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AN EVALUATION OF EULERIAN ADVECTION METHODS FOR THE MODELLING OF LONG RANGE TRANSPORT OF AIR POLLUTION

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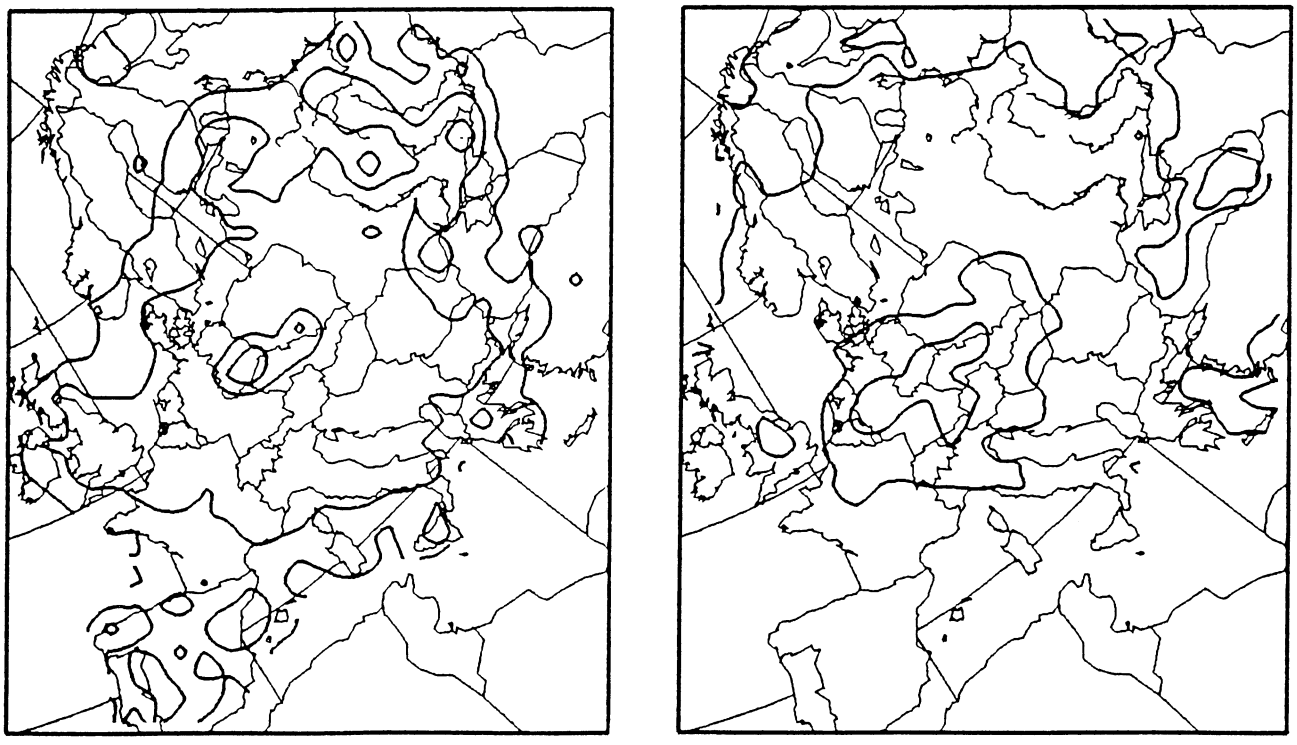

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PREFACE AND ACKNOWLEDGEMENTS

This note was prepared in time for the sixteenth session of the Steering Body of EMEP, in order to give a status of the activity at MSC-W with regard to developement and use of Eulerian models. The note presents an evaluation of numerical solution techniques for solving the advection equation. The experiences gained in this study will be utilized in the further use of the hemispheric scale model and the development of the regional scale multilayer model.

The authors want to acknowledge valuable discussions and suggestions with Professor A. Eliassen and Dr. T. Iversen. We would also like to thank Dr. Z. Zlatev for putting his latest computer version of the pseudospectral method at our disposal.

