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THE EVALUATION OF 'UMKEHR' OBSERVATIONS OF ATMOSPHERIC OZONE BY A MAXIMUM ENTROPY METHOD.

by

P L Read

Met O 19
(High Atmosphere Branch)
Meteorological Office
London Road
BRACKNELL
Berks RG12 2SZ

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1. Introduction

The 'umkehr' technique (Götz, Meetham and Dobson 1934) is widely used to obtain smoothed estimates of the vertical distribution of ozone in the stratosphere. Measurements are made of the ratio of the intensity of sunlight scattered from the clear zenith sky at two wavelengths, the shorter wavelength being absorbed more strongly by ozone than the longer, at a series of elevation angles of the sun near sunrise or sunset. Sunlight at a single wavelength is scattered from a definite, though rather broad layer in the atmosphere. As the solar zenith angle changes from 60° to 90°, the mean scattering height for wavelengths ~ 310 nm rises from ~ 5 km to near 45 km, enabling the distribution of ozone to be sampled throughout the stratosphere up to a height ~ 50 km.

Because the scattering layer at a given solar zenith angle is very broad (typically 15 to 20 km FWHM), the individual observations are strongly interdependent (indeed Mateer (1964) has shown that a typical umkehr curve contains at most 4 linearly independent pieces of information). Thus, the problem of extracting the ozone distribution is numerically ill-posed. A completely unique solution is not possible, and the analysis is unstable unless extra constraints are introduced into the solution scheme (eg Twomey and Howell 1963; Mateer 1964). The most widely accepted solution method for ozone (Mateer and Dütsch 1964) involves linearisation of the scattering integrals about a climatological mean distribution and subsequent smoothing of the resulting solution to suppress the effects of instabilities (ie to a large extent the method assumes the solution before making use of the observations).

The concept of 'Maximum Entropy' has recently received attention in the context of the inversion of Fourier Transform data, particularly in radio astronomy (Wernecke and D'Addario 1977; Gull and Daniell 1978, 1979) and for the analysis of time series power spectra (eg Ulrych and Bishop 1975). The former application is quite general and not limited to the Fourier Transform. Unlike most other methods of treating data, Maximum Entropy (ME) is non-linear and data-adaptive, and its main advantages are that it makes the minimum possible prejudgement regarding the expected solution, and it only generates features in the solution if they are really justified by the data. In this respect it is similar to the Backus-Gilbert method (eg see the review by Parker 1977), but has the added advantage, at least in the cases of deconvolution and the Fourier Transform, of producing a solution which is mathematically unique, and which is the most likely solution given no more information than the observational data.

The umkehr technique could potentially be applied to the investigation of other minor constituents in the stratosphere for which there is not yet sufficient information to define a climatological mean. In these circumstances the Maximum Entropy technique might provide a method of analysing the observations. The purpose of this report is to record the results of a study of the ME technique as applied to ozone, for which comparative results by Mateer's technique and direct measurements of the vertical distribution (by ozonesonde) are available.

2. The Method

2.1 Principles of Maximum Entropy (ME)

The philosophy of ME is derived from Bayes' theorem in probability theory (eg see Gull and Daniell 1979), which expresses the way in which the prior knowledge or prejudice regarding the solution is to be modified given the observational data. Essentially it says that

$$\text{Posterior } P(\text{solution}|\text{data}) \propto \text{Prior } P(\text{solution}) \times P(\text{data}|\text{solution}) \quad (1)$$

(ie the probability of a solution given the observational data is proportional to the product of the *a priori* probability of the solution and the probability of the data given the solution). If it is possible to calculate what an instrument would observe for any given solution, the second term on the right of (1) may be evaluated. For the case where the measurements have independent Gaussian errors, this term may be expressed by the statistic χ^2, where

$$\chi^2 = \sum_k \frac{(E_k - \eta_k)^2}{\sigma_k^2} \quad (2)$$

and where η_k is the data value calculated from the guessed solution, E_k is the kth measurement and σ_k the associated error estimate. The probability that a given solution gives rise to the data is then exp $(-\chi^2/2)$.

The primary limitation in the use of Bayesian statistics is the choice of a suitable expression for the prior probability of a given solution in the absence of data. If this probability is expressed as exp (S/λ), where S is a function of the guessed solution and λ is a fixed constant, the most probable solution given the data may be obtained via (1) by maximising the quantity $S-\frac{1}{2}\lambda\chi^2$. As long as the posterior probability distribution has a well-defined global maximum, the solution corresponding to the maximum probability is, in a fundamental sense, the 'best' solution given the data. The existence and uniqueness of such a solution for the cases of deconvolution and for the Fourier Transform have been proved by Skilling (see Gull and Daniell 1978). The function S is identified as the 'entropy' of the solution (by analogy with statistical mechanics), which therefore represents the prior probability distribution. The different expressions which are used for the entropy of the solution merely represent different prior probability distributions.

Two definitions of entropy are commonly used in the radio astronomical application of Maximum Entropy, given by:

$$S_1 \propto \sum_i \log f_i \tag{3}$$

and

$$S_2 \propto -\sum_i f_i \log f_i \tag{4}$$

where f_i is the value of the solution at position i (eg the number density of ozone in height level i). The former definition S_1 is used by Wernecke and D'Addario (1977) which corresponds more closely to the autoregressive application of ME mentioned earlier. The latter definition S_2 is preferred by Gull and Daniell (1978) and arises from a consideration of the configurational entropy of the solution if the amplitude f_i is quantised. If n_i 'quanta' are placed in the i^{th} level by a random process, the probability that a particular distribution of n_i's occurs is proportional to $N!/\prod_i n_i!$ (N is the total number of quanta). If N and n_i are large, we can apply Stirling's approximation and obtain:

$$\begin{aligned} S &\propto \log \text{(probability)} \\ &\propto -\sum_i n_i \log n_i / N \end{aligned} \tag{5}$$

This expression assumes that all solution values are positive ($n_i > 0$) and, when maximised by itself, it results in a completely uniform solution (ie n_i independent of height). In relating the quantised value n_i to the continuous variables f_i, (5) becomes

$$S \propto -\sum_i \left(\frac{f_i}{\sum_j f_j}\right) \log \left(\frac{f_i}{\sum_j f_j}\right) \tag{6}$$

The method of solution therefore reduces to finding the f_i which maximises $S-\frac{1}{2}\lambda\chi^2$, ie

$$\frac{\partial}{\partial f_k} \left\{ -\sum_i \left(\frac{f_i}{\sum_j f_j}\right) \log \left(\frac{f_i}{\sum_j f_j}\right) - \frac{\lambda}{2}\chi^2 \right\} = 0 \tag{7}$$

This has the solution

$$f_k = \exp\left\{\frac{\sum_j f_j \log f_j}{\sum_j f_j}\right\} \exp\left\{-\frac{\lambda}{2}\frac{\partial \chi^2}{\partial f_k}\right\} \tag{8}$$

where the first exponential term is to normalise the function f. An alternative approach is to regard (7) as the maximisation of the entropy S (given by (6)) subject to the constraint that the solution be consistent with the data. λ is then identified as a Lagrangian Multiplier, and the constraint is obtained by causing χ^2 to be equal to its expectation value, which is the number of degrees of freedom (ie the number of independent measurements). In this manner, adequate account is taken of the effect of random noise, and no attempt is made to obtain an <u>exact</u> fit to the data. (An exact fit would be likely to generate features in the solution due to the noise alone and hence could be misleading.) Because the unconstrained solution is completely uniform, the constrained solution (8) may therefore, in a sense, also be regarded as the most <u>uniform</u> solution consistent with the data.

Provided, therefore, that the entropy definition expressing the prior prejudice concerning the expected solution is kept as simple and as general as possible, the Maximum Entropy solution is, in accordance with the principle of Jaynes (1957a, b), the solution which is 'maximally non-committal with respect to the unavailable information'.

