$-45.05^{\circ}$	169.68°	СО
Wollongong	$-34.45^{\circ}$	150.88°	CO
Kitt Peak	31.90°	$-111.50^{\circ}$	CO
St Petersbourg	59.88°	29.83°	СО
Fairbanks	64.82°	$-147.87^{\circ}$	$CH_4$ , CO
Ny-Ålesund	78.92°	11.93°	CH <sub>4</sub>
Eureka	$80.05^{\circ}$	$-86.42^{\circ}$	CH <sub>4</sub>

<sup>a</sup>The molecule measured is indicated for each station.



**Figure 11.** Comparison of the CO total columns retrieved from IMG/ADEOS data (gray diamonds) and the columns provided by the NDSC (black crosses) for April 1–10, 1997, at the different stations providing measurements collocated to the IMG data. The errorbars correspond to the standard deviation of the available data for the period studied, within a  $2.5^{\circ} \times 2.5^{\circ}$  area around the measurement station for the IMG retrievals.

Northern Hemisphere (North America, Europe and Eastern Asia) and the regions of strong biomass-burning (e.g., Central Africa and South-East Asia). The lowest values are observed in the Southern Hemisphere, where the source regions are less important. The lifetime of CO, is a lot lower than that of CH<sub>4</sub>, less than 2 months [*IPCC*, 2001], but nevertheless allows a transport downwind the polluted areas. CO plumes can be observed above the Northern Pacific and the Northern and tropical Atlantic oceans.

[64] As for CH<sub>4</sub>, the NDSC data have been used to validate the retrieved distribution. The total columns, averaged over the period considered, are represented in the global distributions of Figure 9, and a comparison of the data collocated within a  $2.5^{\circ} \times 2.5^{\circ}$  area is shown in Figure 11. The accuracy associated with the NDSC CO measurements is estimated to 4%.

[65] The agreement between the NDSC measurements and the retrieved IMG columns is good, with a mean bias lower than 8%. Note that the stations of Lauder and St Petersburg do not present well collocated IMG measurements. Here again, the validation is highly limited by the lack of comparison data. A more accurate validation will be undertaken during the IASI mission.

### 5.3. Total Column O<sub>3</sub>

[66] The largest total columns of  $O_3$  (Figure 10) are observed at high latitudes, especially in the Northern Hemisphere and the lowest ones in the tropics. This distribution is mainly controlled by the dynamics of the stratosphere (ascendance in the tropics and the summer hemisphere, subsidence at high latitudes, especially in the winter hemisphere), where the lifetime of  $O_3$  can reach up to several months. Low  $O_3$  columns are retrieved around the North Pole, due to the massive photochemical destruction of polar stratospheric  $O_3$  in spring. The large total columns obtained above the polluted areas of the Northern Hemisphere are attributed to  $O_3$  peaks in the troposphere.

[67] The availability of simultaneous measurements from the Total Ozone Mapping Spectrometer (TOMS) [*Heath et al.*, 1975], present on board ADEOS together with IMG, allowed a representative validation of the total column retrievals. The TOMS Level 2 data with reflectivities lower than 20% (corresponding to clear-sky conditions) and corrected for aerosol interference and sea-glint errors using the Pseudo-Version 7.5 TOMS algorithm (provided by J.-F. Lamarque, by courtesy of the NASA Ozone Processing Team), have been used for the comparison. The accuracy of the TOMS total columns has been estimated at 3% by comparison to ground-based measurements [*Krueger and Jaross*, 1999], and it is evaluated at 6% for reflectivities between 10 and 20% [*Lamarque et al.*, 2002].

[68] A discussion of the algorithm is provided in *Turquety et al.* [2002] for a version of the algorithm restricted to the total column  $O_3$  retrieval. Figure 12 presents the comparison for the current version of the operational algorithm, providing the total column as well as 3 partial columns of  $O_3$ , for data collocated at  $\pm 0.5^{\circ}$  in longitude and latitude and measured within a  $\pm 2$  seconds time interval.

[69] The agreement between the two distributions is very good, with a correlation coefficient (R) better than 0.9 and a root-mean-square (RMS) difference lower than 8%. A bias is however clearly identified with a tendency of IMG to overestimate the total column  $O_3$  with respect to TOMS.

### 5.4. Partial Columns O<sub>3</sub>

[70] The interpretation of the distributions of the partial columns of  $O_3$  (Figure 10) is not straightforward since both tropospheric and stratospheric contributions must be considered, depending on the altitude of the tropopause. The thermal tropopause height can be deduced from the temperature profiles, which will be operationally provided during the IASI mission. It is located at altitudes near 16 km



Figure 12. Comparison of the total columns retrieved from IMG/ADEOS data to the total columns provided by TOMS/ADEOS for April 1-10, 1997.

