

ALGORITHM AND DATA USER MANUAL FOR THE SPECIAL SENSOR MICROWAVE IMAGER/ SOUNDER (SSMIS)

Appendix E: SSMIS UPPER AIR SOUNDING ALGORITHM

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TECHNICAL REPORT

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1 Introduction and Summary

The purpose of the SSMIS UAS algorithm is to retrieve atmospheric temperature (in K) at 8 pressure levels (7, 5, 2, 1, 0.4, 0.2, 0.1 and 0.03 mb), and geometric thickness (in m) for 8 layers (10-7, 7-5, 5-2, 2-1, 1-0.4, 0.4-0.2, 0.2-0.1, and 0.1-0.03mb). These thickness values are then used to determine geometric height (m) based on the 10mb height found with the Lower Air Sounding Temperature algorithm. The algorithm is based on a multivariate regression technique in which the effects of the Earth's magnetic field are treated in a deterministic manner.

2 Scientific Background

The approach to recovering upper stratospheric and mesospheric temperature profiles from spectral brightness temperature measurements is much the same as for recovering lower atmospheric profiles. Such measurements must be made in a spectral region where there is strong dependence of atmospheric absorption with frequency. When this condition holds over an adequately broad region (such as in the 5-mm oxygen band), it is possible to select a set of frequencies and bandwidths with associated weighting functions (Figure 1) that are appropriately sharp, distinct, and properly distributed with altitude to allow successful frequency-domain to space-domain inversions. While there is a practical limit to the number of non-redundant measurements that can be inverted by present day numerical methods, there are other controlling factors which complicate the inversion process, e.g. the stability of the weighting function shape and peak altitude with changing atmospheric state, and above about 40-km altitude, the magnetic line splitting effects on the effective absorption coefficients (the state transitions of the oxygen molecule in the 5-mm band are the magnetic dipole transitions). A successful way to perform the mesospheric inversions has been developed and demonstrated by Aerojet [Stogryn, 1989b]. The resulting algorithm is described below.

Prior to describing the UAS algorithm and the numerical approach to obtaining a stable inversion, theoretical considerations underlying the concept are briefly addressed here. To begin, atmospheric oxygen absorption-line shape is dependent on local pressure, composition (local density and molecular collisions), and the strength and orientation of the local magnetic field. The latter effect is most pronounced near line center where measurements must be made in order to obtain enough absorption (and therefore emission) to sound high in the atmosphere. The use of pressure as the independent height variable eliminates the need for explicit consideration of local density, and relative composition is assumed to be an invariant function of pressure in the altitude range of concern. The effects of magnetic disturbances have been investigated with the finding that their effects are very small, in addition to being unpredictable. Thus, it is only necessary to have a model of the main magnetic field for the vicinity of the soundings. The International Geomagnetic Reference Field (IGRF) has been chosen for this purpose.

Next, the orientation of the planes of polarization of the radiometer antenna with respect to the local magnetic field must be accounted for. This problem is dealt with by utilizing an expansion of the brightness temperatures in terms of the magnitude of the local Earth's field and the square of the cosine of the angle between the field and the propagation vector. It has been shown [Stogryn 1989a] that for the configuration used in the SSMIS, this angular dependence involves at most a quadratic expansion of the cosine squared. The resulting simplicity of this sounding formulation has led to a linear regression approach for high altitude temperature sounding. The use of a manageable look-up table for the local magnetic field with an extrapolation scheme, combined with accurate spacecraft orientation data, make it

possible to compute parts of the regression matrix, thereby simplifying and speeding up the retrieval process.

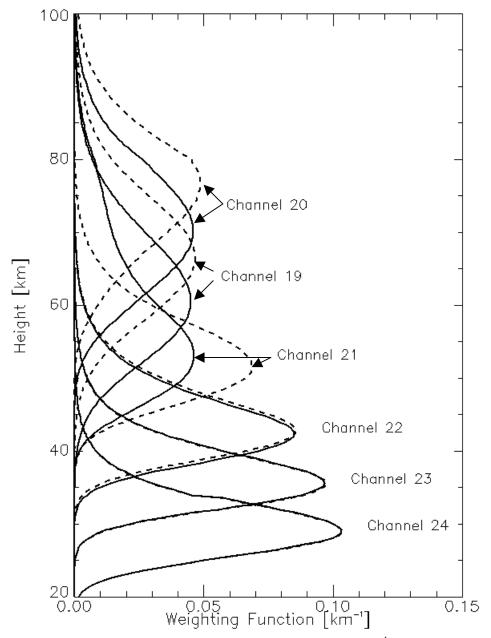


Figure 1. The UAS weighting functions (km⁻¹) for SMISS (solid line: B_e = 65 μ T, θ_B =53°; dashed line: B_e = 25 μ T, θ_B =90°)