2.2 The umkehr effect

Umkehr observations are measurements of the ratio of the intensities of sunlight scattered from the clear zenith sky in two narrow wavelength bands (I and I', the ratio normally expressed as $\log_{10}(I/I')$). The resulting 'umkehr curve' may be derived from the vertical distribution of the absorbing constituent by reference to Fig 1. We consider only Rayleigh scattering by air molecules in the vertical column of atmosphere viewed by the instrument, and we ignore multiple scattering, aerosol scattering and more complex radiative transfer effects. If the intensity of sunlight outside the earth's atmosphere is I_o, the intensity at the scattering point G is given by:

$$I_G = I_o \exp\left\{-\int_z^\infty (s_c n_c + s_R n_a) \sec \zeta \, dh\right\} \tag{9}$$

where S_c is the absorption cross-section of the minor constituent, n_c its number density at height h, S_R the Rayleigh scattering cross-section and n_a the air number density. ζ is the local zenith angle of the sun along the slant path (and depends on θ , z and h). The intensity of light scattered down to the instrument from air molecules in a layer of thickness dz at G is given by:

$$dI_G = K S_R (1 + \cos^2\theta) I_G n_a(z) dz \qquad (10)$$

where K is a constant, $(1 + \cos^2\theta)$ represents the phase function for Rayleigh **scattering,** and θ is the solar zenith angle at the scattering point. The scattered light is further attenuated on its way down to the instrument, the received intensity being

$$dI = dI_G \exp\left\{ - \int_0^z (S_c n_c + S_R n_a) dh \right\} \qquad (11)$$

The total intensity received by the instrument is obtained by integrating (11) over all heights in the atmosphere. Thus, combining (9), (10) and (11),

$$I = I_0 K S_R (1+\cos^2\theta) \int_0^\infty \exp\left\{ - \int_0^z (S_c n_c + S_R n_a) dh - \int_z^\infty (S_c n_c + S_R n_a) \sec\zeta \, dh \right\} n_a \, dz \qquad (12)$$

A similar expression can be derived for the intensity I' at the second wavelength. (12) may be simplified somewhat when the ratio I/I' is considered, in that the terms common to both wavelengths (ie $K(1 + \cos^2\theta)$) will cancel. The integral over $z \rightarrow \infty$ may be split into two components with multipliers 1 and $(\sec\zeta - 1)$. The former can then be combined with the integral between 0 and z to form an integral from 0 to ∞ which is independent of z. The expression may be simplified further if the ratio at a relatively small zenith angle θ_0 is subtracted from each subsequent observation ie

$$\eta_k = \left[\log_{10}(I/I') \right]_{\theta_k} - \left[\log_{10}(I/I') \right]_{\theta_0} \qquad (13)$$

A factor of $K S_R(1 + \cos^2\theta) \exp\left[- \int_0^\infty (S_c n_c + S_R n_a) dh \right]$ is then common to the values of I and I' at θ_k and θ_0, and is therefore eliminated. The quantity remaining is given by:

$$Q(\theta) = \int_0^\infty \exp\left\{ - \int_z^\infty (S_c n_c + S_R n_a)(\sec\zeta - 1) dh \right\} n_a \, dz \qquad (14)$$

The measured quantity represented by η_k is therefore:

$$\eta_k = \log_{10}\left\{Q(\theta)/Q'(\theta)\right\} - \log_{10}\left\{Q(\theta_0)/Q'(\theta_0)\right\} \tag{15}$$

2.3 The numerical scheme

Because n_a, n_c and ζ all depend on height, the numerical evaluation of (14) requires a double quadrature. Provided the atmosphere is divided into a reasonable number of height levels, the errors in the evaluation of the integrals is relatively small. For simplicity, the classical umkehr inversion scheme B (Ramanathan and Dave 1957), which divides the atmosphere between the ground and 50 km into ~10 layers of equal depth (in log pressure), has been adopted. In this scheme the ozone concentration is assumed to be constant within each layer, but for attenuation purposes it is taken to be located at a single level ($\frac{1}{3}$ of the layer thickness above the base of each layer). Thus, the total ozone (per cm^2) in the ray path for light scattered down from the i^{th} layer is given by

$$l_i = \sum_{j=i}^{N} \overline{(\sec\zeta - 1)}_{ij}\, c_j\, z' \tag{16}$$

where c_j is the ozone concentration, z' is the layer separation, and the bar over $(\sec\zeta - 1)$ implies the average over the layer, which may be calculated given i, j, z' and θ from the geometry (cf Ramanathan and Dave 1957). The total air column density (ie the number of air molecules in the ray path) may be calculated using the Chapman grazing incidence function (eg see Craig 1965) and assuming a simple exponential variation of density with height. Thus, the air column density above i is given by:

$$L_i = n_i H\left\{Ch(\theta, x) - 1\right\} \tag{17}$$

where H is the density scale height, Ch represents the Chapman function and x is given by

$$x = (R_0 + z_i)/H \tag{18}$$

where R_0 is the radius of the Earth (see the derivation by Craig 1965). We may represent (14), therefore, by:

$$\begin{aligned} Q(\theta) &= \sum_{i=1}^{N+1} n_i \exp\left\{-S_c l_i - S_R L_i\right\} \\ &= \sum_{i=1}^{N+1} n_0 \exp\left\{-z_i/H\right\} \exp\left\{-S_c l_i - S_R L_i\right\} \end{aligned} \tag{19}$$

where n_o is the air number density at $z = 0$. The $(N + 1)$th layer embraces the entire atmosphere above the Nth layer, in which the ozone density is assumed to be negligible.

As discussed in Section 2.1, the ME method requires the calculation of η_k at each observed zenith angle θ_k for any guessed distribution of ozone density, and also the calculation of $\partial\chi^2/\partial c_i$. From (2), this is given by:

$$\frac{\partial \chi^2}{\partial c_i} = 2 \sum_k \frac{(\eta_k - E_k)}{\sigma_k^2} \frac{\partial \eta_k}{\partial c_i} \tag{20}$$

and $\partial\eta_k/\partial c_i$ may be obtained from the summation given above. Thus, from (15) and (19)

$$\frac{\partial \eta_k}{\partial c_i} = \log_{10} e \left\{ \left[\frac{1}{Q}\frac{\partial Q}{\partial c_i} - \frac{1}{Q'}\frac{\partial Q'}{\partial c_i} \right]_{\theta} - \left[\frac{1}{Q}\frac{\partial Q}{\partial c_i} - \frac{1}{Q'}\frac{\partial Q'}{\partial c_i} \right]_{\theta_0} \right\} \tag{21}$$

and

$$\frac{\partial Q(\theta)}{\partial c_i} = - S_c \sum_{j=1}^{i} \overline{(\sec\zeta - 1)}_{ij}\, n_o \exp\{-z_j/H\} \exp\{-S_c l_j - S_R L_j\} \tag{22}$$

Gull and Daniell (1978) suggest that the Maximum Entropy calculation is carried out using an iterative scheme in which the Lagrangian multiplier λ is gradually increased until χ^2 is equal to its expectation value. The amount by which λ is increased at each iteration depends upon the value of χ^2, and successive iterates are averaged (ie new solution = (raw solution + old average)/2) to reduce possible instabilities and to ensure convergence. Gull and Daniell do not discuss how λ is to depend upon the value of χ^2, but a quasi-Newton method in λ was found to work reasonably well, and was easy to include in the calculation. The increment $\Delta\lambda$ is therefore

$$\Delta\lambda = -(\chi^2 - N_m) \Big/ \frac{\partial \chi^2}{\partial \lambda} \tag{23}$$

where N_m is the number of independent measurements. Because the new guess for c_i is of the form

$$c_i = A \exp(-\lambda u_i) \tag{24}$$

(see (8)) where A is a constant, and

$$u_i = \sum_k \frac{(\eta_k - E_k)}{\sigma_k^2} \frac{\partial \eta_k}{\partial c_i} \tag{25}$$

and we have

$$\begin{aligned} \frac{\partial c_i}{\partial \lambda} &= -u_i A \exp(-\lambda u_i) \\ &= -u_i c_i \end{aligned} \tag{26}$$

Using (25) and (26)

$$\begin{aligned} \frac{\partial \chi^2}{\partial \lambda} &= 2 \sum_k \frac{(\eta_k - E_k)}{\sigma_k^2} \frac{\partial \eta_k}{\partial \lambda} \\ &= 2 \sum_k \left\{ \frac{(\eta_k - E_k)}{\sigma_k^2} \left(\sum_j \frac{\partial \eta_k}{\partial c_j} \frac{\partial c_j}{\partial \lambda} \right) \right\} \\ &= -2 \sum_k \left\{ \frac{(\eta_k - E_k)}{\sigma_k^2} \left(\sum_j \frac{\partial \eta_k}{\partial c_j} u_j c_j \right) \right\} \end{aligned} \tag{27}$$

Reversing the order of the summation,

$$\frac{\partial \chi^2}{\partial \lambda} = -2 \sum_j \left\{ c_j u_j \left(\sum_k \frac{(\eta_k - E_k)}{\sigma_k^2} \frac{\partial \eta_k}{\partial c_j} \right) \right\} \tag{28}$$

which, from (25) is simply

$$\frac{\partial \chi^2}{\partial \lambda} = -2 \sum_j c_j u_j^2 \tag{29}$$

In practice, $\Delta\lambda$ has to be modified from the simple form given by (23) to take account of the averaging process before constructing the next iterate. Also, because the problem is intrinsically non-linear, the value of $\Delta\lambda$ must be further reduced by an empirical factor which depends upon $(\chi^2 - N_m)$ and the number of iterations to achieve smooth convergence. The overall scheme is summarised in the flow diagram shown in Fig 2. Each new iterate is normalised to a total column density of ozone which may be specified at the beginning of the calculation or kept as a free parameter. Most of the tests of the method given in the following sections were made using 12 height levels up to a height of 55 km, and the solution required usually between 30 sec and 1 min of cpu time on an IBM 360/195. While this time may seem excessively large, no particular attempt was made to optimise the program efficiency, and it is probable that the execution time could be reduced by a factor ~ 10 with a method which selects more carefully the direction of convergence in parameter space.