INTRODUCTION

The main objective of EMEP (as stated in terms of reference, ECE/EB.AIR/GE.1/8, Appendix 2) "is to provide Governments with information on the deposition and concentration of air pollutants, as well as on the quantity and significance of long-range transmission of pollutants and fluxes across boundaries". The main tool at EMEP/MSC-W to fullfil this objective has so far been a two-dimensional receptor oriented Lagrangian model. A major reason for chosing such a type of model within the EMEP work has been the high accuracy in calculating the horizontal transport and its simplicity and low computational costs. The Lagrangian approach is also particularly suitable for allocating concentrations and deposition to contribution from different sources whithin the model grid (country to grid square and grid square to grid square allocations). Such calculations have been of considerable importance in assisting the negotiations for new protocols on the reduction of emissions of air pollution under the "Convention on Long-Range Transboundary Air Pollution". A description of the latest version of the Lagrangian model together with the calculated fluxes of transboundary acidifying compounds are found in Sandnes and Styve (1992). Grid square to grid square calculations have also been made, and these are described in Barrett (1992). The most recent application of the Lagrangian approach to photochemical oxidants is found in Simpson (1992).

As our understanding of the physical and chemical processes leading to transboundary transport and deposition of air pollutants is increasing, the need for developing multilayer models in order to handle more complex vertical atmospheric features is enhanced. Tropospheric processes such as exchange mechanisms between the planetary boundary layer and the free troposphere, vertical wind-shear and cloud chemistry, can only be properly treated in a multilayer model. For example, as pointed out in Sandnes and Styve (1992), the underestimation of sulphur compounds in air and precipitation over Scandinavia and the overestimation of the same compounds in source regions may be related to the simplified treatment of the tropospheric processes in the one layer model. Furthermore, the two-dimensional Lagrangian model employs 150km horizontal resolution. This resolution may be too coarse in several situations. For instance, in order to include the non-linear photochemical effects on ozone production a finer grid may be required (see Sillman et al., 1990). In a model with significantly finer resolution

than 150km (for example 50km) a one layer approach can hardly be justified anymore.

In a multilayer model the Lagrangian description is difficult to implement in practice, but instead Eulerian methods have to be used. For this reason the EMEP/MSC-W has initiated a development of a regional scale Eulerian model. For the moment this model is under developement and hence no results on transboundary transport of air pollution are yet available. During this work we benefit from the experience EMEP/MSC-W already has obtained in developing and running a hemispheric scale Eulerian model (Iversen, 1989; Tarrason and Iversen, 1992).

In this note we want to focus on one important aspect of an Eulerian model, namely the errors caused by numerical approximations to the advection equation. The objective of investigating this problem is to gain insight into the expected errors and the applicability of Eulerian methods to the modelling of long range transport of air pollution. Of particular concern is the errors connected to allocating contributions to emissions sources such as countries and grid squares.

We will examine the advection schemes that we presently consider as good candidates for use in the multilayer model. These are the Smolarkiewicz scheme (Smolarkiewicz, 1983), the Bott scheme (Bott, 1989 a, b) and the pseudospectral scheme (Zlatev, 1985). The Smolarkiewicz and the Bott schemes are both so-called flux schemes, which behave quite similarly. Investigations by Berge and Kristjansson (1992) and additional personal experience indicate that the Bott scheme has the less numerical errors of the two. On the other hand the spectral method behaves quite differently from the flux methods. We will therefore concentrate on a comparision between the Bott scheme and the pseudospectral scheme.

As mentioned above a major concern of the Eulerian methods is related to the source allocation calculations. Such calculations require an estimate of the contribution of the emissions in individual grid-squares or countries to the concentrations and deposition elsewhere in the model domain. Hence, one has to model the advection from single point sources rather than all sources together. We now prefer to separate the problems that may arise from applying Eulerian advection schemes to source allocation into (1) approximations to the advection which are non-linear in the concentrations, (2) the numerical errors near the steep gradients associated with the point sources and (3) the dependence of the numerical errors on the orientation of the grid relative to the transport

direction. In fact, when the Lagrangian model was developed nearly two decades ago (Eliassen and Saltbones, 1975; Eliassen, 1978) points (2) and (3) were important reasons for not selecting the Eulerian approach.

