EVALUATION OF TOTAL OZONE RETRIEVAL FROM NOAA-TOVS DATA BY MEANS OF NEURAL NETWORK TECHNIQUES

Anton K. Kaifel
Center for Solar Energy and Hydrogen Research
Hessbruehlstr 21c
70565 Stuttgart, GERMANY

1. INTRODUCTION

As recent research results of different authors (e.g. Manney, 1994 or Gathen, 1995) demonstrated chemical ozone depletion in the stratosphere occurring not only during winter and spring over the Antarctic but also during winter over the Arctic. Therefore it is important to monitor the total ozone and other relevant parameters like temperature profile, moisture and various trace gases especially during the Arctic or Antarctic winter, when there is no sunlight and the temperature of the stratosphere is very low.

In principle there are three different kinds of measurements instruments regarding to the spectral region they are working. The first one observe the backscattered ultraviolet radiation in the solar spectrum and is therefore only applicable during daylight. This are the Total Ozone Mapping spectrometer (TOMS) (Fleig, 1982a) the Solar Backscattered Ultraviolet Spectrometer (SBUV) (Fleig, 1982b) and Global Ozone Monitoring Experiment instrument (GOME) (ESA, 1993) recently launched with the ERS-2 satellite (April 1995). The second kind of instruments measures the thermal radiation emission of the earth-atmosphere system around the 9.6 μm absorption band of the ozone (HIRS/2) and the third one in the microwave spectral range (Microwave Limb Sounder, MLS on the Upper Atmosphere Research Satellite (UARS).

For TOMS and SBUV long term data sets are available and the accuracy of the total ozone retrieval is quite good. Long term comparisons over 8 years with Dobson data show a bias of +1% to -3% for TOMS and -1.8% to -5.5% for SBUV (Fleig, 1988). The disadvantage of this instrument is that daylight is necessary for measurements and therefore no data are available for wintertime in polar regions. The UARS is not an operational satellite and no long term data from the MLS are available for climate change studies.

For the TOVS instrument more than 15 years of data are already available and it is planned to continue the operational NOAA-TOVS system at least for the next decade and ozone retrieval is also possible during nighttime. Therefore the TOVS data has a high potential for use in climate and long term ozone monitoring studies.

For ozone retrieval from NOAA/TOVS data two different basic approaches can be made. First a physical retrieval scheme using TOVS ozone absorption channel 9 (e.g. ITTP TOVS data processing software see this
Kaifel, A.K. EVALUATION OF TOTAL OZONE RETRIEVAL...

proceedings). Over Italy Travaglini (1991) get a root mean square error (rms) of 13.03 Dobson Units (DU) in comparison with three different Dobson and Brewer ground measurement stations. Other studies are carried out with modifications on the retrieval scheme in the southern hemisphere by Li, (1991) and Le Marshall (1991).

Planet 1984 made a nonphysical approach using TOVS data for the total ozone amount retrieval based on multivariate linear regression. He used HIRS channel 1-3, 8 and 9 for linear regression analysis with ground measured Dobson spectrometer data. The standard deviation of the error is about 10-18 DU in the tropics and 18-25 DU in the regions poleward of 30° N and S. This approach did not take the nonlinearities of the relation between TOVS data and the total ozone amount of the atmosphere into account. To overcome this problem and to improve the retrieval accuracy for the total ozone amount Kaifel (1993) made an approach using neural networks instead of multivariate linear regression. The nonlinear behavior of the neural networks are well suited to this kind of approximation tasks.

The approach of using neural networks for total ozone amount retrieval from TOVS data presented at ITSC VII (Kaifel, 1993) will be evaluated for different weather conditions (clear/cloudy) for day and night and applied to a medium term data sets. A case study is carried out for the period of July and August 1993 coverage whole Europe, North Africa and parts of the Atlantic Ocean.

2. NEURAL NETWORK APPROACH

2.1 Topology

For the retrieval of the total ozone amount multilayer feed forward perceptron neural networks are used (Kaifel, 1993). This type of neural networks consists of an input layer, hidden layers and an output layer. Each layer of the network consists of a number of neurons and each neuron of a layer is fully connected with all other neurons in the adjacent layers. The number of input neurons corresponds to the number of input parameters (e.g. used HIRS channel, ...) and the output layer has only one neuron for the ozone retrieval representing the total ozone amount (Fig. 1).