3 Retrieval Procedures

For the purpose of understanding the numerical recipe presented below, a brief overview of mathematical formulations are in order. This overview will be posed in the context of a physically based technique for incorporating magnetic field effects within an otherwise multiple linear regression procedure. In the multiple linear regression procedures, it is assumed that the deviations of the state of the atmosphere *p* (atmospheric parameter vector) from the climatological mean may be expressed as a linear combination of the deviations of the measured data vector *d* from their mean values. Mathematically this statement takes the form

$$\hat{p} - \langle p \rangle = D(d - \langle d \rangle) \tag{1}$$

where $\langle \ \rangle$ indicates the expected value, \hat{p} is the estimated value of p, and D is the regression matrix. The quantities $\langle p \rangle$ and $\langle d \rangle$ are computed from a set of representative cases - the *a priori* data set. If the criterion is imposed that the expected value of the square of the difference between each component of the estimated value \hat{p} and the true value p be a minimum when using the *a priori* data set, then the D matrix is given by

$$D = C(p - \langle p \rangle, d - \langle d \rangle)C^{-1}(d - \langle d \rangle, d - \langle d \rangle)$$
(2)

where C (.....,) denotes the covariance matrix of its two arguments. Sensor inherent noise must also be accounted for in the above computation. This accomplished by writing the data vector as

$$d = d_0 + \delta \tag{3}$$

where d_0 is a noise free data vector and δ is a random error vector with zero expected value. Substitution of (3) into (2) yields

$$C(p - \langle p \rangle, d - \langle d \rangle) = C(p - \langle p \rangle, d_0 - \langle d_0 \rangle)$$

$$C(d - \langle d \rangle, d - \langle d \rangle) = C(d_0 - \langle d_0 \rangle, d_0 - \langle d_0 \rangle) + C(\delta, \delta)$$
(4)

Eqs. (4) reveal that the noise has been relegated to a separate noise matrix.

For the SSMIS, the parameter vector consists of eight air temperatures at selected pressure levels and eight atmospheric thickness between selected pressure levels as described above. The data vector consists of the six brightness temperatures measured by Channels 19-24. Thus (1) is equivalent to expressing the air temperature T_i at the i^{th} pressure level as a linear combination of the brightness temperatures:

$$T_{i} = \left\langle T_{i} \right\rangle + \sum_{j=1}^{N} D_{ij} \left[TB_{j} - \left\langle TB_{j} \right\rangle \right] \tag{5}$$

where TB_j is the measured brightness temperature for the j^{th} channel $(1 \le j \le N = 6)$ and (T_i) and (T_i) are, or are calculated from, a priori values. Here D_{ij} represents the i, j^{th} element of the matrix D. An analogous equation applies to thickness.

In general the elements of D would be derived from a set of the representative air temperature profiles and a corresponding set of computed brightness temperatures. However, for mesospheric sounding, channels with weighting functions peaking above 40 km arise (Fig. 1). The corresponding components of d and < d>> depend therefore on the local value of the magnetic field. Accordingly, the brightness temperature $< TB_j>$ and the matrix element D_{ij} in (5) are functions of B_e . The problem to be addressed is how to incorporate the Earth's magnetic field into the formulation expressed by (1) or (5).

4 Incorporating the Earth's Magnetic Field

The approach taken assumes that the components of the data vector d fall into three cases with respect to their dependence on magnetic field. (Note: it is assumed for all cases that the TB_j correspond to the average of two orthogonal polarized brightness temperatures.)

<u>Case 1</u>: Zeeman effect requires a full description (SSMIS Channels 19-21). These brightness temperatures may be expressed as

$$TB_{j} = \sum_{\alpha=0}^{\infty} a_{\alpha j} \left[B_{e} \cos \theta_{B} \right]^{2\alpha} \tag{6}$$

where in practice the sum may be truncated at $\alpha = 1$ or 2. In (6), θ_B is the angle between the propagation direction and the Earth's magnetic field \mathbf{B}_e . The coefficients of the series are functions of $B_e^2 = \mathbf{B}_e \bullet \mathbf{B}_e$ as well as the air temperature profile and the angle of incidence on the Earth's surface. The B_e^2 dependence is obtained by interpolating to the local value of B_e using a pre-selected set of nodes B_k (k=1,, n) that span the possible magnetic field values. For the computations, a four-point Lagrange interpolation formula in the square of the field is used. The two nodes to the left and right side of the local B_e value are selected except at the extremes where the closest four nodes are used. Then the coefficient in (6) can be expressed as [Stogryn, 1989a, b]

$$a_{cj} = \sum_{l=1}^{4} a_{cjl} L_l (B_e^2) \tag{7}$$

where $L_l(B_e^2)$ is the Lagrange polynomial.

<u>Case 2</u>: Channels whose weighting function peak slightly above 40 km and whose magnetic field dependence may be described by means of small perturbation (SSMIS Channel 22). In this case

$$TB_{j} = b_{0} + b_{1}B_{e}^{2} + b_{2}B_{e}^{2} \cos^{2}\theta_{B}$$
 (8)

where the coefficients b_{α} ($\alpha = 0$ and 2) are dependent only on the air temperature profile and the angle of incidence. The coefficient b_{I} is also a function of the magnetic field and its dot product with two orthogonal polarization vectors.

<u>Case 3</u>: Channels are assumed to be sufficiently removed from the oxygen absorption line centers that their brightness temperatures are independent of the magnetic field (SSMIS Channels 23-24).