Point (1) will be addressed by utilizing the hemispheric scale Eulerian model which assesses the contribution of the North-American sulphur emissions to the sulphur deposition in Europe. This model uses the Smolarkiewicz scheme, and it is linear in the treatment of chemical transformation and removal processes. Therefore, the non-linear properties of the model results are only related to the choice of the advection scheme. Before interpreting one year results, the evaluation of the non-linear effects is obviously important. Points (2) and (3) will be analysed by idealized advection tests, simply because the numerical schemes we want to evaluate are not implemented in a three-dimensional model yet. In addition, the properties we want to check are more easily seen in pure tests than from a complex model.

2 DESCRIPTION OF THE NUMERICAL SCHEMES

During the last decades more than 100 numerical schemes have been proposed for solving the advection equation in Eulerian models (Rood, 1987). The numerical errors involved in the Eulerian formulation have their origin on the discretization problem and the choice of approximations to the differential equations. Their behaviour often depends on the particular problem being addressed. It is therefore not a simple task to select an optimal scheme for long range transport of air pollution. Ideally a scheme must satisfy several criteria; (1) positiveness, (2) mass conservation, (3) shape preservation/small diffusion and dispersion, (4) accurate phase speed, (5) accurate implementation of the boundary conditions and (6) low computational costs on computers. To the authors' knowledge there exists no scheme that fullfil all these criteria completely. However, some of todays methods that we are investigating may meet many of these requirements.

2.1 The pseudospectral scheme.

The pseudospectral scheme (PSS) utilizes trigonometric interpolation to estimate the first order space derivatives at the grid points. All other calculations are carried out in the physical space defined by the grid. Fast Fourier Transforms are used to speed up the computations. The scheme was first proposed by Kreiss and Oliger (1972), and it has been used for air pollution studies by Prahm and Christensen (1977), Zlatev (1985) and Hov et al. (1989). A detailed description of how this scheme is applied to the advection equation can be found in for example Zlatev (1985). The main advantages of the scheme are the perfect phase speed and the ability to preserve very steep gradients. The main disadvantages are the creation of negative values, the non-physical requirement of periodic boundary conditions and the relatively high computational costs. The version of the PSS that we employ at EMEP/MSC-W has been developed by Z. Zlatev and his colleagues at DMU*, partly supported by EMEP.

*DMU - National Environmental Resarch Institute, Denmark.

2.2 The Bott scheme.

The Bott scheme (BOS) was introduced by Bott (1989 a,b), and a refined version of the scheme is presented in Bott (1992). The scheme utilizes polynomial fitting between neighbouring grid points of the concentration field in order to simulate the advective fluxes through the boundaries of adjecent grid boxes. The method consists of a flux limitation of the so-called 'integrated flux form' described in Tremback et al. (1987). The improvements in the BOS are to reduce the phase speed errors and to provide a positive definite scheme without loosing mass conservation properties. The main disadvantages with the scheme is the tendency to over- and undershooting and numerical diffusion near steep gradients. Apart from that, several investigations show that the scheme performs quite satisfactory. The order of the polynomial is optional, but a good compromise between accuracy and computational costs is to use either 2'nd order or 4'th order polynomials (Bott 1989 a). The 2'nd order version is somewhat more diffusive than the 4'th order version, but except for that the two version behave quite similarly. In this report we only present results from the 4'th order version of the scheme.

2.3 The Smolarkiewicz scheme.

The Smolarkiewicz scheme (SMS) was introduced by Smolarkiewicz (1983) and an improved version of the scheme is found in Smolarkiewicz and Grabowski (1990). The scheme has been applied to air pollution models (see e.g., Chang et al. 1987; Brost et al., 1988; Berge, 1990 and Tarrason and Iversen, 1992). The main idea of the SMS is to correct the numerical diffusion in the simpler upstream scheme. After the upstream fluxes have been calculated the numerical diffusion is estimated and, based on this estimate, the scheme calculates so-called "antidiffusion velocities" which are applied by a new upstream step in order to correct some of the numerical diffusion. The scheme has similar properties as the BOS, but the over- and undershooting, the numerical diffusion and the phase speed error are somewhat larger. The antidiffusive velocities depend non-linearly on the concentration fields.