**Table 8.** WMO Ozonesonde Stations Which Provided Measurements Collocated to the IMG/ADEOS Measurements During April 1–10, 1997

WMO Code	Station	Latitude	Longitude
323	Neumayer	$-70.65^{\circ}$	$-8.26^{\circ}$
101	Syoma	$-69.39^{\circ}$	58°
233	Marambio	-64.233°	$-56.717^{\circ}$
29	MacQuarie Isl.	$-54.5^{\circ}$	158.967°
256	Lauder	$-45.044^{\circ}$	169.684°
254	Laverton	$-37.867^{\circ}$	144.75°
441	Easter Isl.	$-27.17^{\circ}$	$-109.42^{\circ}$
438	Suva	$-18.13^{\circ}$	178.4°
432	Papeete (Tahiti)	$-18^{\circ}$	$-149^{\circ}$
191	Samoa	-14.23°	$-170.56^{\circ}$
175	Nairobi	$-1.267^{\circ}$	36.8°
205	Thivanorum	8.483°	76.95°
190	Naha	26.2°	127.683°
10	New Dehli	28.65°	77.237°
7	Kagoshima	31.55°	130.55°
14	Tateno	36.05°	140.1°
107	Wallops Isl.	37.933°	$-75.483^{\circ}$
348	Ankara	39.95°	32.883°
67	Boulder	40.03°	$-105.25^{\circ}$
12	Sapporo	43.05°	141.333°
156	Payerne	46.49°	6.57°
99	Hohenpeissenberg	47.08°	11.02°
242	Prague	50.02°	14.45°
53	Uccle	50.8°	4.35°
318	Valentia Observatory	51.93°	$-10.25^{\circ}$
316	DeBilt	52.10°	5.18°
174	Lindenberg	52.21°	14.12°
221	Legionowo	52.4°	20.967°
76	Goose Bay	53.32°	$-60.3^{\circ}$
21	Edmonton (Stony Pl.)	53.55°	$-114.1^{\circ}$
77	Churchill	58.75°	$-94.07^{\circ}$
43	Lerwick	60.13°	$-1.18^{\circ}$
404	Jokioinen	$60.8^{\circ}$	23.5°
262	Sodankyla	67.39°	26.65°
24	Resolute	74.72°	$-94.98^{\circ}$
89	Ny-Ålesund	78.933°	11.883°
315	Eureka	$80.05^{\circ}$	$-86.42^{\circ}$
18	Alert	82.5°	$-62.3^{\circ}$

in the tropics, 8-12 km at mid-latitudes, and 6-10 km at higher latitudes. The column of  $O_3$  between the surface and 6 km can therefore be considered to be representative of tropospheric  $O_3$  amounts (lower troposphere at mid- and tropical latitudes), but the columns surface - 12 km and surface - 16 km must be studied as a function of the altitude of the tropopause.

[71] The profiles measured by ozonesondes at the different stations of the World Meteorological Organization (WMO) allowed the comparison of the IMG partial columns O3 retrievals with high quality independent observations. The uncertainty associated with the soundings varies between 5 and 10% [Logan, 1999]. The data provided by the World Ozone and Ultraviolet Data Center (WOUDC) have been used, at the different stations providing observations collocated to the IMG measurements within  $\pm 2.5^{\circ}$  in longitude and latitude, indicated in Table 8. Here again, the data have been averaged over the 10 days considered in order to increase the number of comparison points. Figure 13 represents the comparison between the IMG retrievals and the collocated integrated ozonesonde measurements for April 1–10, 1997, for each measurement station studied. It should here be pointed out that the comparison is not statistically representative due to the very limited number

of simultaneous collocated observations (less than 4 observations compared for each station on average).

[72] The two datasets are globally in good agreement, with IMG retrievals within the variation range of the ozonesonde measurements. However, the comparison highlights a clear tendency of the retrievals to underestimate the columns with respect to the sonde data, particularly for the [surface - 6 km] partial column and at the stations located in the mid-latitudes of the Northern Hemisphere. This underestimation is mainly explained by the lack of sensitivity of the IMG instrument to the first layers of the atmosphere, which has a particularly large impact in the polluted areas, where the O<sub>3</sub> concentrations in the boundary layer are high. The fact that global model data are used for the training phase of the NN accentuates this underestimation since the model grid, equal to  $2.8^{\circ} \times 2.8^{\circ}$ , is too large to fully represent the high trace gas concentrations detected by the sondes. In the next version of the algorithm, the training dataset will be enlarged to include regional model simulations and ozonesonde data in order to minimize this effect.