This means that the last two columns of the covariance matrix C(p , d < d >) are independent on the magnetic field. Similarly the lower right-hand comer of the covariance matrix C(d < d >, d < d >) is independent of the Earth's magnetic field.

These considerations have shown that all of elements of the covariance matrices may be computed from constants calculated from *a priori* statistical data and a knowledge of the Earth's field at a point where the measured vector is *d*. When the matrices are assembled from their parts, the parameter vector is calculated by first solving the equation

$$C(d - \langle d \rangle, d - \langle d \rangle)\chi = d - \langle d \rangle \tag{9}$$

for the vector χ . Then \hat{p} is found from

$$\hat{p} = \langle p \rangle + C(p - \langle p \rangle, d - \langle d \rangle) \chi \tag{10}$$

Eq. (9) can be solved very efficiently on a computer since the relevant covariance matrix is positive definite.

5 Description Of The Algorithm

The SSMIS UAS algorithm Functional Flow Chart is shown in Figure 2. Each step is detailed below.

- 1. The sensor Data Records File (SDRF) contains the initial inputs to the algorithm. A distinction is made between the inputs that are part of the SDRF and other external files.
- 2. In Produce Upper Sounding Profile, EDRUSO loops through each scene of a multiple scan buffer to perform steps (c) through (h) to produce a profile. A profile contains all the UAS information (i.e. latitude, longitude, temperature, thickness, magnetic field, and time) for a single scene. Step (i) is then called to output the entire multiple scan buffer to the UAS file.
- 3. In Compute Lagrange Coefficients, LAG computes the coefficients for the four-point Lagrange interpolation used for interpolating *a priori* data to the local magnetic field strength at a given scene. A ten-element array containing squares of the values of the interpolation nodes of the magnetic field is defined in a data statement.
- 4. In Compute Temperature Expected Values, EXPTB computes expected values of brightness temperatures (TBAR = <*d*>) from *a priori* values modified for the local values of the magnetic field components.

- 5. In compute DD Covariance Matrix, COVDD implicitly computes the upper triangle part of data-data covariance matrix based on the magnetic field components.
- 6. In Solve For χ vector, POSDEF solves for χ vector in Eq. 9. Gaussian elimination is used to solve the linear system

$$A\chi = B$$

where A, the data-data covariance matrix, is a positive definite $N * N (N \ge 2)$ matrix which is destroyed by this step.

- 7. In Compute PD Covariance Matrix, COVPD computes the parameter-data covariance matrix using local values of the magnetic field components.
- 8. In Compute Upper Temperature and Thickness, UPPTEM computes the upper temperatures for each of the 8 levels using a linear D-Matrix regression technique, and computes the upper thickness values for each of the 7 layers between the 8 levels plus 10-7 mb thickness. The geometric heights are computed by stacking the thickness values upon the 10 mb height derived in the lower temperature profile processing.
- 9. In Create Upper Atmosphere Sounding Profiles, UPPPRO will create, pack, and write the upper sounding profile for each scene to the UAS file. Each profile is also displayed to ASCII Diagnostic file.

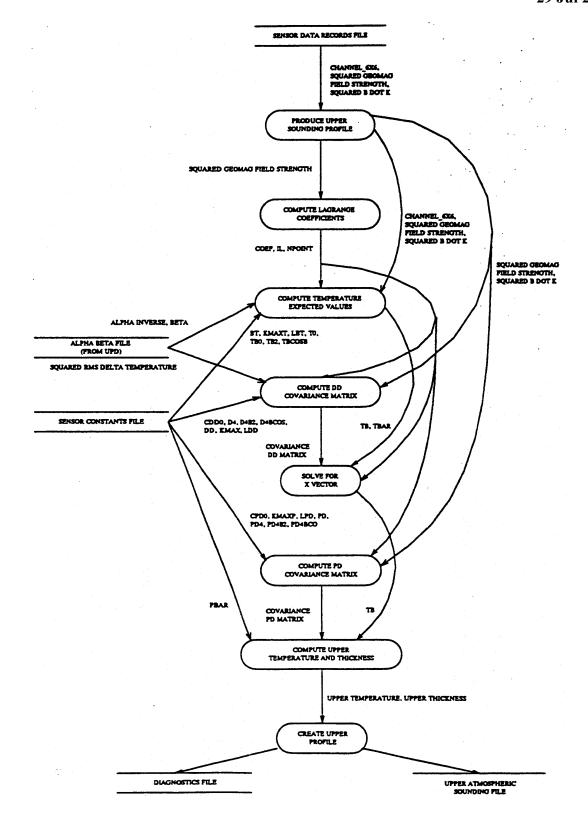


Figure. 2 SSMIS Upper Atmospheric Sounding Functional Flow Chart

6 References

Stogryn, A., The magnetic field dependence of brightness temperatures at frequencies near the O₂ microwave absorption lines, *IEEE Trans. Geoscience and Remote Sensing*, 27, 279-289, 1989a.

Stogryn, A., Mesospheric temperature sounding with microwave radiometers, *IEEE Trans. Geoscience* and Remote Sensing, 27, 332-338, 1989b.

[End of Appendix E]