3 NUMERICAL NON-LINEAR EFFECTS OF ADVECTION SCHEMES IN A HEMISPHERIC MODEL.

An important application of air pollution modelling is to relate concentrations of a pollutant to different emission sources. However, in order to be uniquely determined, this requires a model which is linear in concentrations. The degree of non-linearity can be checked by comparing runs with separate emissions sources with the one with all emissions included simultaneously.

3.1 Model runs.

The following experiment has been designed to assess the importance of non-linear effects in the identification of sources on a hemispheric scale. The Northern Hemisphere has been divided into four large sulphur emission areas: Europe (EMEP area), North America, Asia and the North Atlantic Ocean (natural DMS sources). The hemispheric model has been run separately for one of these emission areas during a certain period. Then, it has been run with the sum of all other emission areas, excluding the first one during the same time period. And finally, the model has been run including all four emission areas. The difference between the sum of the individual sources run and the total sources run are caused by the non-linearity of the advection scheme and it can be expressed by

Non-linear effects = Total sources run - (Source 1 run + (remaining sources run)) (1)

where source 1 run represents a seperate run for one of the four emission areas. Two sources have been isolated for testing and they are North America and the North Atlantic Ocean. The model has been run for the first half year of 1988 and the differences arising from the non-linearity has been assessed on a monthly averaged basis. This analysis can be interpreted as the interaction of 2 large plumes, one situated over for example North America (or the North Atlantic Ocean), the other extending over the rest of the Northern Hemisphere. We can expect the effect of non-linearity to be largest in the region of interaction of the two plumes. For the case of North American sources, the region of

major interaction with the other sources is situated over the mid-Atlantic Ocean. This area can be easily identified in Figs. 1 and 2. The figures show the percentage differences in the monthly averaged SO_2 and SO_4 concentrations in air at 1000m. in June 1988 as given by eq. (1) with source 1 equal to the North American sources. Positive differences indicate that the sum of the individual plumes is smaller than the total plume. Negative differences, on the contrary, indicate an overestimation when adding the individual plumes.

In most parts of the simulation area, the effect of non-linearity on the calculated air concentrations does not exceed 2%. Even in the areas of plume interaction, where these effects are seen to be larger, the percentage is of the order of 5%. These results are also valid for the total deposition fields (see Fig. 3). The fact that over the mid-Atlantic, the effect of non-linearity is generally positive indicates that by separating the different contributions, we might underestimate the deposition values by about 5%. Some very large differences appear at the borders of the plumes, where concentrations are very small (Figs. 6 and 7) and comparable to the model accuracy. Hence, these large differences must not be interpreted as non-linearities, but rather as due to truncation errors of the computer. This truncation effect is especially pronounced in the Arctic areas north of Canada, and as we get to high levels in the atmosphere (not shown).

The presented results are for June 1988, but they are representative of the other analysed months as well. The month of June was selected because it is the month with largest biogenic emission. The effects of non-linearity when isolating natural emissions are shown in Figs. 4 and 5. In this case, the zone of largest percentage differences is less well defined and it affects the west coast of Europe mostly in the neighbourhood of the North Sea, where DMS sources are relatively large.

It can be expected that the effect of non-linear interaction between different sources becomes more important as the number of sources increases. So, for individual isolated plumes over Europe, the non-linear effects introduced by the advection schemes can produce considerable varitiations in the resulting concentration and deposition fields. However, on a hemispherical scale, the results presented here give some confidence on the attempts to identify intercontinental pollution sources within reasonable margins of error.