2.2 Learning Algorithm

For training of the neural networks the Backpercolation algorithm (PERC) is used (Jurik, 1990). Extensive tests of various training algorithms stated (Kaifel, 1992) that Backpercolation is the most stable and fastest algorithm in comparison to Backpropagation (Rumelhart, 1988), Quickpropagation (Fahlmann, 1988) and RProp (Riedmüller, 1993).
Fig. 1: Neural network topology for total ozone retrieval from NOAA-TOVS data with data pre- and post processing (normalization) of input and output data.

2.3 Selection of Input Parameters

For the input of the neural network the TOVS data are calibrated and the brightness temperatures of the HIRS channels are used as input parameters. All infrared HIRS channels are used because it is known that the total ozone is correlated with the temperature in the stratosphere (Craig, 1965). Channel 17, the highest peaking short wavelength infrared channel, was omitted because there is evidence that the atmosphere is not in
thermodynamic equilibrium at the wavelength and altitude \((Planet, 1984)\). In order to take into account that there is a diurnal cycle of the total ozone and the temperature profile in the atmosphere an additional input indicating if it is a day or night overpass of the satellite is introduced (Fig. 1). A second additional input is used for the scan angle (scan point number from nadir) of the TOVS pixel, because no corrections are made during preprocessing for the scan angle. This can be done during the retrieval by the neural network too.

2.4 Training of the Neural Network

All brightness temperatures of the HIRS channels used as input parameters for the neural network are normalized to the interval of \([-1, +1]\) in order to omit saturation effects due to the applied sigmoid transfer function (tanh()) of each neuron in the hidden and output layers (Kaifel, 1993). The scan angle value or pixel number from nadir is coded in the interval \([0,1]\) and for the day/night input parameter the values 0 and 1 are used, respectively.

In the output value interval of the neural network \([-1, +1]\) the total ozone amount of the atmosphere is linear scaled in the Dobson Units (Fig. 1). As target value for the training of the neural network the ground based Dobson Spectrometer measurements collocated with the satellite observations are used. During training the total output error

\[
e = \sum_{k=1}^{N} (o_k - m_k)^2
\]

(1)

of the network is minimized. \(m_k\) represents the measured ozone data, \(o_k\) the corresponding estimates of the network and \(N\) the total number of training data samples, respectively.

For the training all available satellite observations collocated with ground based measurements are divided into a training and a test data set. This means that only about the half of the matchups are randomly selected to be used during training and the remaining data samples are used as an independent test data. This is necessary to test if the neural network does not overfit during training. If this occurs all the training pattern are learned and the network has no generalization ability which means that the error on the test data set is much greater than on the training data set.

3. CASE STUDY

3.1 Data Set

For the evaluation of the proposed ozone retrieval retrieval scheme (Kaifel, 1993) a case study is carried out with about 250 NOAA 11 satellite overpasses from July and August 1993 of the receiving station of the German Weather Service (DWD) in Offenbach, Germany. The coverage area and the number of TOVS pixels on a latitude/longitude grid are shown in Fig. 2. The color indicate the number of TOVS pixels.
The corresponding ground based measurements of the total ozone amount are at from the World Ozone and Ultraviolet Data Center (Woudc) of the Atmospheric and Environment Service Canada in Ontario. The ozone data we get from the Woudc are daily mean values and not preferable single measurement data what can cause some errors because the satellite data are instantaneous measurement data. For the collocation of the ground based data with the satellite data we used the following two criteria:

- Satellite overpass at the same day when a daily mean value of a station is available
- TOVS pixels in a circle of about 150 km around the ground station are used for the corresponding daily mean total ozone amount measurement

With these criteria we get 17899 collocation in total.

Fig. 2: Area coverage with 2-dimensional histogram of all HIRS pixels of about 250 satellite overpasses received at Offenbach, Germany

3.2 Satellite Data Processing

All the TOVS data are used and the cloud detection scheme of the "3I"-System (Scott, 1991, Wahiche, 1986) is applied in order to make different training cycles for the clear and the cloud contaminated collocations. Applying this procedure we got two data sets for clear and cloudy TOVS pixels with the corresponding ground ozone data. For clear case we get 10938 and for cloudy 6961, respectively. The minimum/maximum
measured ozone value is 233 D.U. / 367 D.U. for clear and cloudy cases. The mean and standard deviation value for clear is 307 D.U. and 18.2 D.U. and for the cloudy 319 D.U. and 19.3 D.U., respectively.

For the training 25 % of each data set (clear/cloudy) is used for training of the neural network and the remaining 75% as independent test data set. Tests using about 50% of the data for training stated no improvement in the retrieval accuracy.