3. Tests of the Method

3.1 Synthetic ozone data

The first test to be carried out using the Maximum Entropy program was to make use of 'data' calculated from a series of specified ozone distributions. Ozone wavelengths and absorption cross-sections were used so that the calculated 'umkehr curve' could be checked against the results of other workers. Data generated by this means could be used to test the overall performance of the method, and its reaction to different atmospheric parameters and signal-to-noise ratios (gaussian noise of a known amplitude could be introduced into the data artificially). Some results of this test are illustrated in Fig 3. The method produces plausible solutions with a characteristic peak in the lower and middle stratosphere. The solutions generally agree quite well with the original distributions above the peak at $\sim$25 km, but the maximum in the distribution is usually placed a few kilometres too high, and a large quantity of ozone remains below 12 km. The latter systematic effects are made worse if the total column density is left as a free parameter, although the agreement with the original distribution above 25-30 km is largely unaffected. The ME solutions are also, in general, somewhat smoother than the original distribution, and the peak ozone density tends to be significantly underestimated.

The effect of increased noise on the solution is to reduce the effective height resolution, although the overall shape of the distribution (ie the position of the maximum and the decay with height at upper levels) remains similar. If the noise level in the data is incorrectly assessed in attempting a solution, however, the results may be adversely affected. Significantly overestimating the noise level in the data has the effect of smoothing the resulting solution and placing the ozone maximum even higher than before. Much more noticeable is the effect of significantly underestimating the noise level. Spuriously high resolution features are introduced into the solution, often including more than one maximum in the distribution. In many cases the convergence of the method is severely affected, and a solution is not obtained. This is probably because a noisy umkehr curve contains rapidly varying components which are not characteristic of the physics of the umkehr effect. Whatever the original distribution, the resulting curve will never vary rapidly with solar zenith angle because of the strong smoothing implicit in the scattering integrals (see (12)). In general, however, provided that the signal-to-noise ratio is assessed reasonable accurately (ie within a factor of about +100% - 30%) the solutions are relatively unaffected.

3.2 Ozone umkehr data

A more realistic test of the method was carried out using actual observational data. The results could then be compared with the standard evaluation technique and, by using data which were taken at approximately the same time as an ozonesonde was flown, the results could be compared with an independent measurement of the distribution of ozone up to about 30 km. The data were obtained from the publications of the World Ozone Data Center, which provide unprocessed umkehr observations, umkehr solutions using the standard evaluation method (Mateer and Dütsch 1964), and ozonesonde data for stations all over the world. Data were used only when umkehr and ozonesonde observations were made on the same day at the same station, and when the ozonesonde reached an altitude of at least 30 km. This resulted in a sample of 21 sets of umkehr data from Japanese and Australian stations between 1968 and 1972.

Experiments had shown that there was little difference in the solutions carried out using more than 7 zenith angles, provided that they covered the range in angle from 70° to 90° reasonably uniformly, other than increased computational cost. The solution in the present test, therefore, used the 7 zenith angles suggested by Mateer (1964) viz 70°, 75°, 80°, 84°, 86.5°, 88° and 90°, and θ_o was generally taken as 60°. The raw data were corrected approximately for multiple scattering (see discussion of Mateer 1964). Air number density was obtained using a simple constant-scale-height approximation to the appropriate US standard atmosphere. The total column density was constrained to equal the Dobson measured value (direct sun measurement), and the mean noise level was estimated to be ~ 0.35 N-units (1 N unit $\equiv \log_{10}(I/I') = 0.01$), from a consideration of the residuals quoted as acceptable for the standard evaluation method. The results are shown in Fig 4, which also shows the standard solutions and ozonesonde data for comparison.

The ME solutions are seen to resemble the solutions produced by the standard method, although systematic effects similar to those mentioned in Section 3.1 are evident. The ME solutions are generally smoother, the ozone maximum is placed somewhat higher, and much more ozone is placed in the troposphere than in the standard solutions. This is to be expected, as the ME method was shown in Section 2.1 to produce the most <u>uniform</u> solution consistent with the data. If too much ozone is placed in the lower atmosphere, this is bound to affect the distribution elsewhere, especially if the total column density is constrained to a given value. Because of these systematic effects, the standard solution appears to compare rather better with the ozonesonde profile than does the ME solution. In general, the standard solution places the peak in the distribution at about the same height as the ozonesonde, and it resembles the overall shape of the distribution produced by the ozonesonde more closely. This, again, is to be expected as the standard method employs 'past experience' (ie the climatology of ozonesonde profiles) as well as the observational data to produce its solution.

This situation is not quite so clear, however, when the comparison is made more quantitative. Fig 5 shows plots of the correlation coefficient between the ME solution and the standard solution, and between umkehr solutions and the ozonesonde data. Except around the 25 km level (where an interference effect in interpolating between the sampling grids of the two methods probably reduces the apparent correlation), the ME solution shows a high degree of correlation with the standard solution (the dashed lines P in Fig 5 show the 99.9% confidence level according to the student t-test). On comparing the performance of the two umkehr methods with the ozonesonde data, Fig 5(b) indicates that the ME solutions show a marginally higher degree of correlation than the standard solution, except in the lower stratosphere (15–20 km). While this result is scarcely significant statistically considering the small sample size, it is consistent with the theoretical property of the ME technique that it makes maximal use (and no more!) of the information in the data. The inferior qualitative performance of the technique compared to the standard method is mainly due to predictable (and hence, perhaps, correctable) systematic distortions in the shape of the resulting solution. This may suggest that the entropy definition has not been correctly formulated for this problem. It is possible that an alternative definition could be obtained empirically to produce a better overall fit to the solution, but this would then negate the primary advantage of the method which is its objectivity. This will be discussed further in Section 4.

4. Conclusions

The present study has demonstrated that the Maximum Entropy technique can produce results which are comparable to more conventional methods of analysis for umkehr observations of ozone. In terms of the correlation between the umkehr analysis methods and ozonesonde measurements, the ME technique may even be marginally superior outside the lower stratosphere. It is not suggested, however, that the present formulation of ME should be routinely used in preference to the standard method. ME is computationally more expensive, and the solutions using the currently adopted definition of entropy suffer from gross, though largely predictable, systematic errors of shape and in the position of the peak in the ozone density distribution. The latter problem could be alleviated somewhat by an alternative definition of entropy which did not result in a completely uniform unconstrained solution. An empirical approach could probably produce a solution of sorts to this problem, but it must be emphasised that the primary advantages of ME in this formulation are (a) its objectivity, and (b) its simplicity in the use of a simple, analytically differentiable definition of entropy with a single constraint provided by the data. Further work is really needed to find simple analytic definitions of entropy which could take into account the known (or assumed) physics of any given problem, without compromising the objectivity of the method. It must also be mentioned that further work is required to prove (or otherwise) mathematically the existence and uniqueness of more general solutions of the ME method beyond the currently known cases of the Fourier Transform and deconvolution.

Because of its computational expense, the ME technique is unlikely to find widespread use in routine remote sensing problems where independent information exists for the long term average solution and its expected variability. A more refined version of ME than presented here, however, could well be of some value in situations where little other direct information is available. One may envisage its use in the remote sensing of the atmospheres of other planets, for example, where only the basic physics may be known. Other possible uses may be found in geophysics and other Earth sciences, particularly in situations where it is necessary to make the maximum use of relatively poor and noisy data, and to guard against unjustified conclusions resulting from the 'overinterpretation' of such data.

In this context, an alternative use of ME may be to assess the information content of an observational technique. In the case of umkehr measurements, it is clear that even relatively noise-free data are not sufficient to define the resulting solution completely. The solution is still 'contaminated' by the uniformity imposed by the definition of entropy. This is in contrast to the Fourier Transform case where it has been shown (eg see Gull and Daniell 1979) that two alternative definitions of entropy (S_1 and S_2) resulted in very similar solutions, provided that the initial data were of good quality. This suggests strongly that the umkehr technique needs to rely on climatological information in addition to simple observational data. There is not enough information intrinsic to the technique to define the solution fully. This is particularly noticeable in the ME solutions below about 12 km, which are all virtually identical except for a scale factor related to the total ozone column density (see Fig 4), clearly demonstrating that umkehr observations provide very little information at low levels.

