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Stand-Alone 1D-Var Scheme for the SSM/I, SSMIS and AMSU: User's Guide

Godelieve Deblonde, Meteorological Service of Canada

Stephen English and William Bell, Met Office, UK

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Godelieve Deblonde
Meteorological Service of Canada

Stephen English and William Bell
NWP Group Satellite Applications Section
Met Office

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User's Guide Version 2.0

Godelieve Deblonde
Data Assimilation and Satellite Meteorology Division
Meteorological Service of Canada
2121 Trans-Canada Highway, 5th floor
Dorval PQ
Canada H9P 1J3

Stephen English and William Bell
NWP Group Satellite Applications Section
Met Office
London Road
Bracknell
Berkshire
United Kingdom
RG12 2SZ

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1. Introduction

This document describes the Stand-Alone Variational Retrieval Scheme (SAVRS) for the SSMIS (Special Sensor Microwave Imager Sounder) instrument. This variational scheme also works for the SSM/I (Special Sensor Microwave Imager) and the ATOVS/AMSU (Advanced microwave sounding unit) instruments. A Stand-Alone Variational Retrieval Scheme was developed for the SSM/I (Ridley 2000) and first released to Beta-testers in August 2001. The SSM/I SAVRS was not sufficiently tested and should not be used as is.

The SSMIS SAVRS was developed from the SSM/I SAVRS. The SSMIS SARVS solves for atmospheric temperature, atmospheric water vapour, oceanic surface wind speed and either liquid water path or total water content. The scheme requires as input atmospheric profiles (background profiles) that are spatially and temporally collocated with the satellite observations and returns solution profiles that optimally fit both the observations and the background profiles. The optimal fit is determined by the relative weight of the background error covariances and the observation errors. The forward model (here the radiative transfer model) is RTTOV6.7 modified so that SSMIS, SSM/I and AMSU brightness temperatures and their Jacobians can be computed (see Appendix). The fast emissivity ocean model that should be used is Fastem Version 2.0 (Deblonde and English, 2001, English and Hewison, 1998). This model is included in RTTOV7.

It is assumed that the user is familiar with both variational data assimilation and microwave remote sensing techniques.

This documentation has been updated to include changes introducted at Version 2. The changes for version 2 was primarily to run using RTTOV7 rather than a modified version of RTTOV6. The modified RTTOV6 was distributed with version 1. For vresion 2 users are required to separately acquire RTTOV7 from rttov.nwpsaf@metoffice.com. For more information on RTTOV7 see the RTTOV pages at the NWP SAF website:

http://www.metoffice.com/research/interproj/nwpsaf/rtm/index.html.

Any bugs or suggestions for improvements to the SSMIS SAVRS product should be sent to ssmis.nwpsaf@metoffice.com using the procedure and forms available from the NWP SAF website (http://www.metoffice.com/research/interproj/nwpsaf/ssmi/index.html).

The results of version 1 and version 2 are almost identical. The results of testing of version 2 are available in a separate testing report from the NWP SAF website. The point in the transition to version 2 is future maintainability (the SAF could not support a separate RT code for this deliverable).

2. Background

2.1. Variational Assimilation Technique

A variational retrieval is applied in which the a priori or background information of the atmosphere and surface (x^b), and the measurements y^o (observed brightness temperatures) are combined in a statistically optimal way (with a Bayesian analysis) to estimate the most probable atmospheric state x. The approach is common to a number of areas where non-linear inverse problems are encountered and has been described in detail by many authors (e.g. Rodgers, 1976, Tarantola and Valette, 1982, Lorenc, 1986). Gaussian error distributions are assumed and consequently, obtaining the most probable state is equivalent to minimising a cost function $J(x)$ also referred to as a penalty function. Following the notation of Ide et al. (1997), $J(x)$ may be written as:

$$J(x) = \frac{1}{2}(x - x^b)^T B^{-1}(x - x^b) + \frac{1}{2}[y^o - H(x)]^T (E + F)^{-1}[y^o - H(x)] + J_s \tag{2.1}$$

where B, E and F are respectively, the background, the instrumental, and the representativeness (includes errors of the forward model) error covariance matrices. J_s is a cubic function that limits the supersaturation and acts as a weak constraint (Phalippou 1996):

$$J_s = a(x - x_s)^3 \tag{2.2}$$

x_s is the value of the control variable at saturation. $H(x)$ is the forward operator that maps the control vector x into measurement space. Here $H(x)$ is the radiative transfer model RTTOV6.7. The superscripts T and –1 denote matrix transpose and inverse respectively.

The control vector x consists of temperature (at 43 fixed pressure levels defined by the radiative transfer model), the natural logarithm of specific humidity (defined for the lowest 19 levels of the radiative transfer model) and the oceanic surface wind speed. Optionally, the liquid water path (LWP) defined below can also be added to the control vector.

$$LWP = \frac{1}{g}\int_0^{P_s} q_L(P)dP \qquad (2.3)$$

where g is the gravitational constant, P_s is the surface pressure and q_L is the cloud liquid water content ($kgkg^{-1}$).

If LWP is not chosen as a control variable, then one solves for the natural logarithm of total water content. The total water content is defined as follows:

$$q_{total}(P) = q(P) + q_L(P) \qquad (2.4)$$

where q is the specific humidity ($kgkg^{-1}$).

In general, the minimum of the cost function can be found by the iterative solution of (Newtonian iteration):

$$J''(x_n)(x_{n+1} - x_n) = -J'(x_n) \qquad (2.5)$$

and

$$J'(x_n) \rightarrow 0 . \qquad (2.6)$$

x_n and x_{n+1} are the n^{th} and $(n+1)^{th}$ approximation of x, J' and J'' are the first and second derivatives of the cost function with respect to x. These are given by:

$$J'(x_n) = B^{-1}(x_n - x^b) - H'(x_n)^T(E+F)^{-1}(y^o - H(x_n)) \qquad (2.7)$$

where $H'(x_n)$ is the Jacobian matrix and contains the partial derivatives of $H(x)$ with respect to x. In the linear limit,

$$J''(x_n) = B^{-1} + H'(x_n)^T(E+F)^{-1}H'(x_n) = A^{-1} \qquad (2.8)$$

where A is the error covariance matrix of the solution if $H(x)$ is linear. $J''(x_n)$ is also referred to as the Hessian of the cost function. A is also called the analysis error covariance matrix and in this document A will be referred to as the theoretical error.

2.1.1. Retrieving Liquid Water Path

When the 1D-Var is set up to work for the SSM/I instrument, the retrieval technique is based closely on that developed at ECMWF by L. Phalippou (Phalippou 1996). For this case, the control variable consists of the profile of natural logarithm of specific humidity (lnq), the oceanic surface wind speed (SWS) and the liquid water path. Thus x=(lnq, SWS, LWP).

During the minimisation process of Eq. (2.1), LWP is allowed to vary while the cloud structure S(P) is maintained fixed. The cloud structure S(P) is defined as follows:

$$S(P) = q_L(P)/LWP \qquad (2.9)$$

If there is a cloud in the background profile, then S(P) is given by:

$$S(P) = q_{LB}(P)/LWP_B \qquad (2.10)$$

where q_{LB}(P) is the background profile of cloud liquid water content and LWP_B is the liquid water path of the background profile.

If there is no cloud in the background profile, then a non-zero cloud structure is generated where the relative humidity of the background profile exceeds a pre-set threshold value (e.g. 80%). If there is still no cloud, then a non-zero cloud structure is assigned to the lowest levels of the profile.

In all cases, the first guess LWP is set to 0.1 kgm^{-2}.

The derivative of the brightness temperature (Tb) with respect to LWP is given by:

$$\frac{dTb}{dLWP} = \sum_{i=1}^{N} \frac{\partial Tb(P_i)}{\partial q_L} S(P_i) \qquad (2.11)$$

where N is the number of levels for which the sensitivity of brightness temperature with respect to cloud liquid water content ($\frac{\partial Tb}{\partial q_L}$) is computed by the radiative transfer model (RTTOV6.7).

2.1.2. Retrieving total cloud water content

The idea of retrieving total water content instead of retrieving water vapour content and liquid water path separately came from S. English and follows closely the same concept as that developed in Blankenship et al. (2000). When a water vapour profile is close to saturation, it is quite likely that a cloud will be present and this technique takes advantage of this.

The total water content (q_{total}) is defined as the sum of the water vapour content (q) and cloud liquid water content (q_L). The control variable lnq is replaced with $\ln q_{total}$. Thus the control variable is now x=($\ln q_{total}$, SWS) instead of x=(lnq, SWS, LWP). Each time the radiative transfer code is called, q_{total} is split among its water vapour content and cloud liquid water content. The split contents must be known to compute the sensitivities of Tb with respect to water vapour content ($\frac{\partial Tb}{\partial q}$) and cloud liquid water content ($\frac{\partial Tb}{\partial q_L}$). These sensitivities are needed to compute the sensitivity of Tb with respect to total water content (i.e.):

$$\frac{dTb}{d\ln q_{total}} = q_{total}\frac{dTb}{dq_{total}} = q_{total}\left[\frac{\partial Tb}{\partial q}\frac{\partial q}{\partial q_{total}} + \frac{\partial Tb}{\partial q_L}\frac{\partial q_L}{\partial q_{total}}\right] \quad (2.12)$$

Figure 1 illustrates how q and q_L are defined and also shows the derivatives of q and q_L with respect to q_{total}. The saturation water vapour content q_s depends only on temperature.

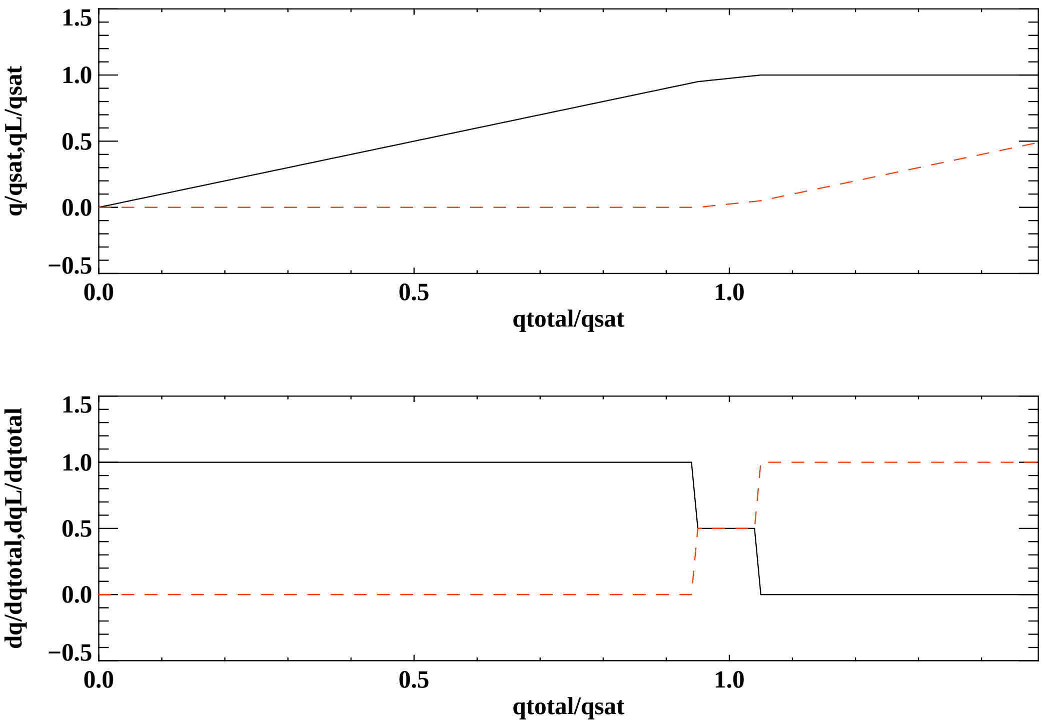

Figure 1: Top plot: dependence of q (water vapour content—black continuous curve) and q_L (cloud liquid water content—red dashed curve) on q_{total} (total water content). Below a threshold value of relative humidity of 95% (the relative humidity is defined as 100*(q_{total}/q_s)), it

is assumed that the water vapour content equals the total water content. Between relative humidities of 95% and 105%, the total water content is split halfway between the water vapour content and the cloud liquid water content. Above 105%, the water vapour content is maintained fixed and any excess water is cloud liquid water content. Bottom plot, derivatives of water vapour content (black continuous curve) and cloud liquid water content (red dashed curve) as a function of total water content.

Note that q and q_L also depend on temperature through the temperature dependence of q_s. In this version of the code (i.e. SSMIS 1D-Var version 1.0), temperature variations when total water content is retrieved is not allowed (i.e. temperature is not part of the control variable). Temperature variations however will be implemented in the next version of the code.

As in Blankenship et al. (2000), the SSMIS channels (Table 2) that were used to do these retrievals are the three water vapour line 183 GHz channels, the 150 GHz channel and the channels 12 to 16 (lowest frequency window channels) for a total of 9 channels.

2.1.3. Minimisation technique

The Levenberg-Marquardt method was implemented for the minimisation . The code based on Press et al. (1989) (See page 523) was kindly provided by Sean Healy from the Met Office.

2.2. Description of the SSM/I and SSMIS instruments

The channel parameter specifications for the DMSP (Defence Military Satellite Project) SSM/I (Special Sensor Microwave Imager) are listed in Table 1 (Hollinger et al. 1990). The SSM/I is a conical scanner with a scan angle (satellite view angle with respect to nadir) of ~ 45^o which corresponds to an earth incidence angle of ~ 53^o. The altitude is ~ 833 km. All channels have dual polarisation except for the 22 GHz channel. The first SSM/I instrument to be launched was the F08 in 1987. The last one sent was the F15.