4 IDEALIZED FLOW FIELD EXPERIMENTS.

In the previous Section we have illustrated the significance of the non-linearities of the Smolarkiewicz scheme in a source allocation study. Similar investigations of the Bott and the pseudospectral scheme will be performed at a later stage when the two schemes are implemented in a three-dimensional model. At present the comparision of the BOS and the PSS is restricted to idealized flow field experiments. As mentioned in the introduction, these tests are constructed in order to focus on particular problems that may arise when Eulerian models are applied to the work at EMEP/MSC-W. Both the PSS and the BOS have been extensively tested out for standard runs in the earlier cited references, and it is clear that the two methods show a quite satisfactory performance in many circumstances. Nevertheless, for the sake of completeness one standard rotational test is included before we discuss the more particular experiments.

4.1 Rotational tests.

A cone resolved by 11 points along the diameter (Fig. 8a) and a square wave resolved by 11*11 points (Fig. 8b) have been rotated with a constant angular velocity equal to 0.625 s^{-1} in a 32*32 grid. Fig. 8c and d show the cone after one rotation (400 time-steps) with the BOS and the PSS. Fig. 8e and f show the same, but for the square wave. Furthermore, in Table 1 we present the maximum (MAX) and minimum (MIN) values during the last quarter of the run, the absolute maximum (AMAX) and absolute minimum (AMIN) values for the whole run, the summed root square error (RSE = $\Sigma(C_{i,j} - C_{true})^2$, change in mass ($\delta M/\delta t = \Sigma C_{i,j} - \Sigma C_{true}$) and change in square mass ($\delta(M)^2/\delta t = \Sigma C^2_{i,j} - \Sigma C^2_{true}$) where N = 32 is the number of grid-points in the x- and y-directions. We have included the time change in the square mass since it tends to be reduced by diffusive processes and hence gives a quantitative measure of the numerical diffusion in the schemes. The quantities RSE, $\delta M/\delta t$ and $\delta(M)^2/\delta t$ are found by comparing with the known exact solution at the end of the run.

Both Fig.'s 8 c,d,e and f and Table 1 show that the two schemes handle the cone much better than the square wave. This is attributed to the very steep gradients at the edges of the square wave, which any scheme will have difficulties in representing. The PSS nearly treats the cone perfectly except for the apperance of some small negative

values. The BOS also shows a quite satisfactory performance, but the shape of the field is somewhat more distorted. For the square wave both schemes yield overshooting of more than 30% and the PSS gives negative values of about 20% of the plateau. The BOS is in this case quite diffusive near the edges of the plateau, while the PSS nearly maintains the steep gradients. Our conclusions from these standard tests are that in the case of uniform fields (a cone distribution) both schemes perform well with the PSS being the most attractive. From the square wave test it is difficult to decide which scheme is preferable. Either one has to face negative values or numerical diffusion near steep gradients together with substantial overshooting. Referring to the criteria listed in Section 2 a scheme ought to satisfy, we now see that both schemes distort the shape of the field (point 3), and the PSS is not positive definite (point 1). Furthermore, the PSS is not necessarily mass conserving (point 2) which is observed from the square wave test in Table 1. This point will be further elucidated in the next section.

4.2 Boundary conditions.

The implemention of the boundary conditions is consider to be a major difficulty with the PSS (see Hov et al., 1989). The decomposition of the spatial field into trigonometric fourier components requires periodic boundary conditions which are unphysical in applications to air pollution modelling on a limited domain. Periodic boundary conditions imply that the advected field appear at the opposite side of the grid at the moment of passing through the boundaries. In order to avoid this problem the fields may be damped toward the background concentration in some domain near the boundaries. In the present version of the PSS we can use either damping or no damping. Figs. 9a and b show an example of the two different conditions applied to advection of a square wave equal to the distribution in Fig 8b. Cleary, the damped version gives the most realistic performance, but it yields some quite strong over- and undershooting at the moment of passing through the boundaries (Table 2). The damping also implies that some mass is lost near the boundaries, and this explains why the PSS is not exactly mass conserving for the square wave rotational test (see Table 1). The boundary conditions are easily fitted to the BOS, and Fig. 9c shows the square wave utilizing this scheme. It is quite obvious that with the present version of the PSS we may create undesired errors near the boundaries.