Rodgers (1976) and Palmer (1979) have shown how climatological information can be incorporated into the Backus-Gilbert method. It may be possible to incorporate such information in an analogous way into a form of the Maximum Entropy method. Such an extension of the method could make it more attractive as a routine retrieval technique.

A further question which should be considered in more detail is whether the χ^2 statistic is the most appropriate to test the 'goodness of fit' of the solution generated by the method. Bryan and Skilling (1980) have shown that the use of χ^2 in the application of ME to deconvolution results in residual errors which are incorrectly (ie non-gaussian) distributed. They suggest the use of a different statistic (the 'E' statistic) designed to fit the expected statistical distribution of residuals and not merely their variance (as fitted by the χ^2 test). The alternative test significantly reduced distortions present in the final solution obtained using the χ^2 test.

Thus, provided that alternative versions of the ME technique can be developed to take account of all the available information, and the measurement error statistics, it is clear that Maximum Entropy could be a useful and simple alternative to more conventional remote sensing inversion methods.

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List of Symbols

E_k	kth measurement (k integer).
η_k	kth data value (calculated from solution, and defined for umkehr observations by equation (13)).
σ_k	error estimate for kth data value.
f_i	value of solution at ith position coordinate.
I_o	Intensity of sunlight outside the atmosphere.
I_G	Intensity of sunlight at scattering point G (see Fig 1).
S_c	Absorption cross-section of minor constituent.
n_c	Number density of minor constituent.
S_R	Scattering cross-section for air (Rayleigh cross-section).
n_a	Molecular number density for air.
ζ	Local zenith angle (see Fig 1).
θ	Zenith angle at the scattering point (see Fig 1)
l_i	Column density (total number per cm^2 along the ray path) of ozone.
c_j	Concentration of ozone (number density) in jth height layer.
z'	Layer thickness.
H	Atmospheric scale height (exponential).
R_o	Radius of the Earth.
N_m	Number of independent measurements.

Figure Captions

Fig 1 Diagram illustrating the geometry of the ray-tracing scheme used to calculate the 'umkehr' effect.

Fig 2 Flow diagram for the Maximum Entropy method as applied to the evaluation of umkehr observations of ozone.

Fig 3 The results of tests using the Maximum Entropy method on sets of artificially generated data. The dashed line shows the distribution of ozone used to generate the data, and the continuous 'histogram' shows the ME solution. Ozone C wavelengths were used (311.4 nm and 332.4 nm). $\overline{\sigma}_N$ is the rms noise level added to the data and assumed for the solution. The ozone column density N_{O_3} was a free parameter in calculating (a) and (b), and was fixed at the appropriate total value for (c) and (d).

Fig 4 The results of tests using the ME method on sets of observational umkehr data for ozone from Japanese and Australian stations. The continuous line shows the corresponding ozonesonde measurement, the continuous histogram shows the ME solution and the dashed histogram shows the standard (Mateer and Dütsch) solution. All sets of data used observations at 7 zenith angles except (a) which used 6. Vertical axes show the geometric height (km) and horizontal axes show number density of ozone in units of 10^{12} cm^{-3}.

Fig 5 Vertical profiles of the correlation coefficient between (a) ME and standard solutions of the umkehr data shown in Fig 4, and (b) between the two umkehr methods and the ozonesonde data. The dashed line P indicates the 99.9 per cent confidence level according to the student-t test (ie the value of correlation coefficient which, for the given number of measurements, has a probability of arising completely by chance of 0.1 per cent).