Table 1: SSM/I Channel Parameter Specifications

Central Frequency (GHz)	First Sideband (GHz)	Half-bandwidth (MHz)	Polarisation	Ground resolution (km)	Ne∆T (K)
19.35	0.13	120	V,H*	70x45	0.8
22.235	0.13	120	V	60x40	0.8

37.0	0.55	450	V,H	38x30	0.6
85.5	0.8	700	V,H	16x14	1.1

* V= vertical polarisation, H= horizontal polarisation

The DMSP SSMIS (Special Sensor Microwave Imager/Sounder) (latest scheduled launch date is for November 2001) is also a conical scanner with a similar earth incidence angle to that of the SSM/I (i.e. ~ 53^o). The altitude is ~ 833 km. The SSMIS will have a larger swath width, 1700 km compared with 1400 km for the SSM/I. The ground resolution will be higher for the SSMIS than that of the SSM/I (compare Tables 2 and 1). The SSMIS instrument incorporates a humidity and temperature sounder as well as an imager (window channels). The sensor noise level of the SSMIS is also lower than that of the SSM/I. The first DMSP satellite to carry an SSMIS instrument is the F16.

Table 2: F16 SSMIS Channel Parameter Specifications

Channel Number	Center Frequency (GHz)	1st IF (MHz)	2nd IF (MHz)	Bandwidth* per passband (MHz)	Polarisation	EFOV** Along scan (km)	EFOV** 90° to scan	Ne∆T (K) For 305K Scene*
1	50.3	0.	0.	380.	H	17.6	27.3	0.21
2	52.8	0.	0.	388.8	H	17.6	27.3	0.20
3	53.596	0.	0.	380.0	H	17.6	27.3	0.21
4	54.40	0.	0.	382.5	H	17.6	27.3	0.20
5	55.50	0.	0.	391.3	H	17.6	27.3	0.22
6	57.29	0.	0.	330.0	H	17.6	27.3	0.26
7	59.4	0.	0.	238.8	H	17.6	27.3	0.25
8	150.0	1250.	0.	1642.	H	13.2	15.5	0.53
9	183.31	6600.	0.	1526.	H	13.2	15.5	0.56
10	183.31	3000.	0.	1019.	H	13.2	15.5	0.39
11	183.31	1000.	0.	512.5	H	13.2	15.5	0.38
12	19.35	0.	0.	355.0	H	44.8	73.6	0.35
13	19.35	0.	0.	356.7	V	44.8	73.6	0.34
14	22.235	0.	0.	407.5	V	44.8	73.6	0.45
15	37.0	0.	0.	1615.0	H	27.5	45.0	0.26
16	37.0	0.	0.	1545.	V	27.5	45.0	0.22
17	91.655	900.	0.	1418.	V	13.2	15.5	0.19
18	91.655	900.	0.	1411.	H	13.2	15.5	0.19
19	63.283248	285.271	0.	1.36	H+V	17.6	27.3	1.23
20	60.792668	357.892	0.	1.35	H+V	17.6	27.3	1.18
21	60.792668	357.892	2.	1.29	H+V	17.6	27.3	0.86
22	60.792668	357.892	5.5	2.62	H+V	17.6	27.3	0.58
23	60.792668	357.892	16.	7.32	H+V	17.6	27.3	0.37
24	60.792668	357.892	50.	26.5	H+V	17.6	27.3	0.38

* Measured for this unit prior to launch
** Raw data resolution (prior to on-board averaging) based on measured half-power beam width and spacecraft altitude of 833 km.

3. Code description

The code and test cases are stored in a file named ssmis1dvar.tar.Z. Type the following commands to unpack the code:

- mkdir ssmis1dvar
- cd ssmis1dvar
- (copy file ssmis1dvar.tar.Z here)
- uncompress ssmis1dvar.tar.Z
- tar xvf ssmis1dvar.tar

3.1. List of directories

/ssmis1dvar/1dvar

Contains ssmi1dvar.sh (script to execute the SSMIS 1D-Var) and SSMI_SAFProg.f90 which calls Standalone1Dvar.f90.

/ssmis1dvar/1dvar/ssmissrc

Contains 1D-Var routines

/ssmis1dvar/1dvar/rttovsrc

This directory contained RTTOV6 source code for version 1. For this version you must place the RTTOV7 source code in this directory.

/ssmis1dvar/1dvar/ssmidata

Contains SSM/I, SSMIS and AMSU related input files (section 3.4.1)

/ssmis1dvar/1dvar/rttovdata

You are required to put RTTOV7 data files into this directory.

/ssmis1dvar/simdat

Contains code to generate true and noisy profile data sets (section 4.1)

/ssmis1dvar/wave

Contains wave procedures to display and process the results (section 4.5)

3.2. List of SSMIS 1D-Var routines

Subroutines new to the SSMIS 1D-Var (not in original SSM/I 1D-Var):

SSMI_CloudStructure.f90
SSMI_ParamsOut.f90
SSMI_Prslev.f90
SSMI_Qtot_to_q_ql.f90
    SSMI_Qtot_to_q_ql_v1.f90
    SSMI_Qtot_to_q_ql_v2.f90
SSMI_Sat_Check.f90

Subroutines NOT changed (from original SSM/I 1D-Var):

SSMI_Cholesky.f90
SSMI_GetUnitNo.f90
SSMI_Linear_Solver.f90
SSMI_OpenFFile.f90
SSMI_svp.f90

List of all SSMIS 1D-Var routines:

Modules:
1 SSMIMod_Background.f90
2 SSMIMod_Emis.f90
3 SSMIMod_Obs.f90
4 SSMIMod_Params.f90
5 SSMIMod_Variables.f90

Subroutines:
1 SSMI_Cholesky.f90
2 SSMI_CloudStructure.f90
3 SSMI_ColumnSum.f90
4 SSMI_CopyX.f90
5 SSMI_DataOut.f90
6 SSMI_Descent.f90
7 SSMI_ErrorCov.f90
8 SSMI_GetUnitNo.f90
9 SSMI_InitRTmodel.f90
10 SSMI_LWP_to_Layers.f90
11 SSMI_LayerK_to_LWPK.f90
12 SSMI_Layers_to_LWP.f90
13 SSMI_Linear_Solver.f90
14 SSMI_MinV.f90
15 SSMI_OneDVar.f90
16 SSMI_OpenFFile.f90
17 SSMI_ParamsOut.f90
18 SSMI_Pen_Func_Sat.f90
19 SSMI_Penalty_Function.f90
20 SSMI_Prslev.f90
21 SSMI_Qtot_to_q_ql.f90
22 SSMI_Qtot_to_q_ql_v1.f90
23 SSMI_Qtot_to_q_ql_v2.f90
24 SSMI_ReadBGCov.f90
25 SSMI_ReadBackground.f90
26 SSMI_ReadSSMI.f90
27 SSMI_Regressions.f90
28 SSMI_Sat_Check.f90
29 SSMI_SetCov.f90
30 SSMI_TranslateDataIn.f90
31 SSMI_eval_derivs.f90
32 SSMI_eval_derivs_sat.f90
33 SSMI_svp.f90

3.3. SSMIS 1D-Var Calling Tree Structure

SSMIS_SAFProg.f90 (calls Standalone_1Dvar)

Standalone_1Dvar

```
SSMI_InitRTmodel
        RTTVI                         -RTTOV7
SSMI_SetCov

For each profile

SSMI_ReadBackground
IF (Op_Mode ==1 ) SSMI_ReadSSMI
SSMI_TranslateDataIn
SSMI_OneDVar

        IF (Op_Mode ==2) RTTOV        -RTTOV7
        SSMI_Descent
                SSMI_CopyX

                For each iteration

                RTTOVK                -RTTOV7

                SSMI_Layers_to_LWP
                IF (.NOT.Lqtotal) SSMI_LayerK_to_LWPK
                IF (Lqtotal) SSMI_Qtot_to_q_ql
                SSMI_CopyX
                SSMI_Penalty_Function
                SSMI_Pen_Func_Sat
                SSMI_eval_derivs
                IF(Lsimdat) RETURN
                SSMI_eval_derivs_sat
                SSMI_Cholesky
                SSMI_Linear_Solver
                IF(.NOT.Lqtotal) SSMI_LWP_to_Layers
                IF(Lqtotal) SSMI_Qtot_to_q_ql

                End for each iteration

        SSMI_CopyX
        SSMI_Sat_Check
        SSMI_ColumnSum
        SSMI_ErrorCov
        SSMI_DataOut

End for each profile

SSMI_ParamsOut
```

3.4. List and description of input and output files

3.4.1. INPUT FILES for RTTOV and SSMIS 1D-Var stored in subdirectories rttovdata and ssmidata

The files needed as input for RTTOV are listed in Table 3 and those needed for the execution of the SSMIS 1D-Var are listed in Table 4.

Table 3: Input files needed by RTTOV7 to run the SSMIS 1D-Var for the SSM/I, the SSMIS and AMSU instruments. The files are stored in ssmis1dvar/1dvar/rttovdata.

File Names	**Content (ASCII Files)**
input_atovs_fastem2.dat input_ssmi_fastem2.dat input_ssmis_fastem2.dat	Contains channel selection flags and default surface emissivity (=-1.0 to activate Fastem 2.0). Note that Fastem 2.0 needs to be activated only for channels that are sensitive to the surface. For the channels that are not sensitive to the surface a value > 0 can be used as input.
refprof.dat	Contains the reference profile on fixed pressure levels (43 levels).
rtcoef_noaa_15_amsua.dat rtcoef_noaa_15_amsub.dat rtcoef_noaa_16_amsua.dat rtcoef_noaa_16_amsub.dat rcoef_noaa_17_amsua.dat rtcoef_noaa_17_amsub.dat rtcoef_dmsp_13_ssmi.dat rtcoef_dmsp_14_ssmi.dat rtcoef_dmsp_15_ssmi.dat rtcoef_dmsp_16_ssmis.dat	Contains all radiative transfer coefficients on 43 fixed pressure levels for water vapour and mixed gas absorption. Also contains Fastem coefficients.

Table 4: Input files needed by the SSMIS 1D-Var to run for the SSM/I, the SSMIS and AMSU instruments. The files are stored in ssmis1dvar/1dvar/ssmidata.

File Names	Content (ASCII Files)
ATOVS_Bmatrix72_43	B matrix file (section 2.1). The format of the file read in is specified in detail in SSMI_ReadBGCov.f90. Although this B-Matrix contains the background error covariances of lnq for the 26 lowest levels of the atmosphere, only values for the lowest 19 levels are used in the SSMIS 1D-Var. The background error variances for SWS and LWP are defined in SSMIMod_Params.f90 by the variables BG_windspeed_SD and BG_LWP_SD respectively.
FILBIASO_atovs FILBIASO_ssmi FILBIASO_ssmis	Contains a listing of brightness temperature biases to be applied to raw brightness temperature observations. Since this version of the SSMIS 1D-Var has been set up for synthetic cases only, the biases have all been set to zero.
FILCOVO_mix2_atovs FILCOVO_mix2_ssmi FILCOVO_mix2_ssmis	Contains the observation errors (E+F), see section 2.1 for the various instruments. The errors must be provided for the number of channels defined by NumATOVS_Chans in the case of ATOVS, NumSSMI_Chans (=7) for the SSM/I and NumSSMI_Chans (=24) for the SSMIS.
gaussian_noise2.dat	A file containing a sequence of gaussian random numbers with mean zero and standard deviation of 1. One random number is read in per Tb observation (for each channel and profile). This "noise" is added to the synthetic brightness temperatures when the SSMIS 1D-Var is solved.
unit_numbers.dat	Contains a list of allowable logical unit numbers which may be used by the I/O calls of the SSMIS 1D-Var. A list of all the files for which I/O occurs in the SSMIS 1D-Var is given in: SSMIMod_Variables.f90.
zero_noise.dat	A file containing zero's. This file is read in when the SSMIS 1D-Var is only used to simulate brightness temperatures only.

3.4.2. INPUT/OUTPUT FILES of the SSMIS 1D-Var

1) Simulating brightness temperatures

Table 5: Output files generated when the SSMIS 1D-Var is used to simulate Tb's only.

File Name (All output files)	Contents (in ASCII format)
FILEOUT	Contains general output and the analysis errors (diagonal elements of the inverse of the Hessian) for the true profile data set.
FILCONVERG	Not Applicable
FILWFORWARD	To be used as FILTB (Table 6) when the SSMIS 1D-Var is solved. Contains synthetic brightness temperatures obtained with the true profile data set.
FILRETRIEVALS	Not Applicable.

2) Solving for the SSMIS 1D-Var

Table 6: Input and Output files when the SSMIS 1D-Var is used to compute the retrievals

File Name (All output files except FILTB)	Contents (in ASCII format)
FILTB	Contains synthetic brightness temperatures generated from the true profile data set (FILWFORWARD in section above).
FILEOUT	Contains general output and the analysis errors (diagonal elements of the inverse of the Hessian) for the retrievals.
FILCONVERG	Contains a listing of convergence criteria information for each profile.
FILWFORWARD	Not Applicable.
FILRETRIEVALS	Contains temperature, q and q_L retrievals at the 43 fixed pressure levels.

4. Running the SSMIS 1D-Var

For purposes of testing the 1D-Var code and for process studies, Version 1.0 of the SSMIS 1D-Var was built so that retrievals are obtained from synthetic brightness temperatures and synthetic background profiles.

First, the instrument configuration has to be set up (section 4.1). Secondly, a data set of true and noisy profiles is created (section 4.2). Thirdly, synthetic brightness temperatures are computed from the true profile data set (section 4.3) and at the same time, the theoretical error (or A, section 2.1) of the true profile data set is computed.

Finally, retrievals are obtained for the noisy profile data set which are used as background field (section 4.4). The observations are the synthetic brightness temperatures (obtained with the true profile data set) to which Gaussian noise is added that reflects the observation error.

4.1. Configuration set-up for AMSU, SSM/I and SSMIS

Changes have to be made to the code to run the 1D-Var for different instruments. Note that the instructions are also listed in the script that runs the SSMIS 1D-Var: ssmis1dvar/1dvar/ssmis1dvar.sh.

Four simple changes are involved:

(1) In **Standalone_1DVar.f90** (ssmis1dvar/1dvar/ssmissrc) set the following:
Set ATOVS or DMSP =true and then the other one MUST be false.
Define the Satellite_ID of the instrument (see comments in subroutine Standalone_1DVar.f90).

Instrument	AMSU	SSMIS	SSMI
ATOVS	.TRUE.	.FALSE	.FALSE.
DMSP	.FALSE.	.TRUE.	.TRUE.