4. RESULTS

First various tests are carried out to find the best network configuration concerning the generalization ability on the test data. We find that with only one output neuron a neural network with two hidden layers get the best results for the test data set. Fig. 1 show the network configuration used with two hidden layers of 15 and 10 neurons. The training of the clear and cloudy data set is carried out separately using HIRS channel 1-16, 18, 19, the scan point number and the day/night flag as input parameter. Tab. 1 shows the root mean square error (rms) and the mean absolute error (mae) for the training (index L) and test (index T) data set. The number of epochs is the number of iterations cycles used for training the neural network with the best generalization ability (minimum rms) on the test data set.

<table>
<thead>
<tr>
<th>data set / # sample sets</th>
<th>number of epochs</th>
<th>training data set (25%)</th>
<th>test data set (75%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>clear / 10938</td>
<td>3687.00</td>
<td>8.06</td>
<td>6.20</td>
</tr>
<tr>
<td>cloudy / 6961</td>
<td>2183.00</td>
<td>11.65</td>
<td>8.74</td>
</tr>
</tbody>
</table>

Tab. 1: Root mean square error (rms) and mean absolute error (mae) of the training and test data set for the clear and cloudy data samples.

As shown in Tab. 1 the differences of the rms and mae between the training and test data set are very low which indicate the good generalization ability of the neural network. Fig. 3a, b shows the rms over the scan point number from nadir of the HIRS instrument of the training and test data for the clear and cloudy learning cycles, respectively. It is shown that without any corrections for scan angle effects (e.g. path length) the neural network is able to correct the scan angle effects during the retrieval process.

With the trained neural networks for clear and cloudy TOVS pixels the whole TOVS data of each satellite overpass can be used for determine maps of the daily, weekly or monthly mean total ozone content of the atmosphere. Fig. 4a, b shows the mean total ozone content of the period from July 6, 1993 to August 10, 1993 for a) cloud free and b) cloudy HIRS pixels. It can be seen that the difference between Fig. 4a and 4b is not
significant which demonstrates that the approach of neural networks for total ozone retrieval is applicable for clear as well as for cloudy HIRS pixels (see also Fig. 4a,b).

Fig. 3: Root mean square error for training and test data of the a) clear and b) cloudy data samples over the scan point number from nadir of the HIRS instrument.
Fig. 4  Mean total ozone content for the period from July 6, 1993 to August 10, 1993 derived from NOAA 11 TOVS data by neural network technique for a) clear HIRS pixels and b) cloudy HIRS pixels. The violet patches at the upper left side of b) are due to missing HIRS data over this area and period.
5. CONCLUSIONS

For all different types of TOVS-Data (day/night, cloud free/cloudy pixels) the neural network technique enables the retrieval of the total ozone content of the atmosphere. The absolute mean error of the test data set for all cases is about 10 D.U.. For cloud free day pixels it is 8.5 D.U. and for cloudy one it is 10 D.U.. This prove that neural networks are a mature and well suited tool for retrieval and forward modelling tasks like the total ozone content as well as for temperature and moisture profiles (Chedin, 1995, Escobar, 1993, Rieu 1993) or radiative budget (Schweiger, 1995).

The study shows that it is possible to retrieve the total ozone content of the atmosphere with an accuracy of better than 2% for different weather conditions. The advantage of the TOVS-Data compared to other satellite instruments for ozone retrieval (TOMS, SBUV, GOME) using the solar spectrum is that also during night good accuracy of the ozone data can be achieved and that each day the retrieval cover the whole earth because it is possible to use for the retrieval the whole scan of the HIRS instrument which result in a better spatial resolution, too (TOMS, SBUV and GOME are only nadir looking spectrometers). Also, the TOVS sensor system which has flown on the NOAA polar-orbiting satellites since 1978 providing a record of 16 years of observations. Therefore TOVS sensor system has the potential to contribute to climate change research.

ACKNOWLEDGMENTS

I would like to dedicate this publication to Prof. Dr.-Ing. W.H. Bloss, the Director of the Institute of Physical Electronics of the University of Stuttgart and member of the managing board of the Center of Solar Energy and Hydrogen in Stuttgart, Germany. He died much too early when I'm writing this publication. He advised me, supported and promoted the work on satellite data processing and especially on ozone retrieval for a long time. I will try to continues the work in accordance with his wishes and ideas.

Sincere thanks are expressed to W. Benesch and T. Böhm from the German Weather Service (DWD) for providing the TOVS data; to E.W. Hare from the Atmospheric and Environment Service (WOUDEC), Canada for providing the ground based total ozone measurements and to B. Heisele from the Center for Solar Energy and Hydrogen Research who did most of the computational work.

6. REFERENCES


Schweiger, A., 1995: A neural network-based approach to the retrieval of the surface radiation budget of the Arctic from TOVS radiances. This proceedings.