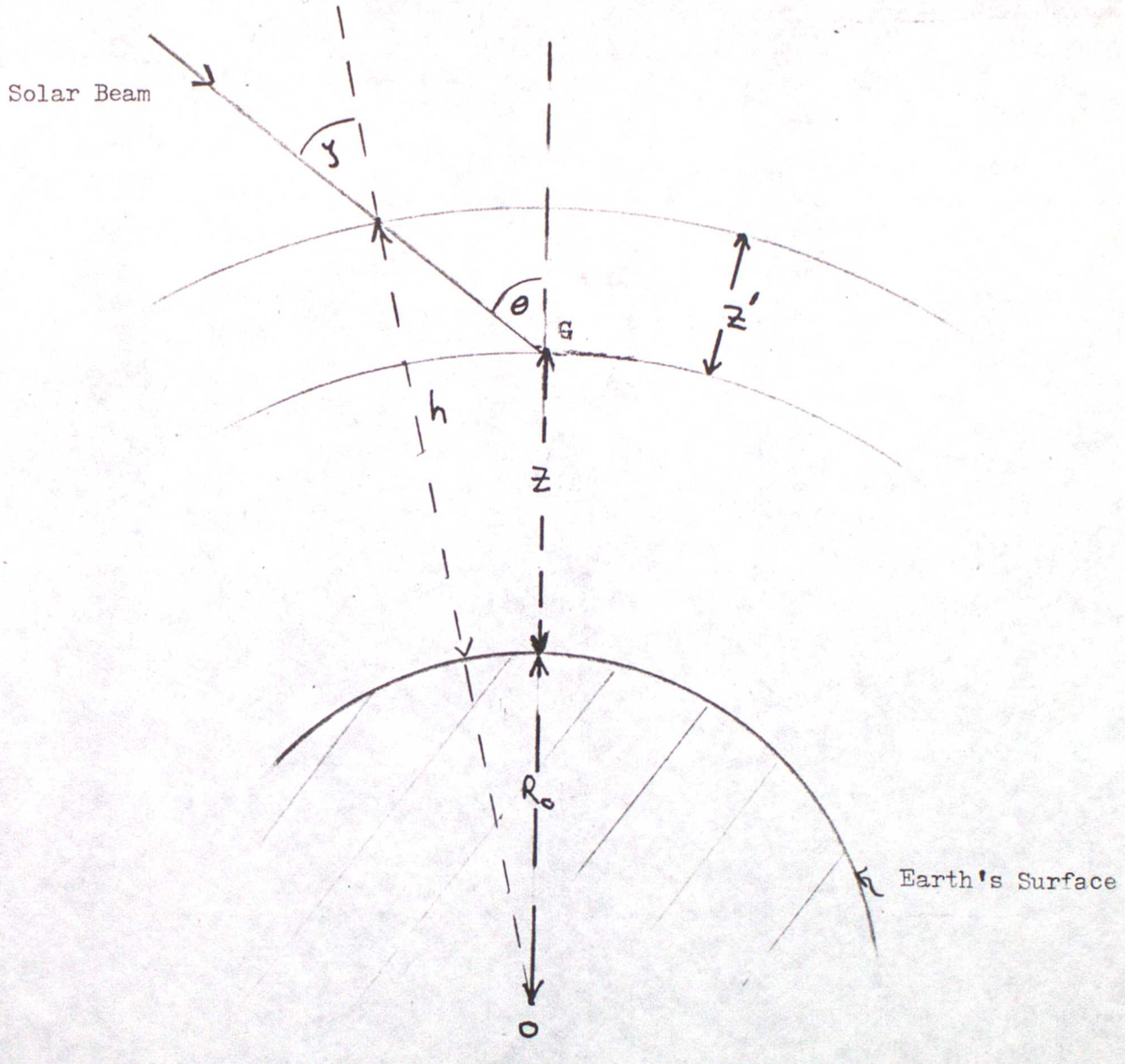


FIGURE 1

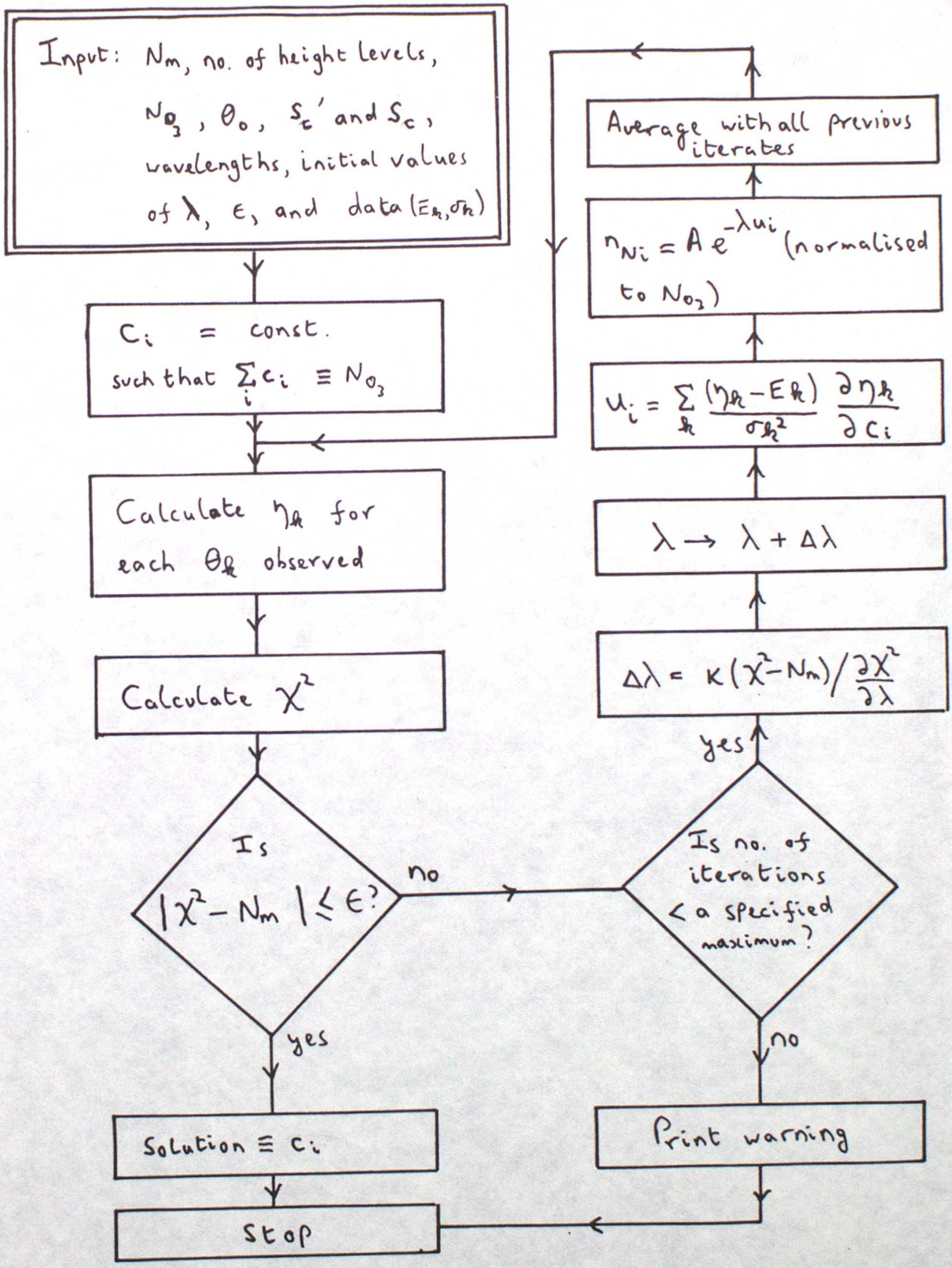
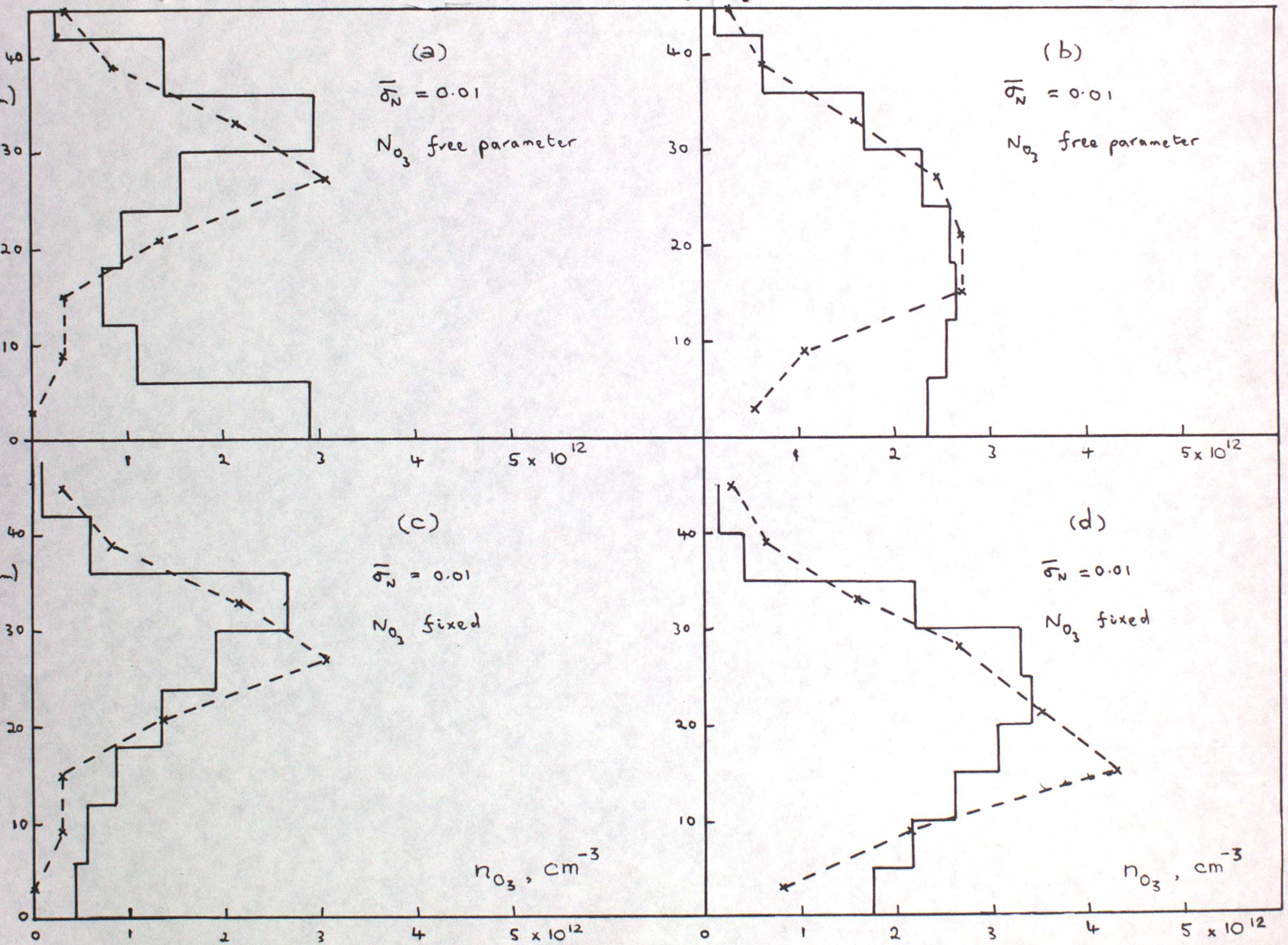

Input: N_m, no. of height levels, N_{O_3}, θ_0, S_t' and S_c, wavelengths, initial values of λ, ϵ, and data (E_k, σ_k)
c_i = const. such that $\sum_i c_i \equiv N_{O_3}$
Calculate η_k for each θ_k observed
Calculate χ^2
Is $|\chi^2 - N_m| \leq \epsilon$?
no
yes
Solution $\equiv c_i$
Stop
Is no. of iterations < a specified maximum?
yes
no
Print warning
$\Delta\lambda = K(\chi^2 - N_m) / \frac{\partial \chi^2}{\partial \lambda}$
$\lambda \rightarrow \lambda + \Delta\lambda$
$u_i = \sum_k \frac{(\eta_k - E_k)}{\sigma_k^2} \frac{\partial \eta_k}{\partial c_i}$
$n_{Ni} = A e^{-\lambda u_i}$ (normalised to N_{O_3})
Average with all previous iterates

FIGURE 2

FIGURE 3.