(2) In **cparam.f90** (/ssmis1dvar/1dvar/rttovsrc) set the following:

AMSU: jpchus= Number of channels selected (≤ 20) in input.dat (ssmis1dvar/1dvar /rttovdata). Remember that the SSMIS 1D-Var only works for microwave channels.
SSMIS: jpssmi=24 and jpchus = Number of channels selected (≤24) in input.dat (ssmis1dvar/1dvar /rttovdata)
SSMI: jpssmi=7 and jpchus = Number of channels selected (≤7) in input.dat (ssmis1dvar/1dvar /rttovdata)

(3) In **SSMIMod_Params.f90** (/ssmis1dvar/1dvar/ssmissrc) set the following:

AMSU: Num_Chans_Used = # of channels selected (≤20) in input.dat (ssmis1dvar/1dvar /rttovdata)
SSMIS NumSSMI_Chans=24 and Num_Chans_Used = # of channels selected (≤24) in input.dat (ssmis1dvar/1dvar /rttovdata)
SSMI NumSSMI_Chans=7 and Num_Chans_Used = # of channels selected (≤7) in input.dat (ssmis1dvar/1dvar /rttovdata)

IMPORTANT: jpchus MUST EQUAL Num_Chans_Used

(4) The zenith angle is defined in ssmis1dvar/1dvar/ssmissrc/**SSMI_ReadBackground.f90**.

Since the SSM/I is a conical scanner and the zenith angle is not provided with the satellite data, the zenith angle should be set equal to a fixed value of ~53.1^{o} for all observations.

The SSMI/S is also a conical scanner and the zenith angle will be provided with the satellite data. The zenith angle is expected to vary by a few degrees around 53^{o}. The RTTOV SSMIS optical depth regression coefficients were developed for a zenith angle valid between 50 and 56^{o} (see Appendix) and thus the zenith angle specified ***must not be outside this range***.

AMSU is a cross-track scanner and the zenith angle varies between 0 and 70^{o}.

4.2. Generating true and noisy profile data sets

The method used to simulate the background profiles closely follows that presented in Eyre (1989). The background profiles (x^b) are generated from a single true profile (x^{true}) by adding noise to the latter. Thus $x^b=x^{true}$+noise. The covariance matrix of the noise has to be the same as that of the background error covariance matrix B introduced in section 2.1.

To generate the noisy profiles, one first computes the eigenvectors (E_i) and eigenvalues (λ_i) of the B matrix. The noise for each profile p and variable v in the control vector of dimension V is then defined as follows:

$$Noise(v,p) = \sum_{i=1}^{V} \varepsilon(p,i)\lambda^{1/2}(i)E(v,i) \tag{4.1}$$

ε is a random number drawn from a Gaussian distribution with zero mean and unit standard deviation. The eigenvalues are equal to the background error variance: the diagonal elements of the B matrix.

The size of the sample N of noisy profiles (need at least 500 samples from experience with the SSMIS 1D-Var) has to be large enough to reproduce the B matrix with sufficient accuracy. It is also very important to reproduce the off-diagonal elements of B accurately since they represent vertical correlations among the variables being modelled. Here we only consider vertical correlations between like variables (e.g. error correlations between temperature and specific humidity are ignored) and therefore the retrievals or analyses are referred to as univariate.

For simplicity of coding in the 1D-Var, even if there is only one true profile, it is duplicated N times to create a true profile data set of size N. It also possible to add a different cloud drawn from a distribution of clouds (uniform random distribution for example) of size N to the true profile and thus again creating a data set of N true profiles.

The code to generate the true and noisy profiles is stored in ssmis1dvar/simdat. Parts of the code are based on Press et al. (1989) and were kindly provided by Sean Healy from the Met Office.

The main program is called prepare_profiles.f90 and the script that generates the profile data sets is called prepare_profiles.sh.

Parameter settings to generate the true and noisy profiles are listed in detail in Table 7.

Table 7: Parameter settings to generate true and noisy profile data sets. N is the number of samples (or profiles) contained in the true and noisy profile data sets.

Parameter	Description
LTEMP	IF TRUE: Add noise to temperature profiles
LWAT	IF TRUE: Add noise to specific humidity profiles (flag not used if both ADDCLOUD and LQTOTAL are true)
LWIND	IF TRUE: Add noise to surface wind speed
ADDCLOUD	IF **FALSE**, the true profile data set will simply contain N times the single true profile read in. **IF ADDCLOUD=TRUE AND LQTOTAL=FALSE*:** ➢ *True profile data set:* (1) A cloud structure function is chosen S(P), see section 2.1. (2) The single true profile is saturated at the levels where a cloud is added (where the cloud structure is non-zero). (3) This single true profile is then repeated N times in the true profile data set but a different cloud liquid water path is assigned to each true profile. The cloud structure S(P) always remains the same but the LWP is drawn from a uniform random distribution such that $q_L(P,j)=LWP(j)\ S(P)$ where P is the pressure and j is the sample number (j ranges between 1 and N). ➢ *The noisy profile data set* contains the same profiles of cloud liquid water content as the true data set. The temperature profiles, specific humidity profiles and surface wind speed may have noise added to them depending on the logical value set for LTEMP, LWAT and LWIND respectively. **IF ADDCLOUD =TRUE and LQTOTAL=TRUE*:** ➢ *True profile data set:* (1) A single cloud liquid water content profile is chosen. (2) The single true profile of specific humidity is saturated at the levels where the cloud liquid water content > 0. This single true cloudy profile is then repeated N times to form the true profile data set. ➢ *Noisy profile data set:* (1) The total water content is computed for the single true cloudy profile: add water vapour content with cloud liquid water content. (2) Noise with the same statistical properties as lnq is then added to the total water content. Hence, the noisy profile data set contains profiles of temperature, total water content and surface wind speed. Temperature profiles and surface wind speed may have noise added to them depending on the logical value set for LTEMP and LWIND. For version 1.0 of the SSMIS 1D-Var, LTEMP must be set to FALSE since when the total water content is retrieved, temperature variation is not allowed.
LQTOTAL	See ADDCLOUD
BmatFaclnQ	Factor multiplying only the B matrix values of lnq. Normally should be =1. WARNING: If BmatFaclnQ is changed in the SSMIS 1D-Var code, then it **must** also be changed in the code that creates the true and noisy profile data sets and in the wave code that plots and processes the output of the SSMIS 1D-Var.

*If LQTOTAL is true, then one solves for total water content (q_{total}) and not LWP in the SSMIS-1D-Var.

4.3. Computing synthetic brightness temperatures

To compute synthetic brightness temperatures and the theoretical error (A, section 2.1) for the true profiles, the parameter Op_Mode in SSMIMod_Params.f90 must be set to 2 and Lsimdat which is a logical flag must be set to true.

If Op_Mode=2, the FORTRAN statement CALL RTTOV is activated and the brightness temperatures are computed by RTTOV. In SSMI_Descent, the routine is exited after the derivatives of the cost function are evaluated. The latter are needed to compute the matrix A. The square root of the diagonal elements of A are an estimate of the theoretical error, which is, read in by the post-processing and graphics procedures in wave (p1dvar.pro and hessian.pro)

In **SSMIMod_Params.f90**: Op_Mode=2 and Lsimdat=.TRUE.

4.4. Solving the SSMIS 1D-Var

The 1D-Var problem is solved with (1) the background profiles read in from the noisy profile data set and (2) the observations (synthetic brightness temperatures) read in from the file generated as per instructions given in section 4.3. Gaussian noise (uncorrelated between channels) with mean zero and standard deviation of one is read in during the execution of the SSMIS 1D-Var and is multiplied by $(E+F)^{1/2}$ where E+F (section 2.1) is a vector since we assume that the instrument and forward model errors are not correlated between channels. This noise is then added to the synthetic brightness temperatures. To activate the retrieving mode of the SSMIS 1D-Var, Op_Mode must equal 1 and Lsimdat must be set to false.

In **SSMIMod_Params.f90**: Op_Mode=1 and Lsimdat=.FALSE.

Parameters in SSMIMod_Params.f90 that require frequent adjustment depending on the problem solved are listed in Table 8. The logical parameter setting which allows one to solve the problem for either LWP or total water content is listed in Table 9.

Table 8: Description of parameters in SSMIMod_Params.f90 that often require to be changed depending on the instrument and channel selection.

PARAMETER	Description
Super_saturation_switch	If TRUE: Adds a penalty term to the cost function in order to limit the supersaturation (See section 2.1).
CutsatBG	If TRUE: forces the background water vapour to be less or equal to its saturation value.
Lqtotal	If TRUE, solve for Total Water Content.
DebugMode2	If TRUE: print out for debugging of the minimisation is activated.
Lforcecloud	If FALSE: The cloud structure function S(P) will only be non-zero if there is a cloud in the background profile. Thus if the background profiles do not have clouds, the LWP retrieved will always be zero. If TRUE: A cloud structure function will be created whether or not there is a cloud in the background profile and thus non-zero LWP will be retrieved (same approach as in Phalippou 1996) For a definition of the cloud structure function S(P), see section 2.1.1.
LwindVar	If FALSE, dTb/dSWS is set to zero.
LlnQVar	If FALSE, dTb/dlnq is set to zero.
LtemperatureVar	If FALSE, dTb/dT is set to zero.
LtskinVar	If FALSE, dTb/dTskin is set to zero. Never tested in TRUE mode.

Table 9: Logical parameter settings in SSMIMod_Params.f90, which allow one to solve for LWP (Liquid water path in kgm-2) or total water, content (kgkg^{-1}).

PARAMETER	Solving for LWP	Solving for total water content
Lforcecloud	TRUE or FALSE	***MUST BE FALSE***
Lqtotal	***MUST BE FALSE***	***MUST BE TRUE***
CutsatBG	Preferably TRUE	***MUST BE FALSE***
Super_saturation_switch	Preferably TRUE	***MUST BE FALSE***
LtemperatureVar	TRUE or FALSE	***MUST BE FALSE***
LwindVar	TRUE or FALSE	TRUE or FALSE
LlnQVar	TRUE or FALSE	***MUST be TRUE***

Two subroutines are provided to split the total water content into water vapour content and cloud liquid water content. These routines also calculate the derivatives of the two latter variables with respect to total water content.

The first of these routines is called SSMI_Qtot_to_q_ql_v1.f90. It uses discontinuous thresholds to specify the water vapour content and cloud liquid water content. The second routine called SSMI_Qtot_to_q_ql_v2.f90 is a “continuous” version of the first one and uses tangent hyperbolic functions. To use either one, copy the one selected to SSMI_Qtot_to_q_ql.f90. While version 2 uses continuous functions, version 1.0 is more robust numerically.

4.5. Wave routines to process/display results

Users must have a valid licence of wave to use these procedures. The main procedures are p1dvar.pro and hessian.pro.

5. Test Cases

All test cases have been performed with the US standard atmosphere profile (Figure 2). The total column integrated water vapour (TCWV) for this profile is 14.2 kgm^{-2}. The oceanic surface wind speed was set to 7 ms^{-1}.

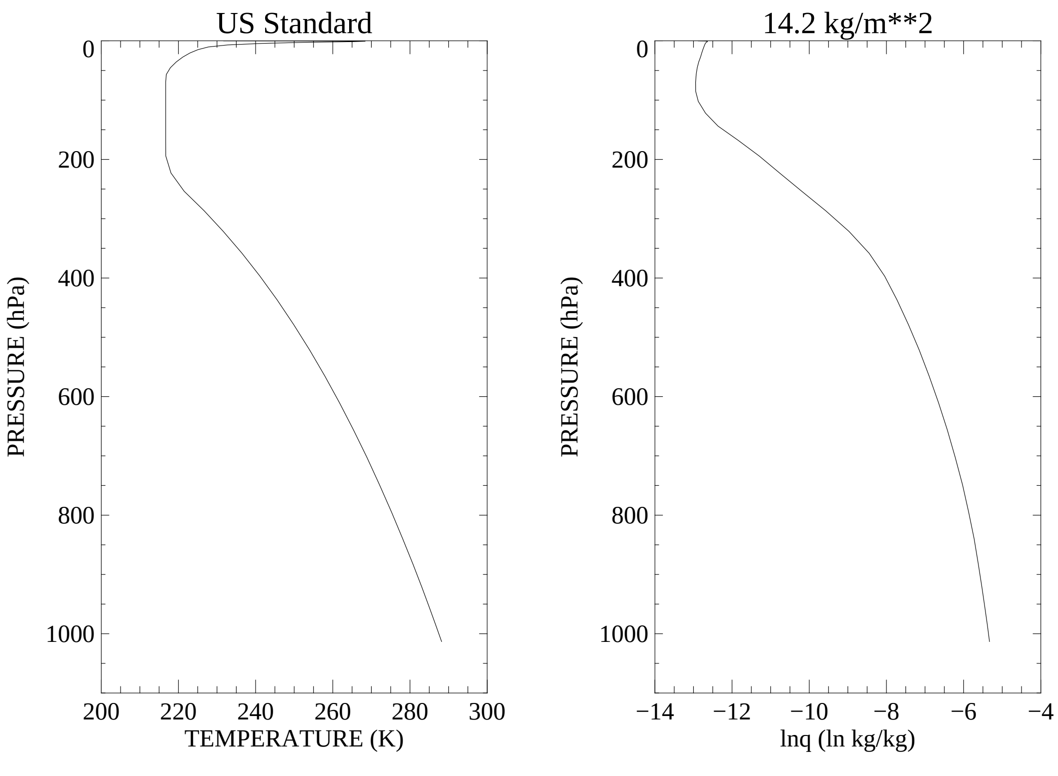

Figure 2: US standard atmosphere used as a true profile for all experiments presented in this user's guide. The value of the true surface wind speed is 7 ms^{-1}.

5.1. AMSU

Temperature retrievals using channels 6 to 11 (Num_Chans_Used=6) for the AMSU-A instrument were performed. The parameters for the generation of the true and noisy profile data sets were as follows: LTEMP=T, LWAT=F, LWIND=F, ADDCLOUD=F and LQTOTAL=F. Thus, noise is added only to the temperature profile. The parameter settings for the SSMIS 1D-Var (in SSMIMod_Params.f90) are as follows: Super_saturation_switch=F, cutsatBG=F, Lqtotal=F, Lforcecloud=F, LwindVar=F, LlnQVar=F, LtskinVar=F and LtemperatureVar=T.