4.3 Advection of isolated plumes and plumes from continuous sources in a grid-point.

The following examples will concentrate on the advection of an isolated grid-point plume (step functions) and plumes generated by grid-point sources. These are the most severe tests that can be employed and they are included in order to evaluate whether or not it is realistic to utilize the Eulerian methods in the regional scale source allocating calculations. First, we will consider the advection of a plume starting in grid-point x=y=5 with a concentration equal to 1 and zero background concentrations (Fig. 10a) which moves parallel to the x-axis with C=0.2. Hence, this is a one-dimensional test. Fig. 10b and c and Table 3 show that the PSS preserves the shape of the step function much better than the BOS. About 30% and 94% of the peak values reamain with the BOS and the PSS respectively. But the PSS still yields quite large negative values (about 25% of the peak, Table 3). In two dimensions the solution of the advection equation is found by splitting the problem into two one-dimensional operations in each spatial directions. If the scheme is diffusive we will employ the diffusive operator twice per time step, and hence make a more diffusive scheme compared to the one dimensional case. This implies that the numerical diffusion will depend on the orientation of the grid relative to the transport direction. In Figs. 10d and e the isolated plume is advected along the diagonal the same distance and at the same velocity as in the one-dimensional case. The diffusivity in both schemes is increased, and the BOS has now reduced the peak value to only about 10% of the exact solution. The peak value is well preserved in the PSS, but still quite large undesired positiv and negative values are seen. For the PSS, the RSE value is considerable increased (Table 3) which is due to the increased number of fictitious positive and negative values in the multi-dimensional case.

In air pollution applications we will mainly have to deal with continuous sources rather than isolated plumes. Therefore we have repeated the simulations from Figs. 10 introducing a continuous source at x=y=5. The source strength is constant and made so that we know the exact solution after a certain number of time-steps. The source is added to the concentration after each advective step. This is straightforward for the BOS, but it is more uncertain if it is an acceptable numerical procedure together with the PSS (Zlatev, personal communication). The results must therefore be interpreted bearing this in mind. Moreover, along the diagonal we find two ways of interpreting the form of the exact solution. First, if we assume all the mass in x=y=5 to be evenly distributed in that grid-

square, we would expect the plume from a continous source to be confined by the two diagonal lines in Fig. 12a. Consequentely, half of the mass must be contained in the grid-squares adjecent to the squares on the diagonal. On the other hand, we may assume that all the mass is confined to the grid-square where the center of the mass is situated. In such a case the exact solution must be equal to the one shown in Fig. 12b. The flux-scheme will obviously interpret the movement of the plume in accordance with Fig. 12a. The numerical experiments show that the PSS will give a solution following the center of the mass. Hence, we find it most reasonable to evaluate the BOS and the PSS based on Figs. 12a and b respectively. The plume from the continous source moving along the diagonal (Figs. 11c and d) are presented in two-dimensional plots to facilitate the comparison with the exact solutions.

The performance of the BOS is considerably improved compared to the isolated plume test above (see Figs. 11a and c). For instance, the RSE is not changing much implying that the average RSE is strongly reduced (Table 4). Still, for the most diffusive case along the diagonal we encounter a 50% reduction at the "downstream front" as compared to the exact solution. In Table 4 we observe that both mass and the square mass (amplitude) increase during the one-dimensional PSS run. This may be related to the above mentioned numerical treatment of the source. Unfortunately, we did not have time to look further into this matter. But we intend to examine this in the near future.

4.4 Computational costs.

The computational costs will always depend on the particular coding and the compiler that are used. We here present CPU-times obtained on a work-station without any vectorizing or parallelizing properties. Thus we may expect somewhat different results in real applications where a vector machine with several processors is used. The CPU has been measured for the standard rotational test and we find that the BOS and the PSS require respectively 4 and 6.5 times more CPU than the simple upstream scheme. Thus, there is no large difference between the two schemes, but the flux-method is somewhat less CPU demanding.