(a)
$\bar{\sigma}_N = 0.01$
N_{O_3} free parameter
(b)
$\bar{\sigma}_N = 0.01$
N_{O_3} free parameter
(c)
$\bar{\sigma}_N = 0.01$
N_{O_3} fixed
(d)
$\bar{\sigma}_N = 0.01$
N_{O_3} fixed
Z(km)
0
10
20
30
40
0
1
2
3
4
5 x 10^12
n_{O_3}, cm^{-3}

FIGURE 4 a-d

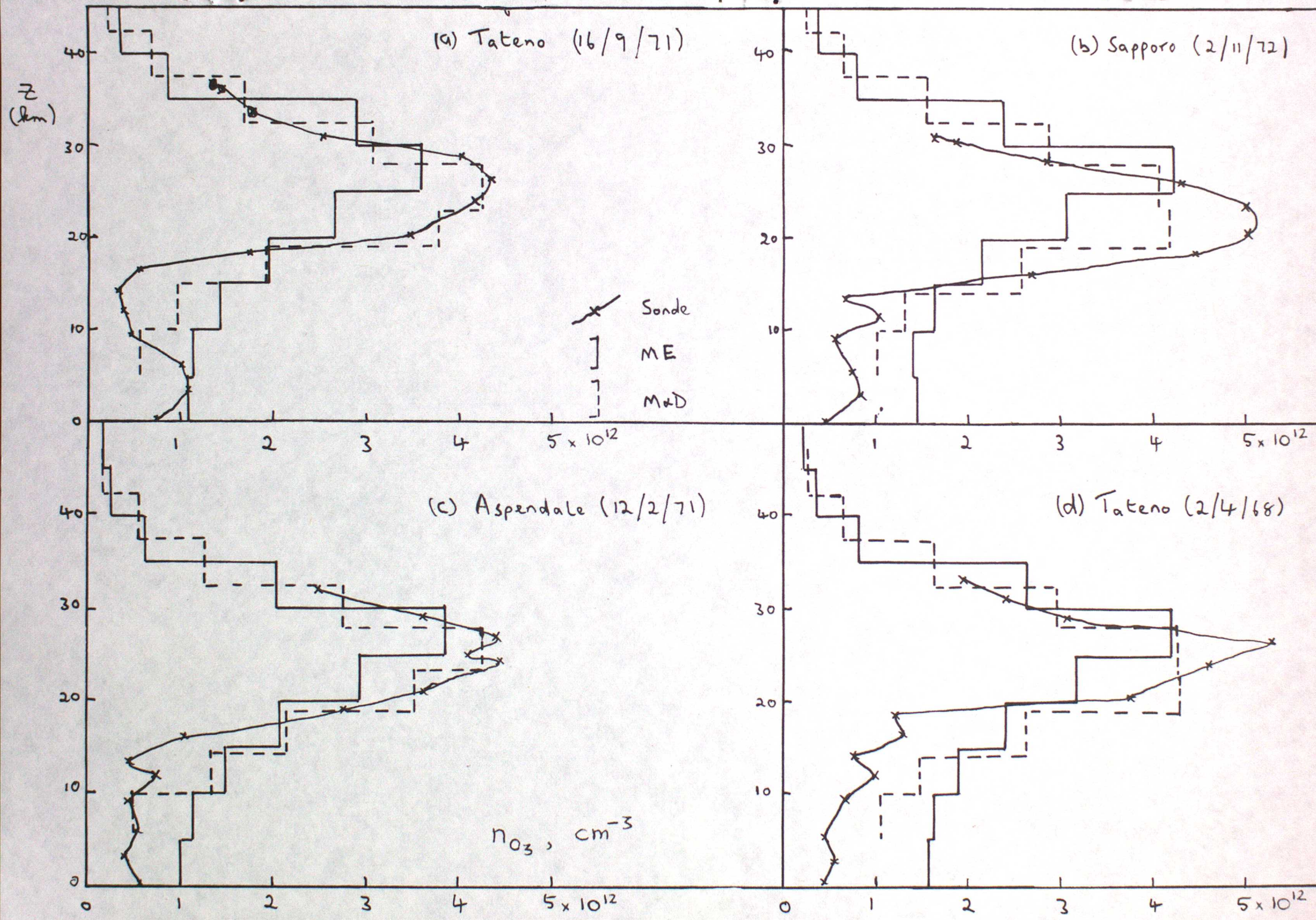
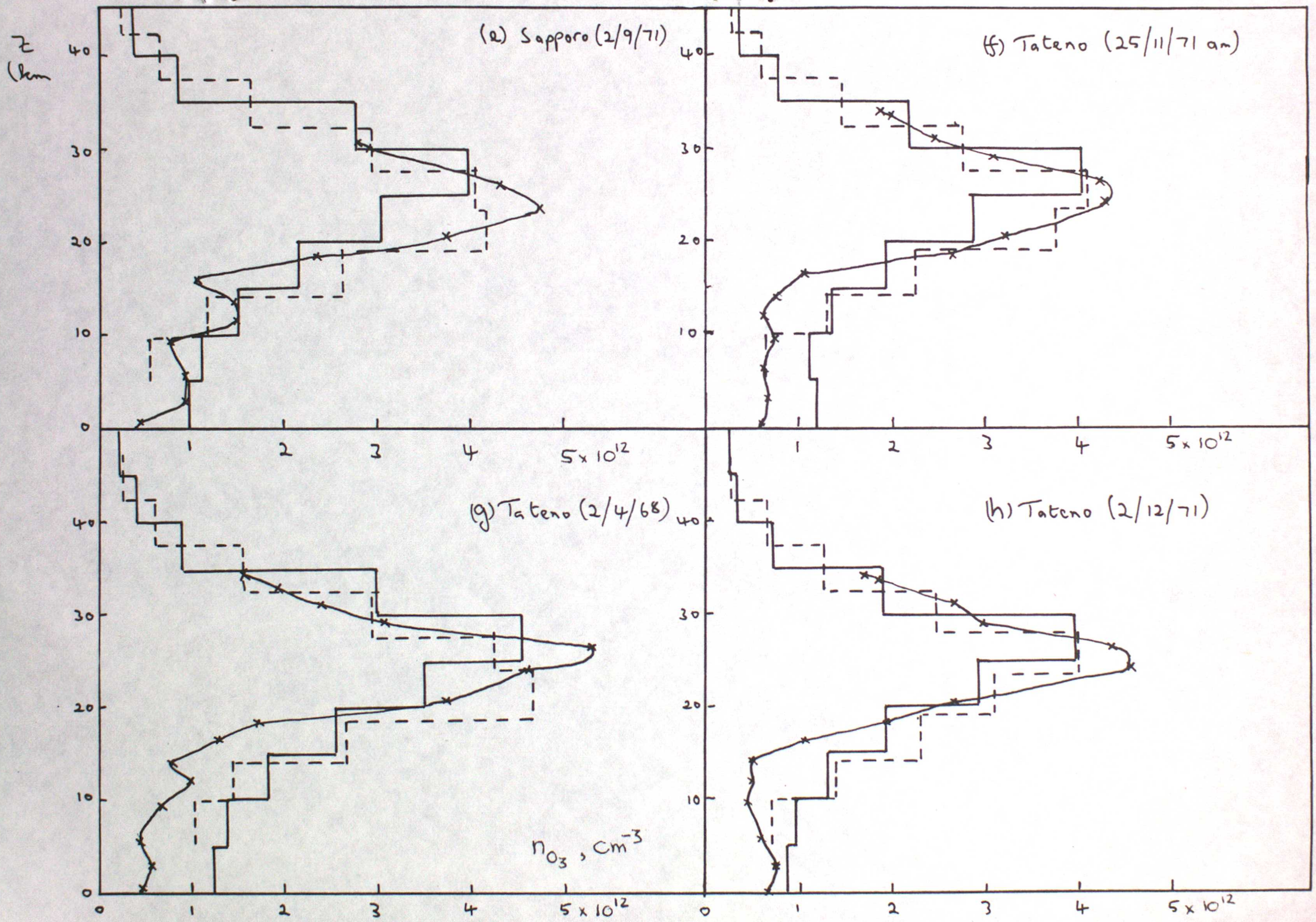
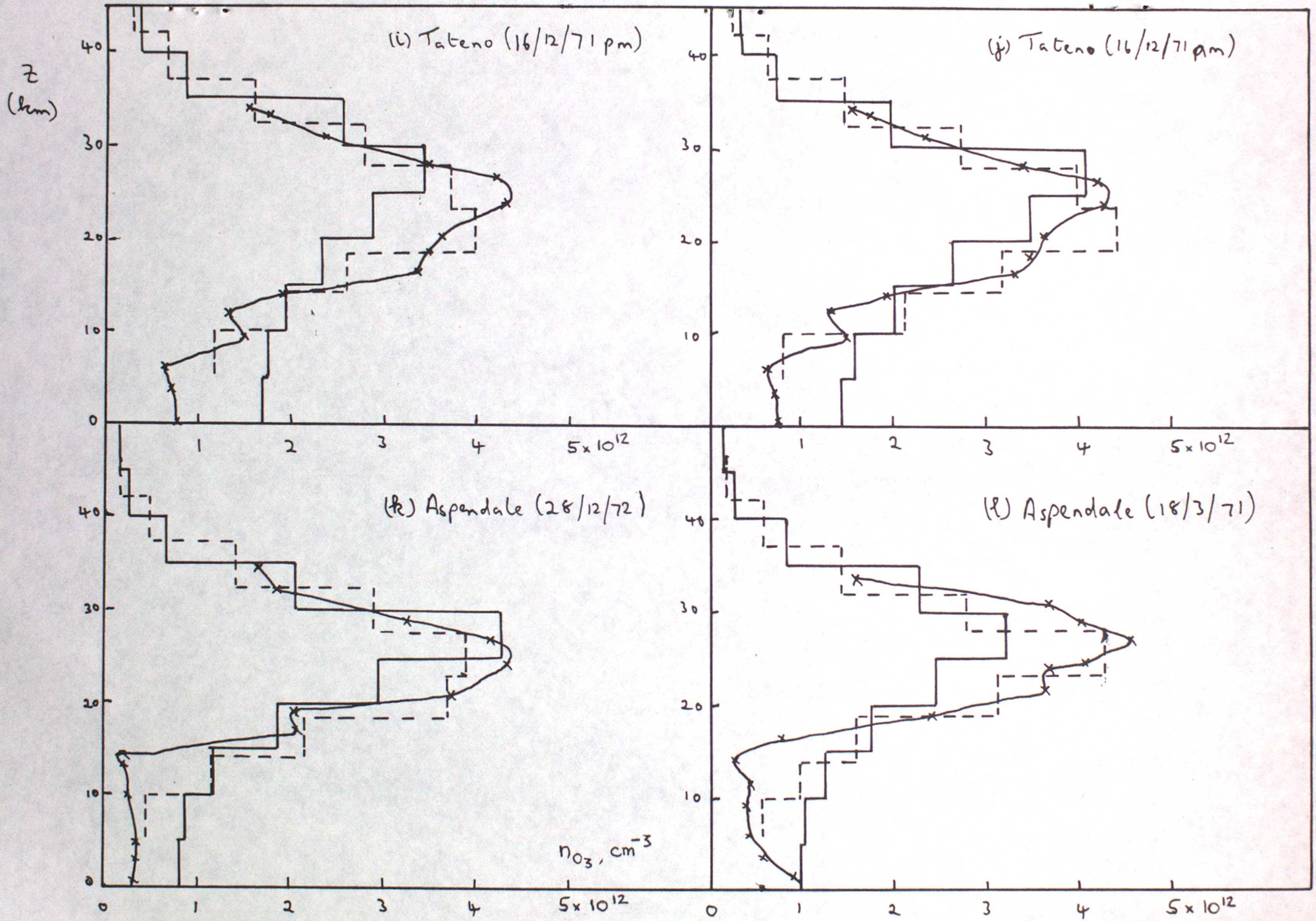