Retrieving temperature is a linear problem ($H(x)$ is linear) and therefore, the error variances computed between the retrieved temperature profiles and the true profiles should be very similar to those obtained from the diagonal elements of the analysis error matrix A (section 2.1). This is illustrated in Figure 3 for two different zenith angles: 53.1^{o} and 0^{o} (or nadir). The sample size N is 3000. The number of iterations for all retrievals was 3. The observation cost function (second term on the right hand side of Eq. (2.1) of the solution for linear $H(x)$ has a chi-square distribution with mean equal to ½ the number of degrees of freedom. As expected, the mean computed for this experiment equals 3.0 which is equal to 0.5* Num_Chans_Used.

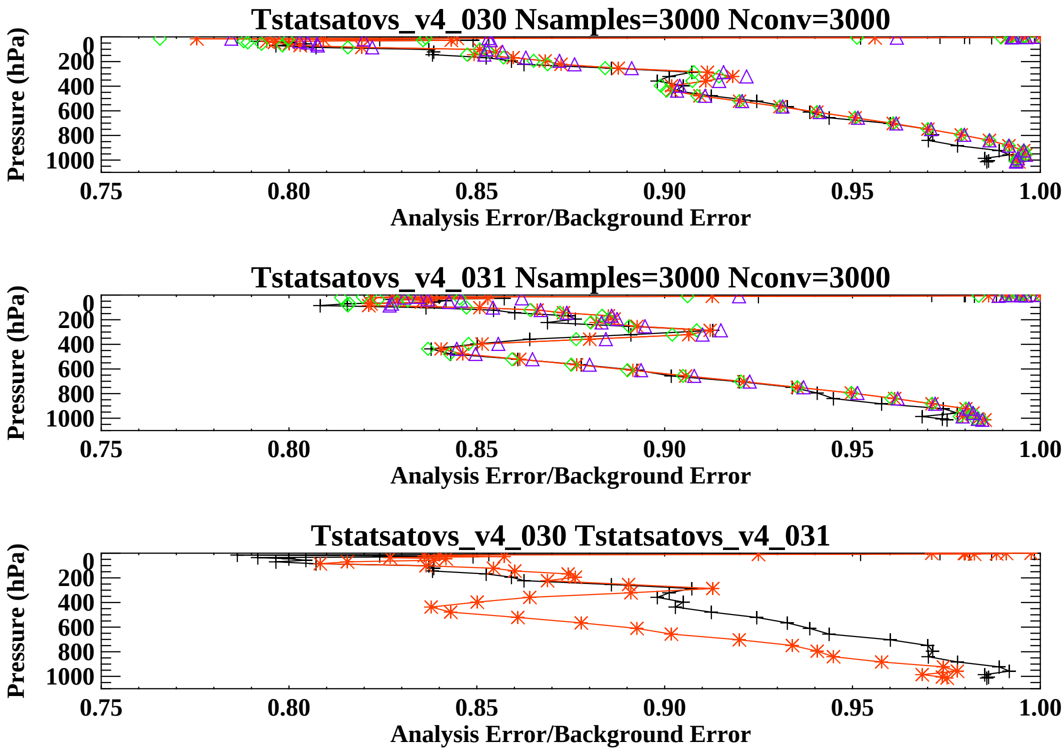

Figure 3: Normalised error standard deviations for AMSU-A (channels 6 to 11) temperature retrievals as a function of pressure. The sample size N is 3000. In the top plot, the error statistics are illustrated for a zenith angle of 53.1°. The red curve (with stars) illustrates $\sqrt{A_{ii}/B_{ii}}$ for the true profile (analysis error divided by the background error). The black curve (with plus signs) illustrates the error computed between the retrievals and the true profile (or standard deviation of (x-x_{true})) and divided by the background error. The green and purple diamonds illustrate respectively the minimum and maximum values of $\sqrt{A_{ii}/B_{ii}}$ for the retrieved profiles. The middle plot illustrates the same statistics as in the top plot but for a zenith angle of 0°. In the bottom plots, only the normalised computed errors are displayed for both zenith angles (53.1° –black curve with plus signs and 0° –red curve with stars).

5.2. SSM/I

The theoretical error is an accurate estimate of the retrieval error only if the forward problem is linear or weakly non-linear at best (for a linear example of forward problem, see the AMSU temperature retrieval problem in section 5.1). In the case of a non-linear forward problem such as the retrieval of water vapour, it is not possible to verify that the 1D-Var works correctly by comparing the error computed from the retrievals with that from the A matrix (section 2.1) or theoretical error.

However, as suggested by John Eyre (personal communication 2001 and Eyre and Collard 1999), if one reduces the size of the elements of the B matrix (or background error covariance matrix), then the two quantities (computed errors from the retrievals versus analysis error A) should become closer since the effect of reducing the size of the elements of the B matrix is to reduce the non-linearity of the problem.

Another impediment to a direct comparison of computed errors from the retrievals with the analysis error from A is the fact that background and retrieved water vapour profiles should not be supersaturated since these are not observed in the atmosphere. If supersaturation is not allowed, this introduces a bias in the retrieved quantities. The only way to strictly compare the computed errors from the retrievals with the analysis error from A is thus to allow for supersaturation but only do so to test that the 1D-Var code is working properly.

5.2.1. Retrievals in the absence of clouds

Water vapour and oceanic surface wind speed retrievals using all SSM/I channels (Num_Chans_Used=7) were performed. The parameters for the generation of the true and noisy profile data sets were as follows: LTEMP=F, LWAT=T, LWIND=T, ADDCLOUD=F and LQTOTAL=F. Thus, noise is added only to the water vapour profile and the surface wind speed. The parameter settings for the SSMIS 1D-Var (in SSMIMod_Params.f90) are as follows: Super_saturation_switch=F, cutsatBG=F, Lqtotal=F, Lforcecloud=F, LwindVar=T, LlnQVar=T, LtskinVar=F and LtemperatureVar=F. To reduce the size of the elements of the B matrix (as discussed above), the B matrix for lnq was multiplied by BmatFaclnQ=0.25. This parameter needs to be set in the 1D-Var code (SSMIMod_Params.f90) and in the code that generates the true and noisy profile data sets. The sample size was 3000. This experiment will be referred to **SSMI1**.

The number of iterations required varied between 2 and 5 with only a few cases with 2 or 5 iterations. The average value of the cost function was 3.35 ($H(x)$ is non-linear). The results for the retrievals of water vapour are shown in Figure 4 (for the first 500 and all 3000 samples). The computed error from the retrievals is indeed similar to that of the analysis matrix A and more so as the sample size increases. For the wind speed retrievals, the error computed from the retrievals was 1.44 ms^{-1} which is the same as that obtained from the analysis error matrix A. The background error for the surface wind speed was set to 2 ms^{-1} (Table 4).

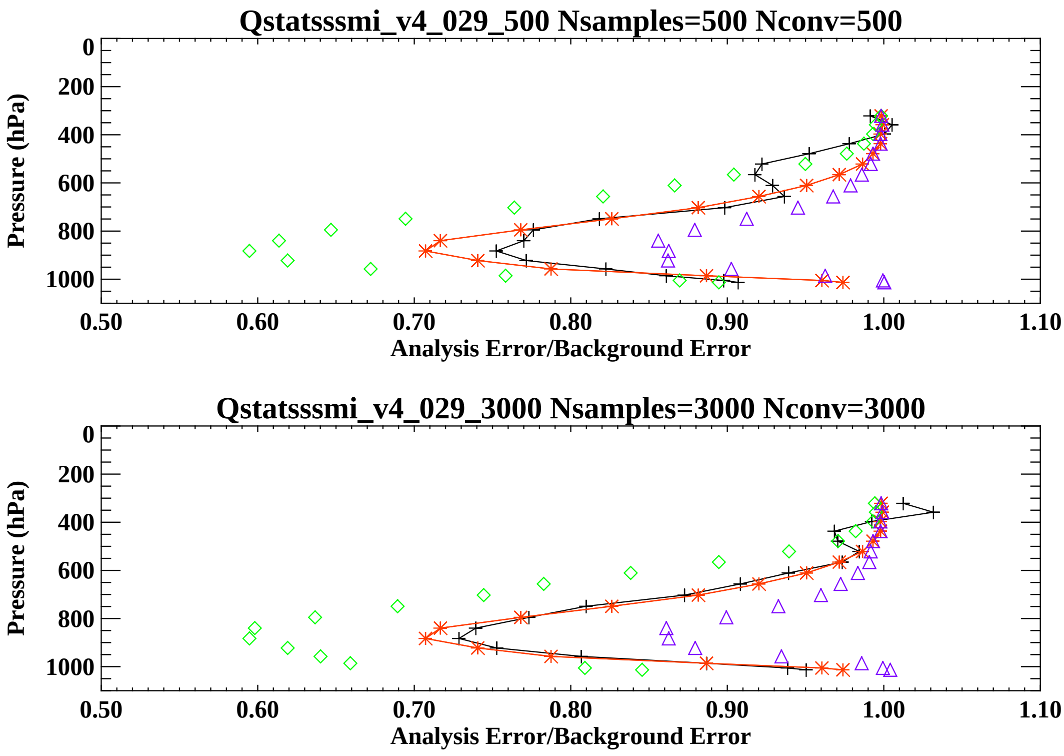

Figure 4: Normalised error standard deviations for SSM/I (all channels) natural logarithm of specific humidity retrievals as a function of pressure (Experiment SSMI1). The zenith angle is 53.1° and BmatFaclnQ=0.25. The error statistics are illustrated as a function of pressure. The red curve (with stars) illustrates $\sqrt{A_{ii}/B_{ii}}$ for the true profile (analysis error divided by the background error), the black curve (with plus signs) illustrates the error computed between the retrievals and the true profile (or standard deviation of ($x-x_{true}$)) divided by the background error. The green and purple diamonds illustrate respectively the minimum and maximum values of $\sqrt{A_{ii}/B_{ii}}$ for the retrieved profiles. The top plot shows the errors for the first 500 samples and the bottom plot for the 3000 samples.

The minimum of the theoretical error of the solution (or retrieval) is obtained for the most humid profiles (green diamonds in Fig. 4) and the minimum is obtained for the driest profiles purple triangles in Fig. 4). This is because the sensitivity of Tb with respect to lnq is:

$$\frac{dTb}{d\ln q} = q\frac{dTb}{dq} \tag{5.1}$$

and the specific humidity itself amplifies the sensitivity of Tb with respect to q.

Figure 5 illustrates the errors for experiment SSMI1 and for experiment **SSMI2**. Experiment SSMI2 is the same as SSMI1 but with BmatFaclnQ=1.0. As expected, for SSMI2 the computed error from the retrievals is further apart from the analysis error obtained from the A matrix. The surface wind speed computed error and theoretical error are now 1.454 and 1.458 ms^{-1} respectively which is very similar to that of experiment SSMI1.

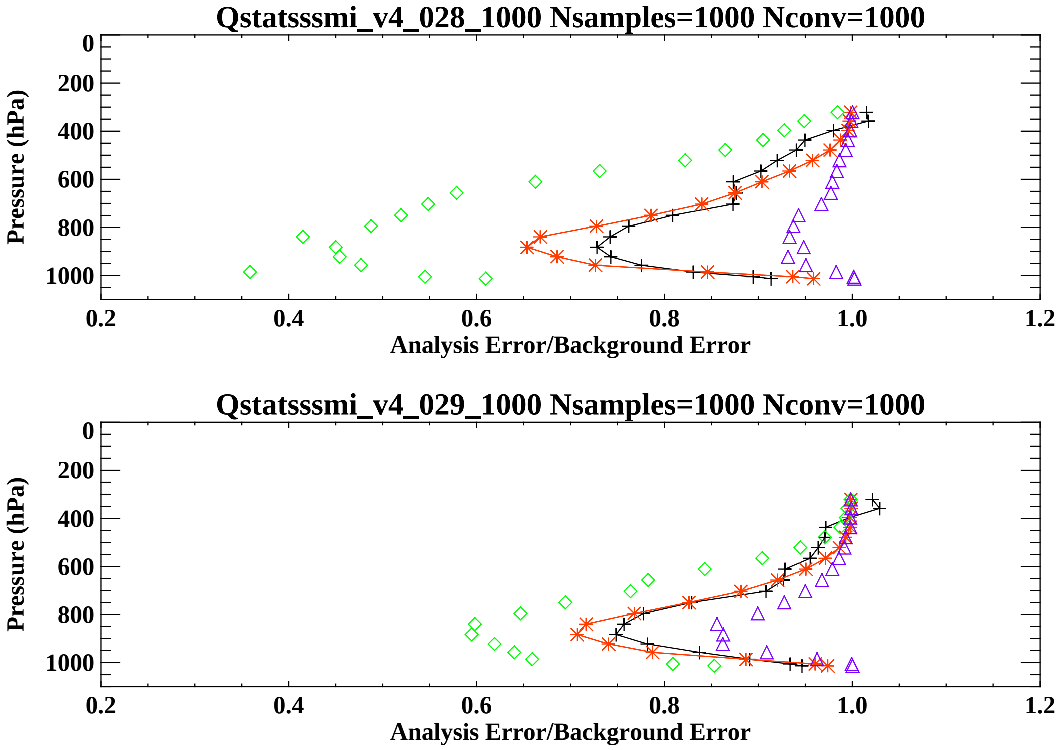

Figure 5: Normalised error standard deviations for SSM/I (all channels) natural logarithm of specific humidity retrievals as a function of pressure. The zenith angle is 53.1^{o} In the top plot, BmatFaclnQ=1.00 (Experiment SSMI2) and in the bottom plot, BmatFaclnQ=0.25 (Experiment SSMI1). The number of samples is 1000. The error statistics are illustrated as a function of pressure in the same way as in Fig. 4.