### 6. Summary and Conclusions

[73] We have developed a fast, neural network based algorithm for the near real time retrieval of ozone and its precursors, CH4 and CO, from the IASI IR radiance measurements. Neural networks are well adapted to the operational processing of satellite data since, in addition to being the fastest inversion method currently available, they are adaptable techniques which can easily integrate new variables or new conditions. A neural algorithm was used to model the global, non-linear, transfer function linking the IASI Level 1 radiances and Level 2 temperatures to the trace gas concentrations. The retrieved products are the total columns of O<sub>3</sub>, CH<sub>4</sub>, and CO, partial columns of O<sub>3</sub>, integrated between the surface and altitudes of 6, 12, and 16 km to provide information on the  $O_3$  vertical distribution and two test radiances, used to check the internal consistency of the retrievals. The transfer function has been calibrated using a set of selected modeled trace gas profiles (from the MOZART CTM and connected to climatologies and/or standard profiles above the tropopause) coupled to the LBLRTM high resolution line-by-line radiative transfer code, with the ECMWF surface and atmospheric temperatures. The input selection (radiances and temperatures) and the trace gas retrieval require less than 0.007 second (on a regular PC).

[74] The statistical inversion error has been evaluated to be about 28%, 15%, and 9% for the  $O_3$  partial columns between the surface and 6, 12, and 16 km, respectively, 1.5% for the  $O_3$  total column, 2% for the CH<sub>4</sub> total column, and 5% for the CO total column, which exceed the IASI Science Plan requirements [*ISSWG*, 1998] and is more adequate in terms of chemical variability of each gas [*Clerbaux et al.*, 2003]. A parallel module has been developed for the evaluation of the uncertainty associated to each retrieval, using the classical error analysis formalism [*Rodgers*, 2000]. The error analysis has shown that the largest inversion error is due to the sensitivity of the observing system itself (instrument and algorithm). The uncertainties on the input parameters will also have an



**Figure 13.** Comparison of the  $O_3$  columns retrieved from IMG/ADEOS data (gray diamonds) and the columns integrated from ozonesonde data (black crosses) for April 1–10, 1997, at the different WMO stations providing measurements collocated to the IMG data. The errorbars correspond to the standard deviation of the available data for the period studied and on a  $2.5^{\circ} \times 2.5^{\circ}$  area around the measurement station (for IMG retrievals).

important impact, which can be accurately estimated using the error analysis module.

[75] A first version of this algorithm is implemented at EUMETSAT for an integration to the ground segment of the EUMETSAT Polar System (EPS). The algorithm (coded in Fortran) is available upon request through the team web site (http://www.aero.jussieu.fr/themes/PCT/NNIASITraceGases/index.html). The NN parameters will be regularly updated to account for upgraded versions of the spectroscopic database, of the atmospheric chemistry

model, and of radiative transfer code. An improved version of the algorithm is under development to include several additional parameters (surface emissivity, topography) and enlarge the training data sets by including ozonesonde profiles for ozone, and regional model simulations and artificial extreme situations for the three trace gases. The possibility of directly retrieving a tropospheric column of ozone is also explored, but the complication of a spatially and temporally varying tropopause height has to be taken into account. The NN algorithm will be confronted with the different  $O_3$  concentration inversion methods developped in the framework of the IASI mission, following the preliminary intercomparison undertaken for the retrieval of the total column of CO by *Clerbaux et al.* [2002].

[76] A first validation exercise has been undertaken using the data provided by the IMG/ADEOS remote sensor, allowing the restitution of global distributions of  $O_3$ ,  $CH_4$  and CO. Although IMG/ADEOS provides an important tool for testing the developments, a complete validation could not be undertaken due to the lack of available independent measurements and to the short periods of time considered (which do not allow a comparison of the temporal variability represented in the data). However, this preliminary study has shown that a good performance can be expected. During the IASI mission, a very good spatio-temporal coverage will be achieved, allowing a full validation of the trace gas observation system (of the ability of the instrument to capture the temporal variation in particular).

[77] Clerbaux et al. [2001] have used data assimilation techniques to compare the model surface CO constrained by the IMG total columns with the surface measurements provided by the NOAA/CMDL (Climate Monitoring and Diagnostic Laboratory) [Novelli et al., 1992], showing that the IMG CO allow a better agreement between the model and the CMDL data. A systematic assimilation tool is currently being developed at Service d'Aéronomie for a coupled integration of  $O_3$ , CO, and CH<sub>4</sub> during the IASI mission, in order to provide high quality 3D Level 3 distributions and to facilitate the validation and interpretation of the retrieved columns.

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