(a) Tateno (16/9/71)
(b) Sapporo (2/11/72)
(c) Aspendale (12/2/71)
(d) Tateno (2/4/68)
Z (km)
Sonde
ME
M&D
n_{O_3}, cm^{-3}
0
1
2
3
4
5×10^{12}
10
20
30
40

FIGURE 4 e–h



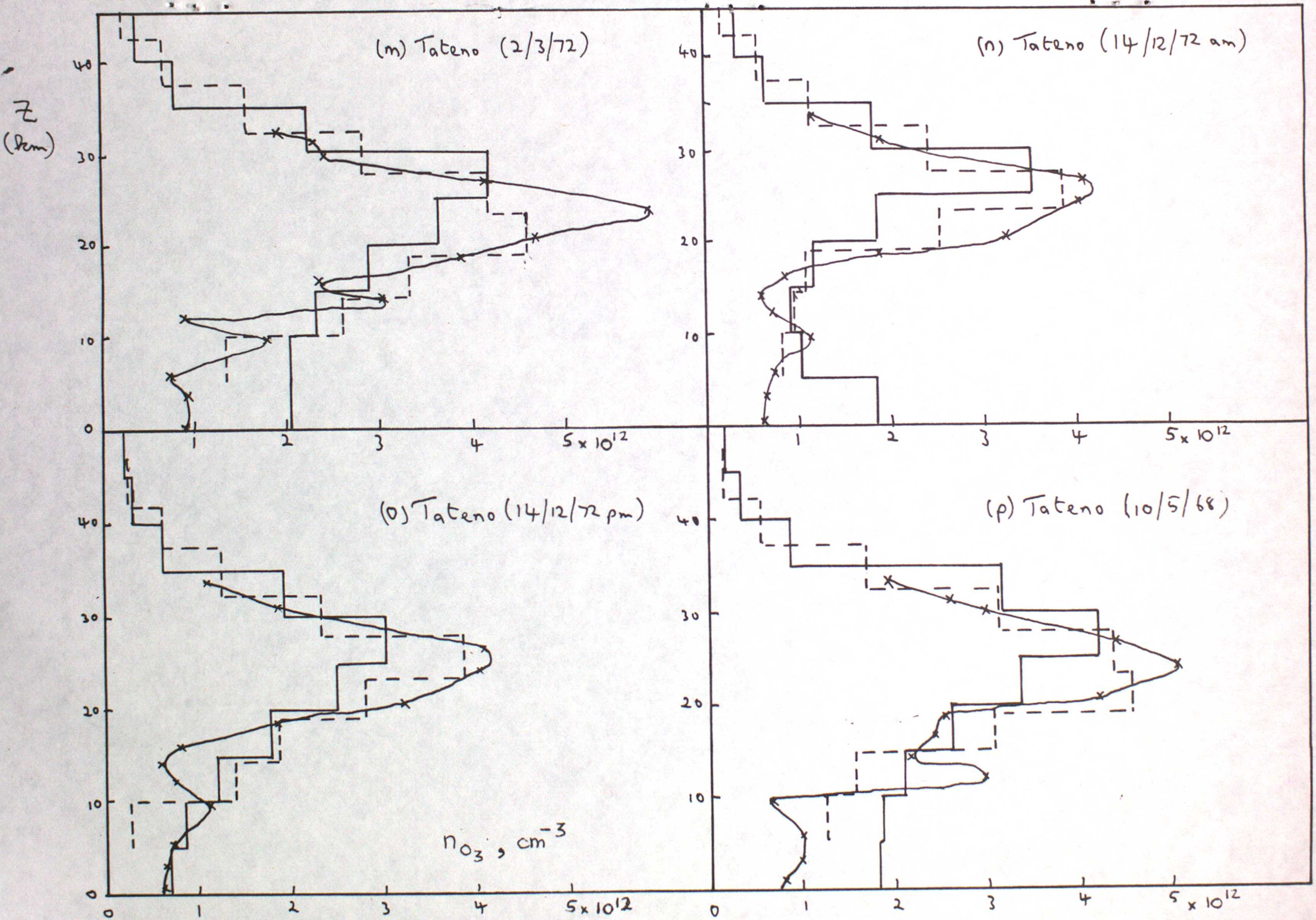
z
km
(e) Sapporo (2/9/71)
(f) Tateno (25/11/71 am)
(g) Tateno (2/4/68)
(h) Tateno (2/12/71)
n_{O_3}, cm^{-3}
5 x 10^12