In the next experiment (**SSMI3**), supersaturation of water vapour profiles is no longer allowed: the background water vapour was cut off to its saturation value and so was that for the retrievals by applying a weak constraint to the cost function (section 2.1). Thus cutsatBG=T and Super_saturation_switch=T. The presence of clouds is not allowed by setting Lforcecloud=F and since there are no clouds in the background fields, no clouds are retrieved either. Lforcecloud is defined in Table 9 of section 4.4.

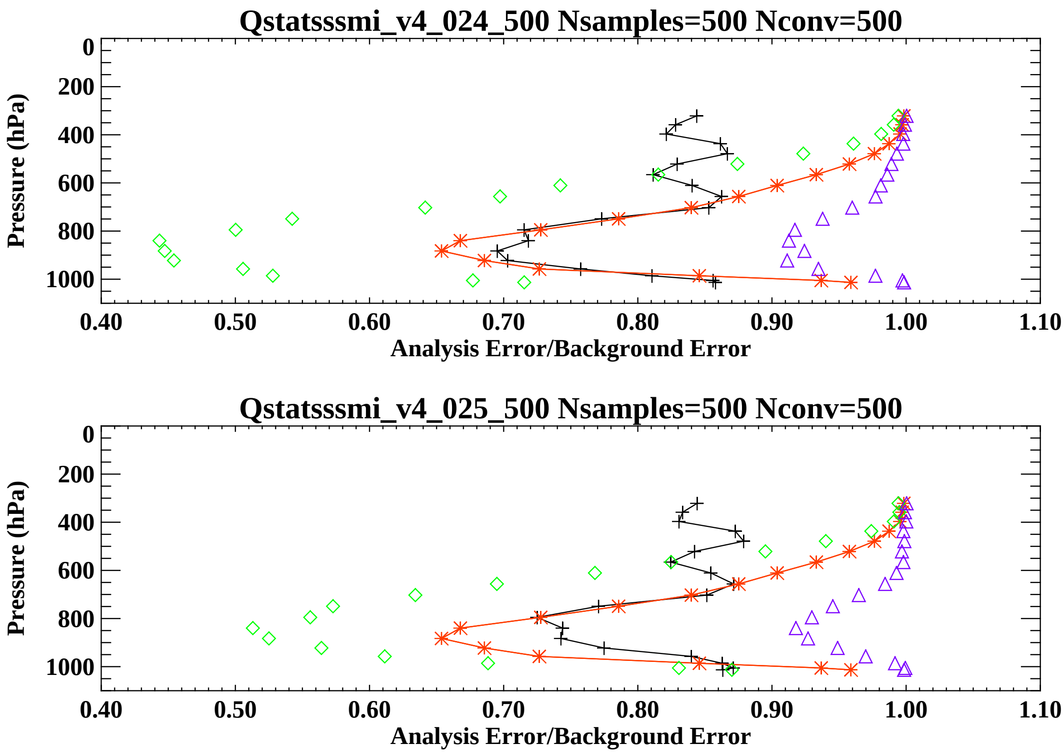

Figure 6: Normalised error standard deviations for SSM/I (all channels) natural logarithm of specific humidity retrievals as a function of pressure. The zenith angle is 53.1°. The number of samples is 500. In the top plot, supersaturation is no longer allowed and clouds are not allowed to form (Experiment SSMI3). In the bottom plot, same experiment as in top plot but now clouds are allowed to form (Experiment SSMI4). The error statistics are illustrated as a function of pressure in the same way as in Fig.4

As illustrated in the top plot of Figure 6, the computed error now is quite different from the theoretical error in particular for levels above 700 hPa.

Experiment **SSMI4** is the same as SSMI3 but clouds are allowed to be retrieved by setting Lforcecloud=T (Lforcecloud is defined in Table 9 of section 4.4). There are no clouds in the background field but a cloud structure is artificially created to allow formation of a cloud. The first guess LWP is set to 0.1 kgm^{-2} and since there are no clouds in the true profiles, the retrievals should only contain small amounts of LWP. In the original code (Ridley 2000), the retrieved LWP was forced to > 0 at each iteration. It was found that this condition led to a lot of profiles that had not converged after the maximum number of iterations was attained. Therefore, this condition was removed. In anycase, for the SSMI channels (with frequencies up 85 GHz, Table 1), the brightness temperatures are not sensitive to small amounts of LWP. Also, a large background error (Table 4) is assigned to LWP (0.200 kgm^{-2}) because the model clouds are quite different from those observed and also less accurate.

Figure 7 illustrates a histogram of the retrieved LWP for experiment SSMI4. As expected, the retrieved LWP is small (-0.04 < LWP< 0.04 kgm^{-2}) and the distribution is almost symmetrical about the zero value. Only 500 samples were retrieved for this experiment. As shown in Figure 6 (bottom plot), the computed retrieval error is somewhat larger around 900 hPa for this experiment but otherwise there are no differences.

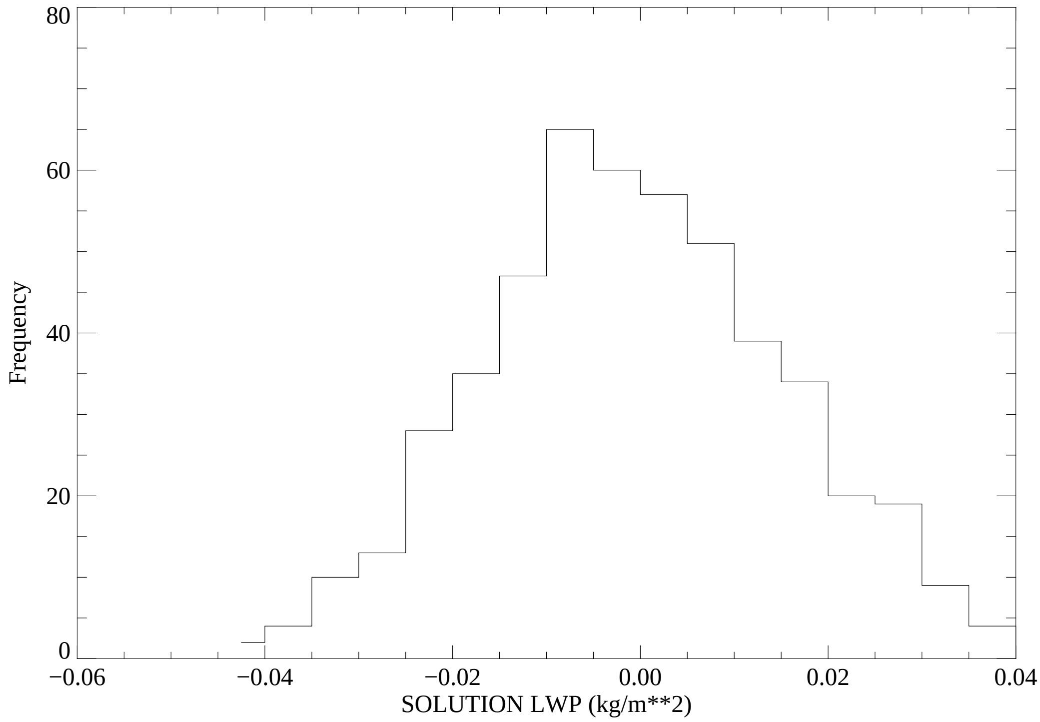

Figure 7: Histogram of retrieved LWP for experiment SSMI4.

5.2.2. Retrievals in the presence of clouds (LWP retrievals)

For experiment **SSMI5**, clouds were added to the true profile to create a cloudy true profile data set in the following manner (also see Table 7 in section 4.2):

- (1) A cloud structure function S(P) is chosen, see section 2.1. For this experiment, the cloud structure was non-zero between 700 and 750 hPa.
- (2) The single true profile is saturated (100% in relative humidity) at the levels where a cloud is added (where the cloud structure is non-zero).
- (3) This single true profile is then repeated N times in the true profile data set but a different true cloud liquid water path is assigned to each profile. The cloud structure S(P) always remains the same but the LWP is drawn from a uniform random distribution such that $q_L(P,j)=LWP(j)\ S(P)$ where P is the pressure and j is the sample number (j ranges between 1 and N). The LWP for all the profiles is comprised between 0.0 and 0.3 kgm^{-2}.

The noisy profile data set contains exactly the same profiles of cloud liquid water content as the true data set. The parameter settings to generate the true and noisy profile data sets were as follows: LTEMP=F, LWAT=T, LWIND=T, ADDCLOUD=T and LQTOTAL=F. The parameter settings for the 1D-Var (SSMIMod_Params.f90) are the same as those of experiment SSMI4.

Figure 8 illustrates the relative LWP retrieval error in % for each sample (total of 500 samples) as a function of true LWP. The relative LWP retrieval error is defined as follows:

$$E(LWP) = 100\frac{LWP^{retrieved} - LWP^{true}}{LWP^{true}} \quad (5.2)$$

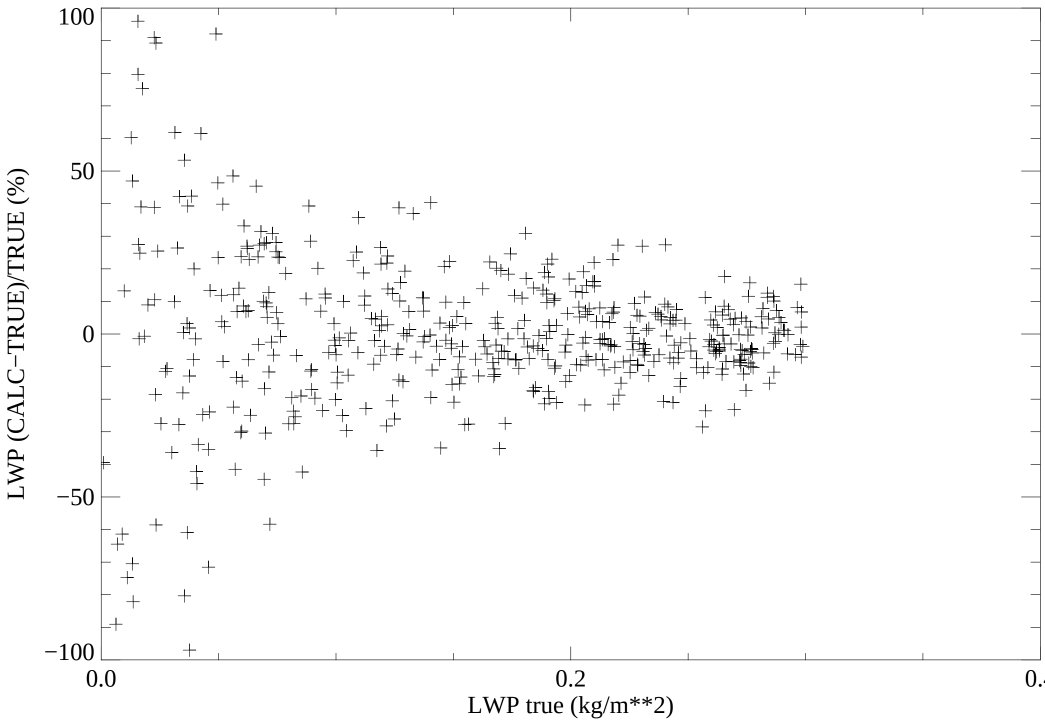

Figure 8: Relative LWP retrieval error in % for experiment SSMI5 (Eq.(5.2))

For values of LWP < 0.1 kgm^{-2}, E (LWP) increases very quickly (>50%) as LWP decreases. This is consistent with the fact that the SSM/I brightness temperatures are not sensitive to low amounts of LWP. Figure 9 illustrates the computed and theoretical errors for experiment SSMI5. The computed and theoretical errors are quite close except above 700 hPa where the differences are due to not allowing supersaturation, and close to the surface.

From experience with prior experiments, it is very likely that the gap close to the surface would decrease as the number of samples is increased. Note that there is no longer a single value for the theoretical error of the true profile data set. There is now a different value for each true profile since a different cloud (drawn from a random distribution) is assigned to each profile.

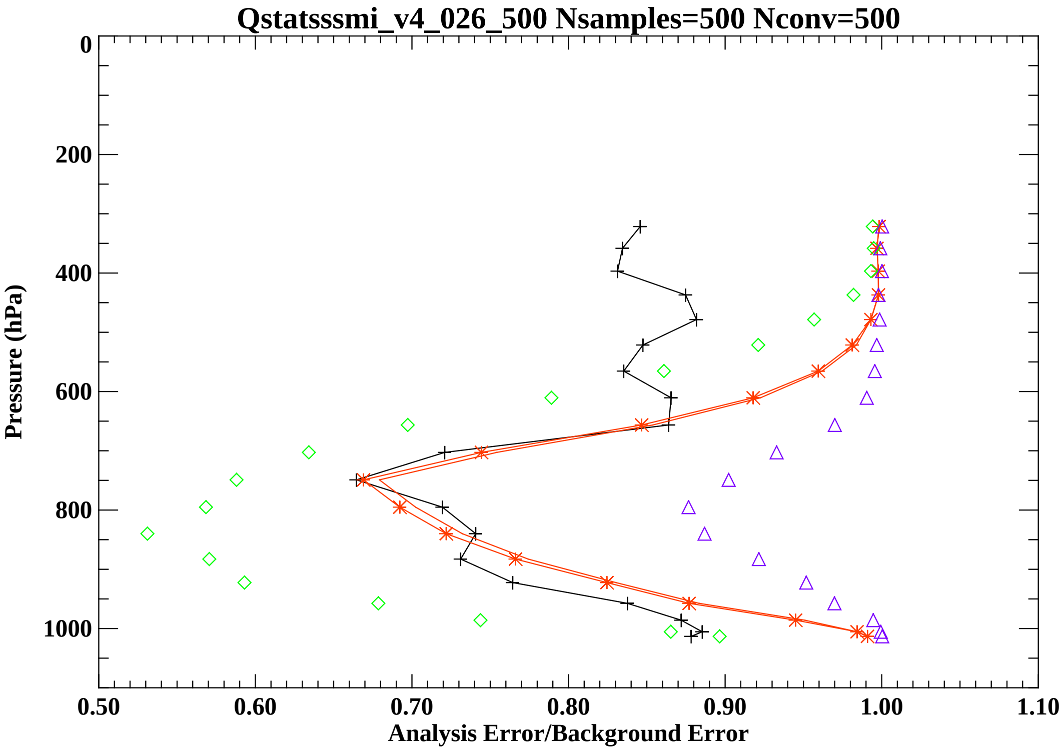

Figure 9: Normalised error standard deviations for SSM/I (all channels) natural logarithm of specific humidity retrievals as a function of pressure (Experiment SSMI5). The true and noisy profile data sets both contain the same clouds. The zenith angle is 53.1°. The number of samples is 500. The error statistics are illustrated as a function of pressure in the same way as in Fig. 4. Note that there is no longer a single value for the theoretical error of the true profile data set. There is a different value for each true profile since a different cloud (drawn from a random distribution) is assigned to each profile. The minimum and maximum values are illustrated by the two distinct red curves (one with stars and one without).

5.3. SSMIS

5.3.1. Retrievals in the presence of clouds (LWP retrievals)

The first of the SSMIS experiments is referred to as **SSMIS1**. All the input, output and result files for this experiments are provided with the SSMIS 1D-Var code as a test case (files containing 041 as job identification number). The SSMIS channel selection for this experiment are: Channels 1-18 and channel 24, this gives a total of 19 channels (Num_Chans_Used=19). The weighting functions of the temperature channels 19 to 23 peak too high in the atmosphere (stratospheric channels) and are not used.

First, the true and noisy profile data sets have to be generated. This is done by setting the parameters in prepare_profiles.f90 as follows: LTEMP=T, LWAT=T, LWIND=T, ADDCLOUD=T and LQTOTAL=F. This setting is the same as for experiment SSMI5 (also see Table 9 in section 5.1) except that noise is now also added to the temperature profile by setting LTEMP=true.

Secondly, parameters that control the execution of the SSMIS 1D-Var and defined in SSMIMod_Params.dat (see section 4.4) are set as follows: Super_saturation_switch=T, cutsatBG=T, Lqtotal=F, Lforcecloud=T, LwindVar=T, LlnQVar=T, LtskinVar=F and LtemperatureVar=T. These are the same settings as for experiment SSMI5 except that now temperature variation is also allowed.

For the majority of profiles, the number of iterations is 4 and 0.5% of profiles did not satisfy the convergence criterion when the maximum number of iterations was reached. The mean cost function for all profiles was 9.2 (Num_Chans_Used/2 = 9.5).

Figure 10 illustrates the computed and theoretical retrieval errors for temperature. The clouds that were added to the true profiles are the same as those for experiment SSMI5 described in section 5.2.2. The cloud always has the same cloud structure S(P) that is non-zero for pressure levels between 700 and 750 hPa. Again, there is no longer a single value for the theoretical error of the true profile data set. There is now a different value for each true profile since a different (random) cloud is assigned to each profile. The maximum and minimum values are shown in Figure 10. The theoretical error extrema of the true profiles always lie within the range of the extrema of the theoretical error for the retrievals. As expected the computed error is similar to the theoretical error (away from the cloud location) since temperature is linear in the forward operator.

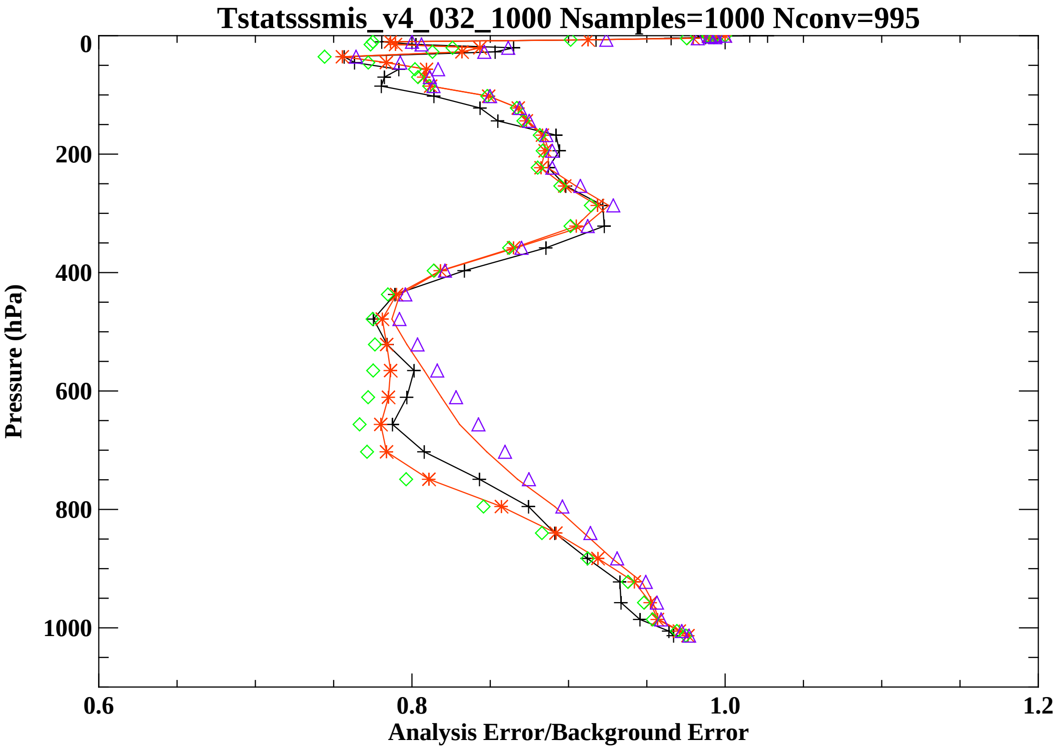

Figure 10: Normalised error standard deviations for SSMIS temperature retrievals as a function of pressure (Experiment SSMIS1). The sample size N is 1000 and the zenith angle of 53.1°. The red curves illustrate the minimum (curve with stars) and maximum values (curve without stars) of $\sqrt{A_{ii}/B_{ii}}$ for the true profiles (analysis error divided by the background error). The black curve (with plus signs) illustrates the error computed between the retrievals and the true profile (or standard deviation of (x-x_{true})) and divided by the background error. The green and purple diamonds illustrate respectively the minimum and maximum values of $\sqrt{A_{ii}/B_{ii}}$ for the retrieved profiles.

Figure 11 illustrates the computed and theoretical retrieval errors for the natural logarithm of specific humidity (lnq). As for the SSMI5 experiment, there is good agreement between the computed and theoretical retrieval errors except above 700 hPa where the differences are due to not allowing for supersaturation of the profiles. Figure 12 illustrates E(LWP) defined in section 5.2.2 (See Eq. (5.2)). Again, the retrieval error increases dramatically for LWP < 0.1 kgm^{-2}. Finally, Table 10 lists the computed and theoretical retrieval errors for LWP and SWS. The computed error lies between the extrema of their theoretical counterparts.

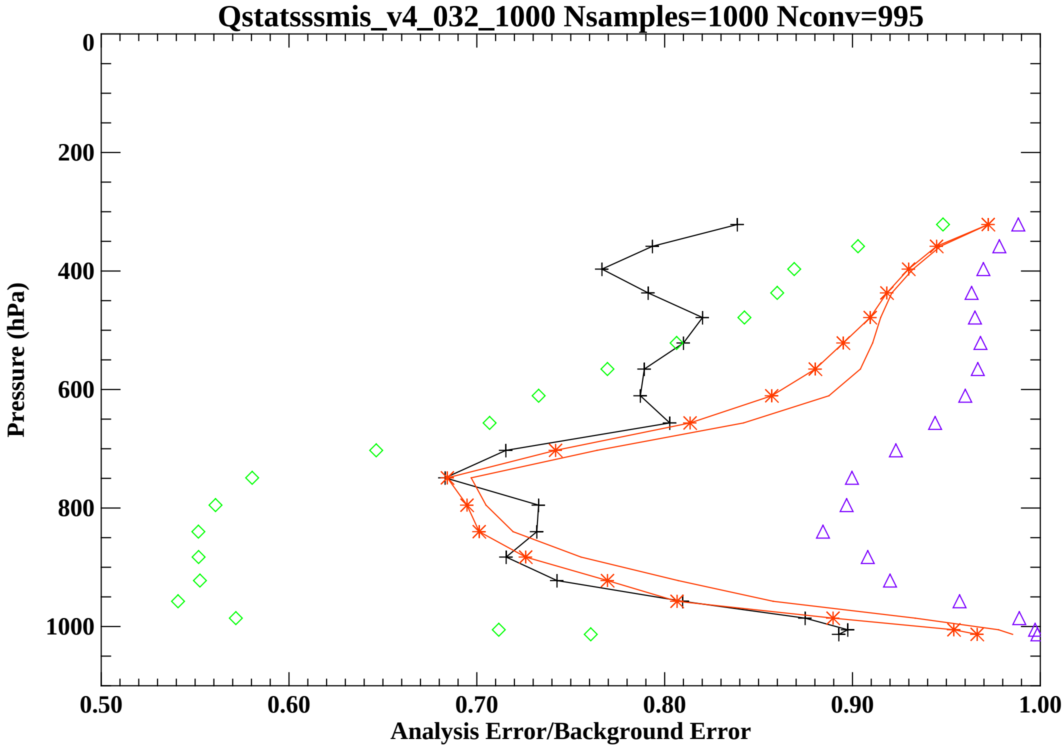

Figure 11: Same as in Fig.10 (Experiment SSMIS1) but for the natural logarithm of specific humidity.

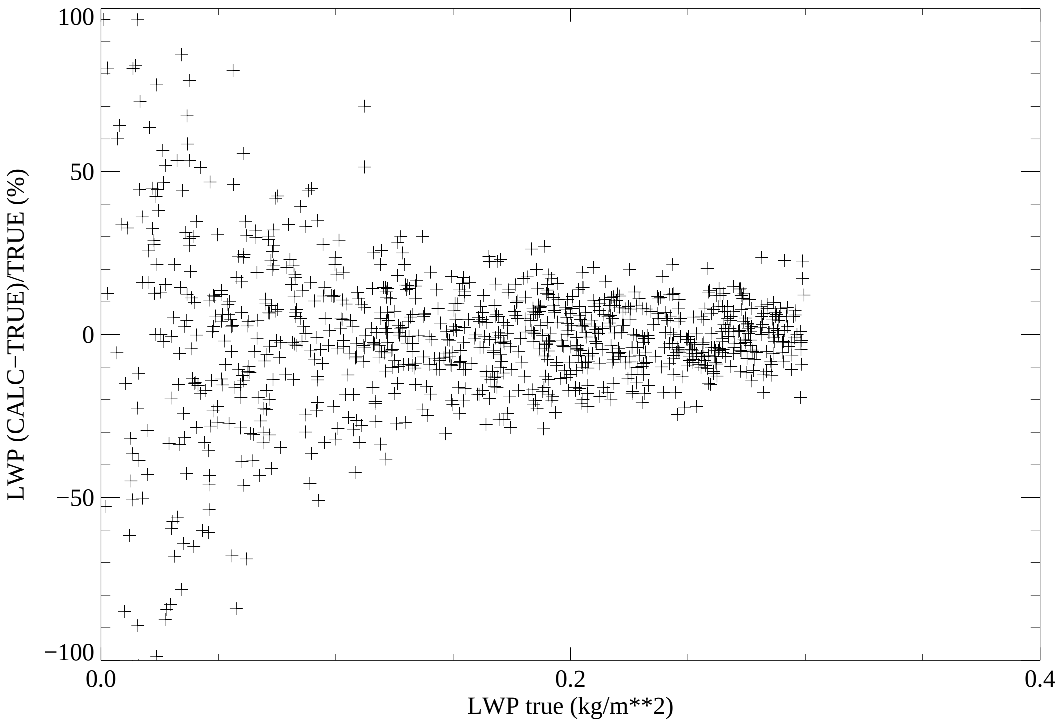

Figure 12: Relative LWP retrieval error in % (See Eq.(5.2)) for experiment SSMIS1.

Table 10: Computed and theoretical retrieval errors for LWP and SWS for experiment SSMIS1. Nsamples=1000. 0.5% of profiles did not converge when the maximum number of iterations was reached. The statistics listed below are for all the 1000 samples and were extracted from the file Gstatsssmis_041.

Control variable	Computed Error	Theoretical Minimum Error for retrieved values	Theoretical Maximum Error for retrieved values
LWP (kgm^{-2})	0.021	0.016	0.025
SWS (ms^{-1})	1.53	1.44	1.58

5.3.2. Retrieving total water content

As in Blankenship et al. (2000), the SSMIS channels (Table 2) selected to compute retrievals of total water content (and optionally also oceanic surface wind speed) are the three water vapour line 183 GHz channels, the 150 GHz channel and the channels 12 to 16 (lowest frequency window channels) for a total of 9 channels.

5.3.2.1. In the absence of clouds

Retrievals in the absence of clouds imply that there are no clouds in the “true” profile data set. The true and noisy profile data sets were created by setting the parameters in prepare_profiles.f90 as follows: LTEMP=F, LWAT=T, LWIND=F, ADDCLOUD=F and LQTOTAL=F. Thus no noise has been added to the wind speed field.

Parameters that control the execution of the SSMIS 1D-Var and defined in SSMIMod_Params.dat (see section 4.4) were set as follows: Super_saturation_switch=F, cutsatBG=F, Lqtotal=T, Lforcecloud=F, LwindVar=F, LlnQVar=T, LtskinVar=F and LtemperatureVar=F.

The first experiment with BmatFaclnQ=1.0 is referred to as **SSMIS2**. The number of iterations to satisfy the convergence criterion is usually 4. 13.6% of the 500 samples did not satisfy the convergence criterion after 20 iterations. The top plot in Figure 13 illustrates the computed and theoretical errors for lnq_{total}. For pressure levels situated below 800 hPa, the computed retrieval error is considerably larger than its theoretical counterpart and the reverse is true for pressure levels above 600 hPa. Retrieving the natural logarithm of total water content (lnq_{total}) also ensures that retrieved cloud liquid water content will always be positive and this is illustrated by positive only LWP retrievals (column integral of the retrieved $q_{L,}$ Eq. (2.3)) in the histogram of LWP (Fig. 14). Non-zero values of LWP are to be expected even if the true profiles are cloudless. This results from the fact that the background $\ln q_{total}$ profiles are noisy and noise was also added to the synthetic brightness temperatures.