FIGURE 4 i-1



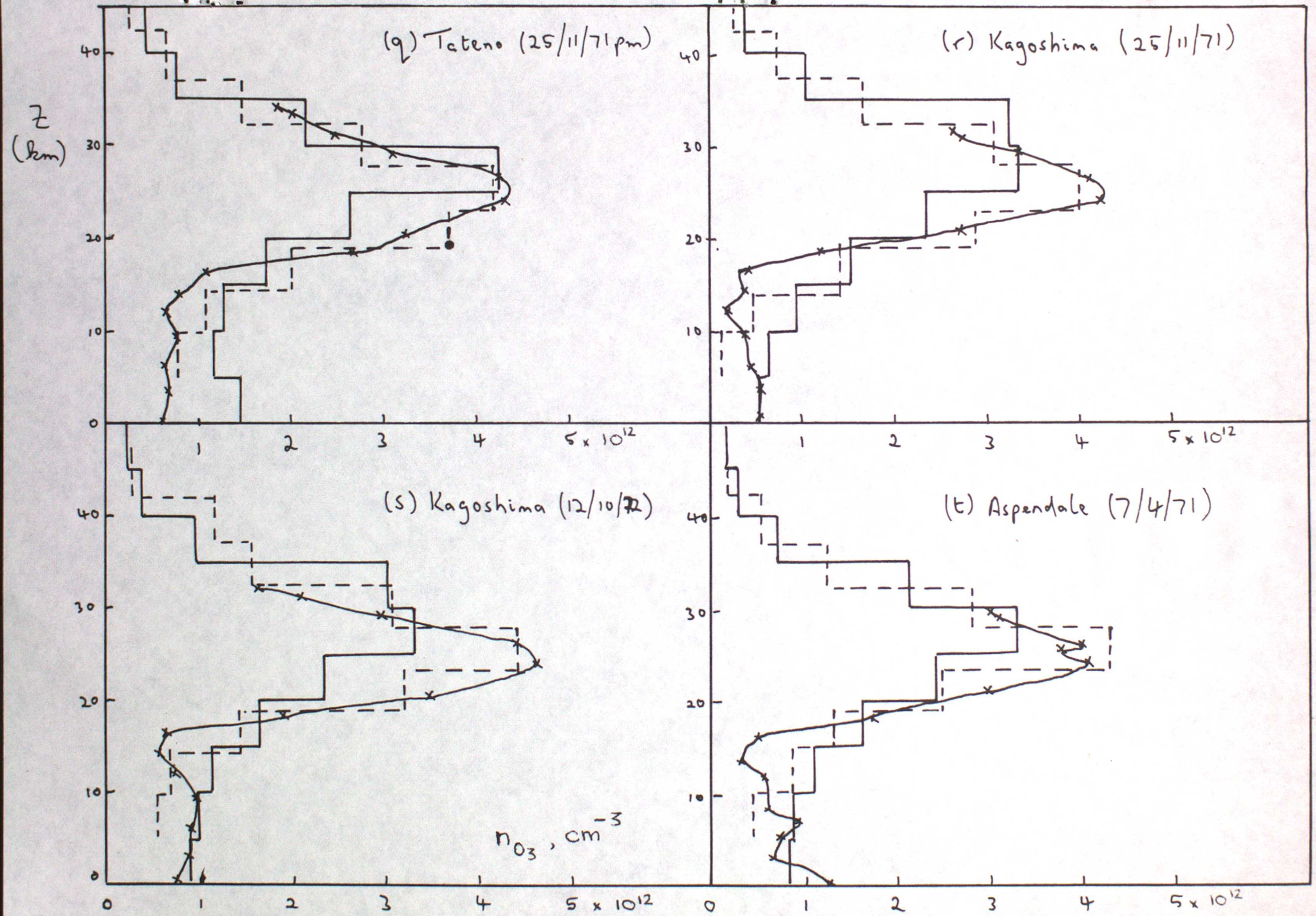
(i) Tateno (16/12/71 pm)
(j) Tateno (16/12/71 am)
(k) Aspendale (28/12/72)
(l) Aspendale (18/3/71)
z (km)
0
10
20
30
40
1
2
3
4
5 x 10^12
n_{O_3}, cm^-3

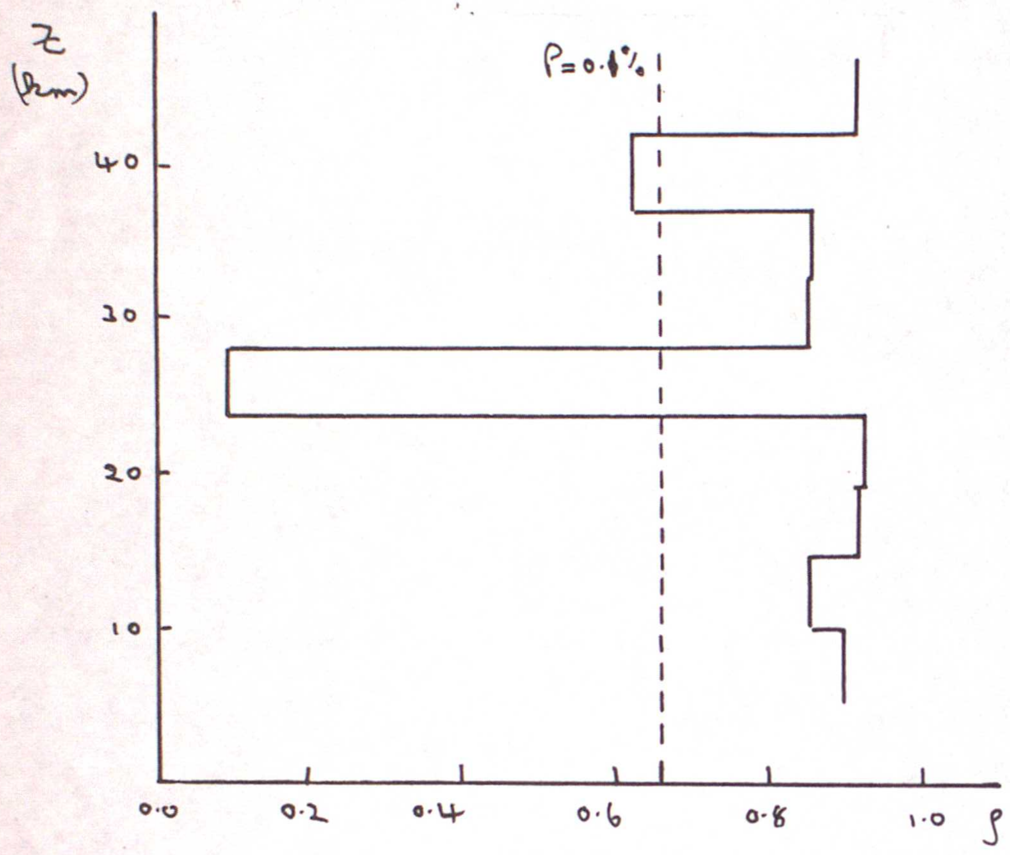
FIGURE 4 m-p



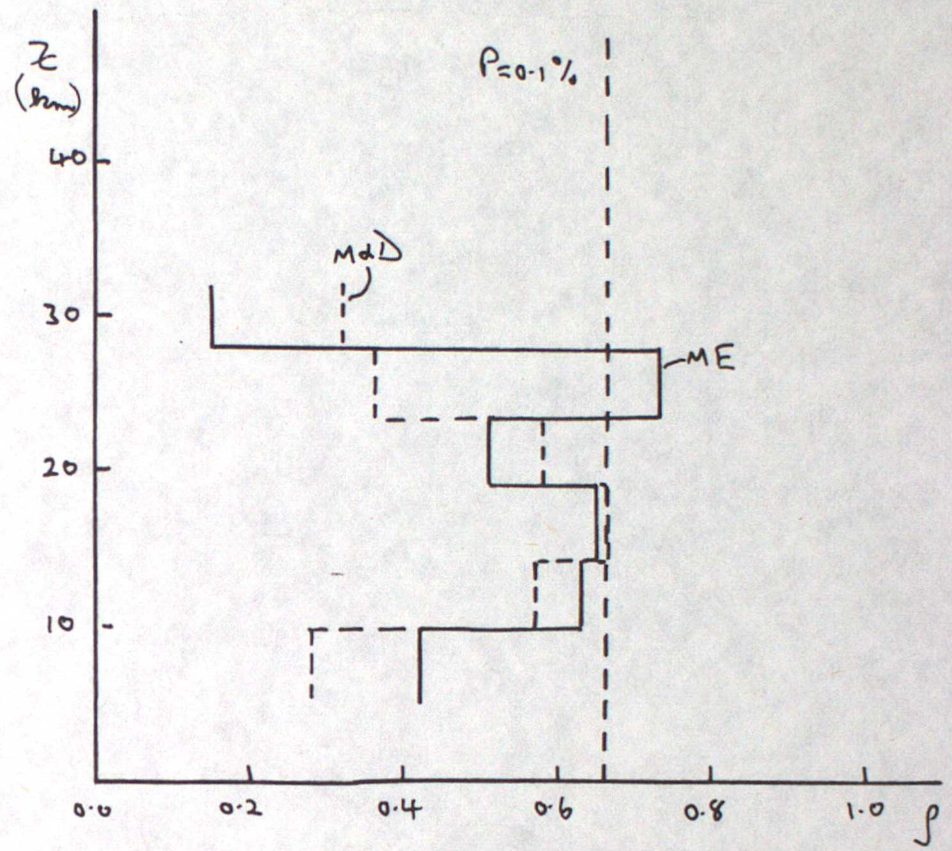
(m) Tateno (2/3/72)
(n) Tateno (14/12/72 am)
(o) Tateno (14/12/72 pm)
(p) Tateno (10/5/68)
Z
(km)
n_{O_3}, cm^{-3}
5×10^{12}

FIGURE 4 q–t


(q) Tateno (25/11/71 pm)
(r) Kagoshima (25/11/71)
(s) Kagoshima (12/10/72)
(t) Aspendale (7/4/71)
Z (km)
n_{O_3}, cm^{-3}
0
10
20
30
40
1
2
3
4
5×10^{12}



a) ME versus Mateer & Dutsch umkehr solution



b) ME and Mateer & Dutsch solutions versus ozone sonde.

FIGURE 5