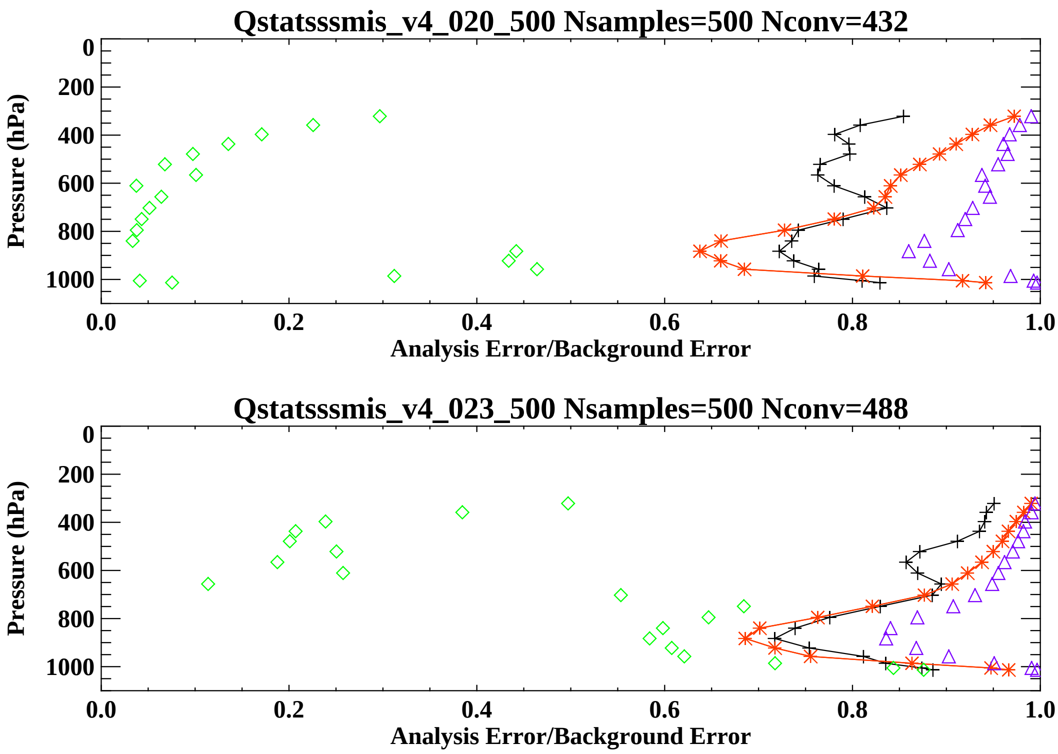

Figure 13: Normalised error standard deviations for SSMIS natural logarithm of total water content retrievals. The zenith angle is 53.1°. The sample size N is 500. The error statistics are illustrated as a function of pressure in the same way as in Fig. 4. The top plot illustrates the results for experiment SSMIS2 and BmatFaclnQ=1.0. The bottom plot illustrates the results for experiment SSMIS3 and BmatFaclnQ=0.25.

Experiment **SSMIS3** is exactly the same as experiment SSMIS2 except that now BmatFaclnQ=0.25 to reduce the non-linearity of the retrieval problem. As was the case for the SSM/I experiments (section 5.2), reducing the values of the elements of the B matrix results in computed errors being closer to their theoretical counterparts (bottom plot in Figure 13). This also confirms that the retrieval scheme works as expected. Furthermore, only 2.4% of the 500 samples did not satisfy the convergence criterion after 20 iterations.

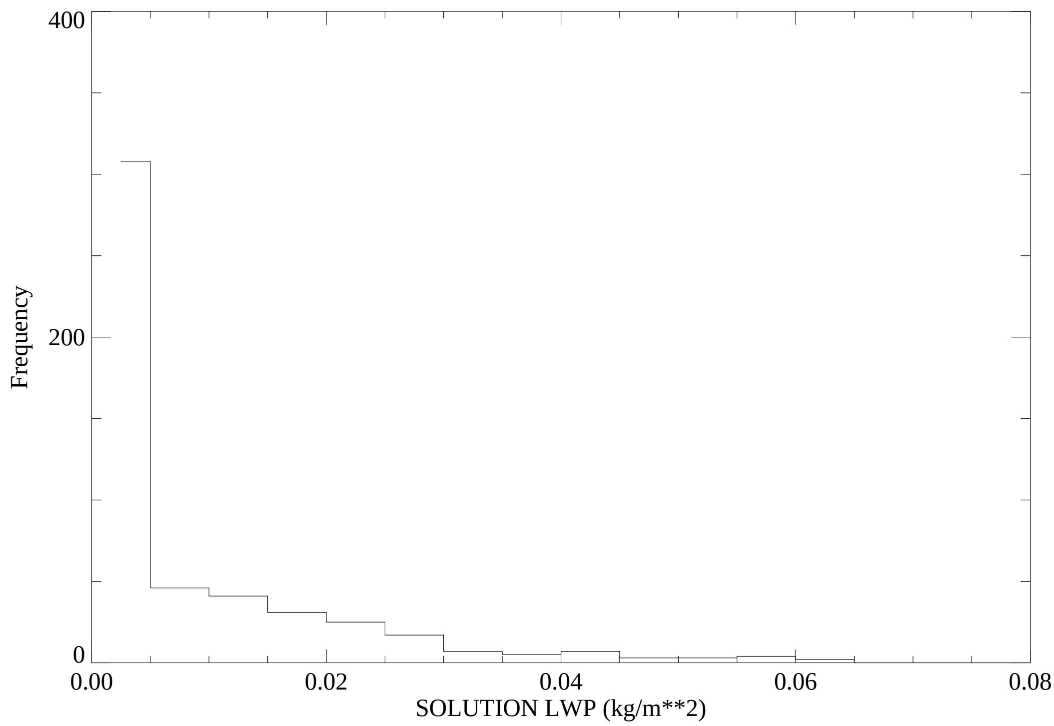

Figure 14: Histogram of retrieved LWP for experiment SSMIS2 for all 500 samples.

5.3.2.2. In the presence of clouds

In this section, three experiments (**SSMIS4**, **SSMIS5** and **SSMIS6**) are described that retrieve total water content (q_{total}(P)) in the presence of clouds. Surface wind speed is not a control variable in the first two experiments but is in the last one. BmatFacInQ=1 for experiments SSMIS4 and SSMIS6 but is equal to 0.25 for SSMIS5.

For all three experiments, a cloud profile was added to the true profile to create a cloudy true profile data set in the following manner (also see Table 7 in section 4.2):

- (1) A single cloud liquid water content profile was chosen with a non-zero cloud structure S(P) for pressure levels between 700 and 750 hPa and a LWP of 0.1 kgm^{-2}.
- (2) The single true profile of specific humidity is saturated (100% relative humidity) at the levels where the cloud liquid water content > 0. This single true cloudy profile is then repeated N times to form the true profile data set.

For the noisy profile data set:

- (1) The total water content is computed for the single true cloudy profile: add water vapour content with cloud liquid water content.

- (2) Noise with the same statistical properties as lnq is then added to the total water content. Hence, the noisy profile data set contains profiles of temperature, total water content and surface wind speed. The parameter settings to generate the true and noisy profile data sets are : LTEMP=F, LWAT=T, LWIND=F, ADDCLOUD=T and LQTOTAL=T. LWIND=T for experiment SSMIS6.

Parameters that control the execution of the SSMIS 1D-Var and defined in SSMIMod_Params.dat (see section 4.4) have to be set as follows: Super_saturation_switch=F, cutsatBG=F, Lqtotal=T, Lforcecloud=F, LwindVar=F, LlnQVar=T, LtskinVar=F and LtemperatureVar=F. LwindVar =T for SSMIS6. BmatFaclnQ also has to be adjusted.

The number of iterations needed for convergence for SSMIS4 is quite variable with 15% of the 500 samples not satisfying the convergence criterion after 20 iterations. The nonlinearity of the total water content variable is clearly visible (Figure 15, top plot) by the large difference between the theoretical and computed retrieval errors especially where the cloud is located (700 to 750 hPa). The distribution of retrieved LWP is shown in Figure 16 for the 500 samples. After splitting the total water content into its water vapour and cloud water contents (section 2.1.2), the column integrated cloud water content of the true profile is 0.15 kgm^{-2}. The total water content splitting function starts creating cloud water when the relative humidity exceeds 95% and that is why the LWP after the splitting function has been applied is larger than that of the original profile (LWP of 0.1 kgm^{-2} with 100% saturation where the cloud structure is non-zero).

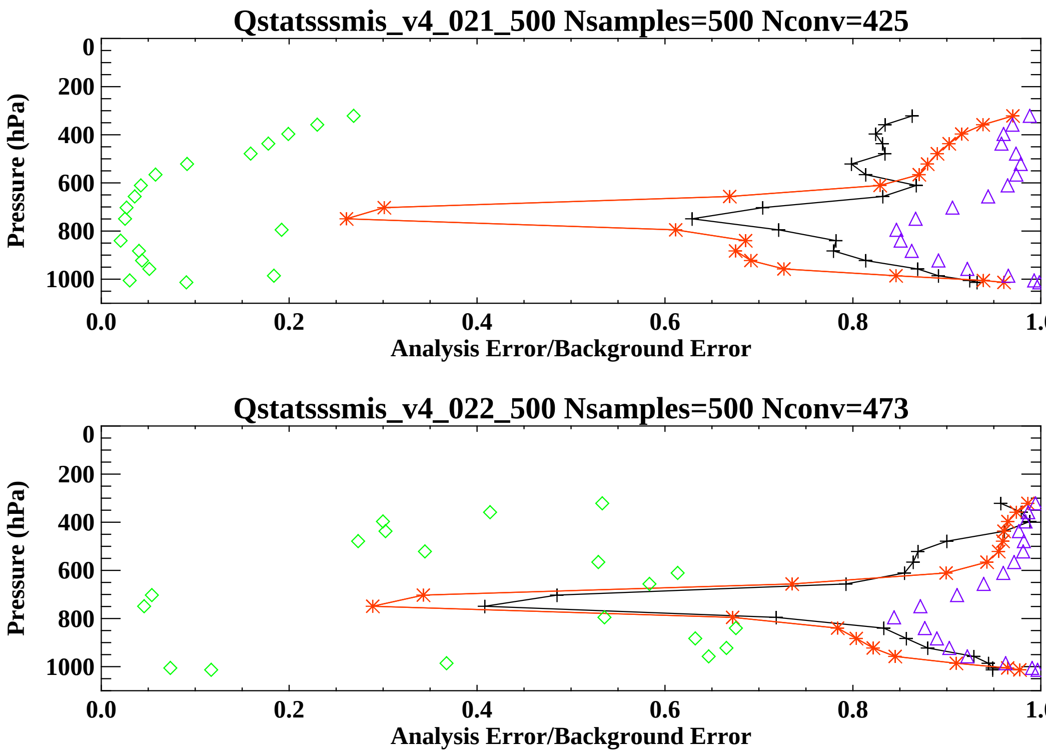

Figure 15: Normalised error standard deviations for SSMIS natural logarithm of total water content retrievals. The zenith angle is 53.1^{o}. The sample size N is 500. The error statistics are illustrated as a function of pressure in the same way as in Fig. 4. The top plot illustrates the results for experiment SSMIS4 and BmatFaclnQ=1.0. The bottom plot illustrates the results for experiment SSMIS5 and BmatFaclnQ=0.25.

Again, to verify that the SSMIS 1D-Var works properly, the value of the elements of the B matrix was reduced (in order to reduce the non-linearity of the problem) for experiment SSMIS5. As expected, the computed and theoretical retrieval errors are now closer (Figure 15, bottom plot) and the percentage of non-converging cases is now only 5.4%. The distribution of LWP retrieved is illustrated in Figure 17 and now has a clear peak in frequency at LWP=0.15 kgm^{-2} which is the LWP of the true profile.

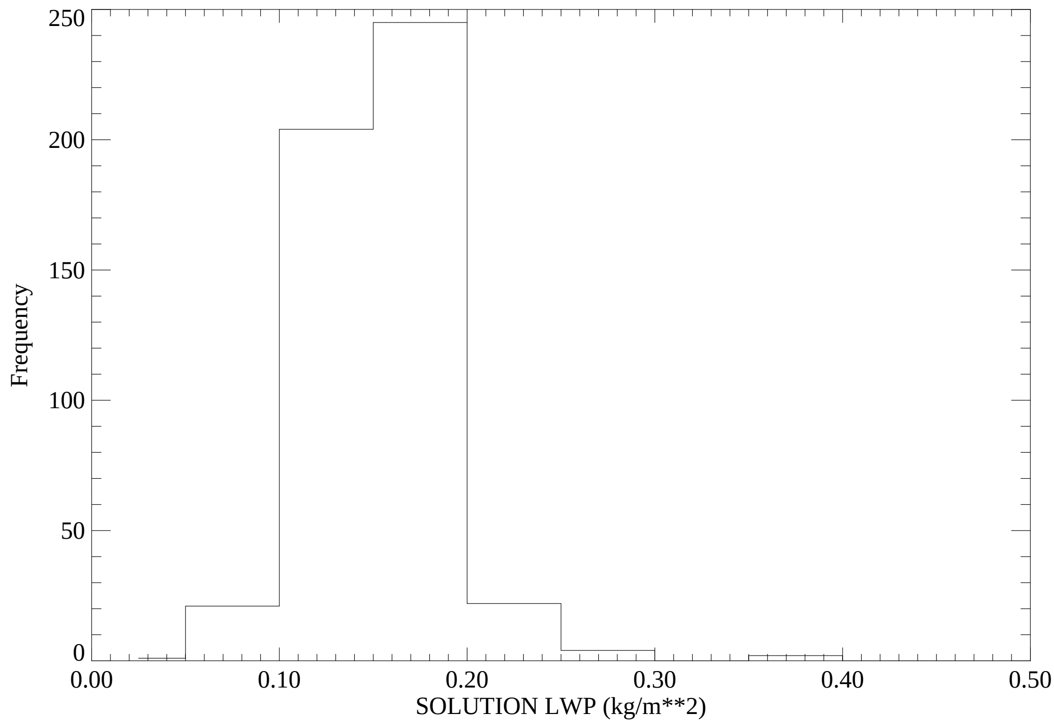

Figure 16: Histogram of retrieved LWP for experiment SSMIS4 for all the 500 samples.

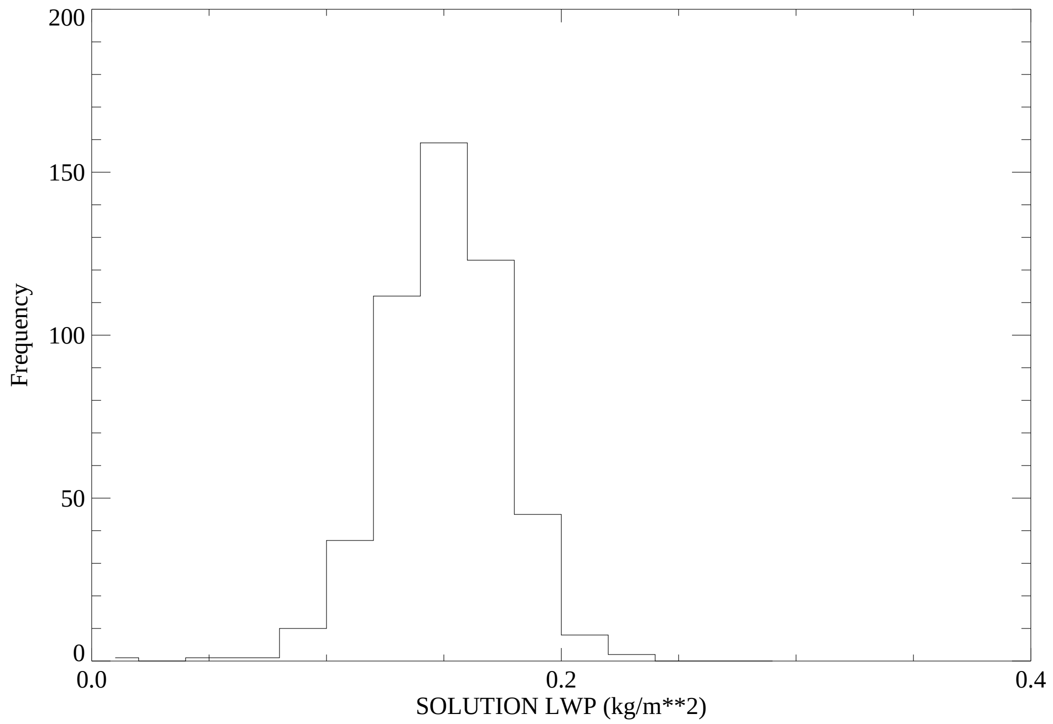

Figure 17: Histogram of retrieved LWP for experiment SSMIS5 for all the 500 samples.

Finally, in the last experiment, surface wind speed was also allowed to vary. The retrievals of $\ln q_{total}$ are very similar to those when the wind speed is not allowed to vary (Figure 15 top plot) and the computed retrieval error for wind speed is 1.547 ms^{-1} compared with 1.586 ms^{-1} for the theoretical error of the retrievals for all 500 samples.

6. Future developments

6.1. Total water content retrievals with temperature variation

The SSMIS 1D-Var version 1.0 cannot solve simultaneously for total water content and temperature because the sensitivity of the brightness temperature with respect to temperature coming from the dependence of q and q_L on temperature has not been included. Both q and q_L depend on temperature through the saturation water vapour, which depends only temperature. This sensitivity is given by:

$$\frac{\partial Tb}{\partial T} = \frac{\partial Tb}{\partial q}\frac{\partial q}{\partial q_s}\frac{dq_s}{dT} + \frac{\partial Tb}{\partial q_L}\frac{\partial q_L}{\partial q_s}\frac{dq_s}{dT} \qquad (6.1)$$

and will be implemented in the next version of the code. The derivative of q_s with respect to temperature is given by Eq. (6.9) in section 6.4.

6.2. Allowing for incomplete profiles

The current version of the SSMIS 1D-Var requires as input complete background profiles that are specified on the 43 fixed pressure levels. The code RTTOV requires that the atmospheric profile be provided at all levels above that of the surface and at the level just below the surface. Thus, the profiles need not be provided at the lower levels. Some of the routines have been changed to function with a reduced number of levels (all levels above the surface and the level just below the surface) but not all of the routines.

6.3. Solving the SSMIS 1D-Var with observed brightness temperatures

Solving the SSMIS 1D-Var with observed brightness temperatures is entirely possible and would require very minor changes to the code. It is suggested that Op_Mode=3 be used to identify this case.

6.4. Weak supersaturation constraint dependent on temperature

When the first and second derivatives of the cost function are computed, the dependence of J_s (Eq. (2.1)) on temperature has been ignored (Eqs. (6.5) and (6.6)). It would be worthwhile to investigate whether neglecting this dependence significantly affects the retrievals when the natural logarithm of specific humidity (x=lnq) and temperature (T) are retrieved simultaneously. The saturation cost function $J_s(x)$ (Eq.(2.2)) and its first and second derivatives with respect to x and T are given by:

$$J_s(x) = (x - x_s)^3 \qquad (6.2)$$

$$\frac{\partial J_s}{\partial x} = 3(x - x_s)^2 \qquad (6.3)$$

$$\frac{\partial^2 J_s}{\partial x^2} = 6(x - x_s) \qquad (6.4)$$

$$\frac{\partial J_s}{\partial T} = -3(x - x_s)^2 \frac{dx_s}{dT} \qquad (6.5)$$

$$\frac{\partial^2 J_s}{\partial T^2} = 6(x - x_s)\left[\frac{dx_s}{dT}\right]^2 - 3(x - x_s)^2 \frac{d^2 x_s}{dT^2} \qquad (6.6)$$

The subroutine (SSMI_svp.f90) that calculates saturation specific humidity q_s [$q_s = \exp(x_s)$] in SSMIS 1D-Var uses a look-up table. The look-up table approach could be replaced with a continuous function to compute saturation specific humidity. Such a function *(that computes saturated specific humidity with respect to water only*) is given by: (see subroutine wsat.f written by P.D. Watts, version 3.00 #240484)

$$
\begin{aligned}
q_s &= a\varepsilon_s (P - d\varepsilon_s)^{-1} \\
d &= (1-\varepsilon) \\
\varepsilon_s &= e^{f(T)} \\
f(T) &= a_1 - (b_1 T + c_1) T^{-2} \\
\varepsilon &= 0.622;\ a = \varepsilon \\
a_1 &= 19.2082 \\
b_1 &= 4086.19 \\
c_1 &= 181961.0
\end{aligned}
\qquad (6.7)
$$

where P is pressure (in hPa), T is temperature (in K) and ε_s is saturation vapour pressure in hPa. The first and second derivatives of x_s with respect to temperature are given by Eqs. (6.8) to (6.12).

$$
\begin{aligned}
\frac{dx_s}{dT} &= q_s^{-1} q_s' \\
\frac{d^2 x_s}{dT^2} &= q_s^{-1} q_s'' - q_s^{-2} (q_s')^2
\end{aligned}
\qquad (6.8)
$$

$$
q_s' = a\varepsilon_s' [(P - d\varepsilon_s)^{-1} + d\varepsilon_s (P - d\varepsilon_s)^{-2}] \qquad (6.9)
$$

$$
\begin{aligned}
\varepsilon_s' &= f' \varepsilon_s \\
f' &= -b_1 T^{-2} + 2(b_1 T + c_1) T^{-3}.
\end{aligned}
\qquad (6.10)
$$

$$
\begin{aligned}
q_s'' = a\varepsilon_s'' &\left[(P - d\varepsilon_s)^{-1} + d\varepsilon_s (P - d\varepsilon_s)^{-2} \right] + \\
&(\varepsilon_s')^2 2ad \left[(P - d\varepsilon_s)^{-2} + d(P - d\varepsilon_s)^{-3} \varepsilon_s \right]
\end{aligned}
\qquad (6.11)
$$

$$
\begin{aligned}
\varepsilon_s'' &= f' \varepsilon_s' + f'' \varepsilon_s \\
f'' &= 4b_1 T^{-3} - 6(b_1 T + c_1) T^{-4}
\end{aligned}
\qquad (6.12)
$$

where ‘ denotes $\frac{d}{dT}$ and ‘’ denotes $\frac{d^2}{dT^2}$.

6.5. Forcing LWP and SWS to be positive

For each iteration during the minimisation, the NWP SAF SSM/I 1D-Var LWP and SWS (surface wind speed) are reset to a small positive value if they reach a value less than this small positive value. In the SSMI 1D-Var developed by Phalippou (1996), a NAG routine was used that included special treatment for variables with bounds. The simple resetting of values for LWP as used in the NWP-SAF SSMI 1D-Var leads to multiple cases of non-convergence. When this condition was removed (SSMIS 1D-Var), negative LWP were retrieved but the values remained small. The condition on SWS in this version of the code has also been removed and has not been thoroughly tested since in the experiments that were performed the true SWS was set to 7 ms^{-1} and so retrieved SWS rarely reached values close to zero.

7. References

Blankenship, C.B., A. Al-Khalaf, and T.T. Wilheit, 2000: Retrieval of Water Vapor Profiles using SSM/T-2 and SSM/I data, *J. Atmos. Sciences*, **57**, 939-955.

Deblonde, G., 1999: Variational assimilation of humidity using the SSM/T-2 brightness temperatures. Proc. Tenth Int. TOVS Study Conf., Boulder, CO, 154-165. [Available from Bureau of Meteorology Research Center, GPO Box 1289K, Melbourne UIC 3001, Australia.]

Deblonde, G. and S.E. English, 2000: Evaluation of the Fastem2 fast microwave oceanic surface emissivity model. Proc. Eleventh Int. TOVS Study Conf., Budapest, Hungary, 20-26 September 2000.

English, S.J. and T.J. Hewison, 1998: A fast generic millimeter-wave emissivity model, Proceedings of SPIE, 3503, 288-300.

Eyre, J.R., 1989: Inversion of cloudy satellite sounding radiances by nonlinear optimal estimation. I. Theory and simulation for TOVS., *Q. J. R. Meteorolol. Soc.*, **115**, 1001-1026.

Eyre, J.R., and A.D. Collard 1999: The effects of nonlinearity of retrieval errors: implications for the interpretation of advanced infra-red sounder data. Technical Proceedings of ITSC-X, Boulder, CO, 27 January – 2 February 1999.

Hollinger, J., J.L. Pierce, and G.A. Poe, 1990: SSM/I instrument evaluation. *IEEE Trans. Geosci. Remote Sens.*, **28**, 781-790.

Ide, K., P. Courtier, M. Ghil, and A.C. Lorenc, 1997: Unified notation for data assimilation: Operational, sequential, variational, *J. Meteor. Soc. Japan*, **75**, 181-189.

Liebe, H.J., 1989: MPM—An atmospheric millimeter wave propagation model. *Int. J. Infrared Millimeter Waves*,**10**, 631-650.

Liebe, H.J., P.W. Rosenkranz, and G.A. Hufford, 1992: Atmospheric 60-GHz oxygen spectrum: New laboratory measurements and line parameters*. J. Quant. Spectrosc. Radiat. Transfer*, **48**, 629-643.

Lorenc, A.C., 1986, Analysis methods for numerical weather prediction*, Q. J. Royal Meteor. Soc.*, **112**, 1177-1194.

Phalippou, L., 1996: Variational retrieval of humidity profile, wind speed and cloud liquid-water path with the SSM/I: Potential for numerical weather prediction. *Q. J. R. Meteor. Soc.*, **122**, 327-355.

Press, W.H., Flannery, B.P., A.A. Teukolsky and W.T Vetterling, 1989: Numerical Recipes, The art of scientific computing (Fortran version), Cambridge university press, Cambridge, 702 pp.

Ridley, J., 2000: Stand-Alone 1DVAR scheme for the SSM/I. NWP-SAF documentation.

Rodgers, C.D., 1976, Retrievals of atmospheric temperature and composition from remote measurements of thermal radiation, *Reviews of Geophysics and Space Physics*,**14**, 609-624.

Rodgers, C.D., 2000: Inverse Methods for Atmospheric Sounding, Theory and Practice, In Series on Atmospheric, Oceanic and Planetary Physics-Vol2. World Scientific, London. 238pp.

Tarantola, A.T. and B.. Valette, 1982: Generalised nonlinear inverse problems solved using the least squares criterion*, Reviews of Geophysics and Space Physics*, **20**, 219-232.

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Table 10: Computed and theoretical retrieval errors for LWP and SWS for experiment SSMIS1. Nsamples=1000. 0.5% of profiles did not converge when the maximum number of iterations was reached. The statistics listed below are for all the 1000 samples and were extracted from the file Gstatsssmis_041. 36
Table A.1: List of experiments for the computation of LbL transmittances.**Error! Bookmark not defined.**
Table A.2: Extrema of transmittance differences between experiments p43_narrow_z and p43_narrower_z for the 24 SSMIS channels. p43_narrow_z - p43_narrower_z. The zenith angle is 50^o. .... **Error! Bookmark not defined.**
Table A.3: Extrema of transmittance differences between experiments p43_narrow_z and p43_narrower_z for the 24 SSMIS channels. p43_narrow_z - p43_narrower_z. The zenith angle is 56^o. .... **Error! Bookmark not defined.**
Table A.4: RTTOV6.7 predictors for water vapor. The profile variables are as defined in the RTTOV-6 SCIENCE AND VALIDATION REPORT........... **Error! Bookmark not defined.**
Table A.5: Statistics of brightness temperature differences between the LbLmodel and the fast model. The columns entitled Zero X_8,X_9 refer to the case where the AMSU window water vapor channel predictors were used (Table A.4) and those entitled Non-Zero X_8,X_9 refer to the case where the SSMI/SSMIS window water vapor channel predictors (Table A.4) were used. .... **Error! Bookmark not defined.**