4.5 Discussions of the idealized tests.

Following the six criteria listed in Section 2 we find that the most serious

disadvantages with the PSS is related to the negative values (point (1)) and the implementation of the boundary conditions (point (5)). In addition we find some distortion of the shape of the fields (point (3)), and that the mass is not fully conserved for the most attractive boundary treatment. The most serious problems with the BOS is the distortion of steep gradients through the numerical diffusion (point (3)). The BOS do satisfy the other criteria. We observe that the numerical errors in BOS are related mainly to one of the criteria while the PSS do not satisfy several points.

Our final impression is therefore that the BOS is preferable in a regional scale Eulerian model since to many disadvantages are connected with the PSS. However, the present analysis also show that the Eulerian methods may give different results depending on the transport direction, and that in the case of the BOS on may argue that these errors are probably too large to be tolerated. The major advantage with the PSS is the ability to maintain the steep gradients of step functions. But, still the numerical errors are substantial and it is probably not recommendable to apply the PSS to grid square to grid square calculations.

5 SUMMARY AND CONCLUSIONS.

At EMEP/MSC-W an Eulerian model is used to assess the sulphur transport on the northern hemisphere and a regional scale Eulerian model is under development with the purpose of calculating transboundary fluxes and deposition of air pollution within Europe. An important aspect of an Eulerian model is the numerical errors related to the solution of the advection equation, and in this note we have evaluated three different numerical advection schemes that we either presently apply or consider to apply to our models.

The hemispheric scale model uses the Smolarkiewicz scheme which has been analysed with regard to numerically induced non-linear interactions between the plumes from the major sulphur emission areas (North America, Europe and the North Atlantic Ocean). Our model calculations show that the non-linear interactions are small (less than 2%) over most parts of Europe. We can therefore conclude that the model is suitable to assess the contribution from for example North America to the sulphur deposition in Europe within reasonable margins of errors.

However, the more detailed calculations of the contribution from grid-point sources to other (also neighbouring) grid-points will certainly give rise to much stronger non-linear interactions. Such calculations will also suffer from the numerical errors related to the treatment of very steep gradients and the fact that the numerical errors will depend on the orientation of the grid relative to the transport direction. The two schemes that we presently are implementing in the regional scale Eulerian model (the Bott scheme and the pseudospectral scheme) have been analysed for these two latter problems. Our conclusions are that the numerical errors are considerable in both schemes when isolated grid-point plumes and sources are treated. However, in most transport simulations including all sources we will hardly find the very steep gradients associated with isolated grid-point sources. Under these circumstances both schemes may perform satisfactory and among the two the Bott scheme is probably preferable. This is due to the disadvantages encountered in the boundary treatment and the apperance of negative values when the pseudospectral method is applied. A general advice, based on the limitations set by the advection schemes, is to concentrate the applications of the Eulerian model to calculations where the numerical errors are expected to play a minor role. Such calculations should include all sources and thereby reduce the strength of the gradients. We then obtain an optimal use of the benefits a three-dimensional approach may give the modelling work in EMEP/MSC-W. For the purpose of the grid square to grid square allocations including the treatment of isolated sources, the Lagrangian methods will probably still be the most appropriate.

Since we here only present idealized tests of the Bott and the pseudospectral scheme, we intend to follow up the evaluation of the numerical schemes during the implementation procedure in the regional scale multilayer model.

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7 TABLES

Table 1. Results from the standard rotational test show in Fig. 8. The presented quantities are the maximum (MAX) and the minimum (MIN) values during the last quarter of the run, the absolute maximum (AMAX) and absolute minimum (AMIN) values for the whole run, the summed root square error ($RSE = \Sigma(C_{i,j} - C_{true})^2$, change in mass ($\delta M/\delta t = \Sigma C_{i,j} - \Sigma C_{true}$) and change in square mass ($\delta(M)^2/\delta t = \Sigma C^2_{i,j} - \Sigma C^2_{true}$). N = 32 is the number of grid-points in the x- and y-directions.

Table 2. Same as Table 1, but for a square wave passing through the boundaries shown in Fig. 9.

Table 3. Same as Table 1, but for the isolated puff experiment shown in Fig. 10.

Table 4. Same as Table 1, but for the continous source experiment shown in Fig. 11.

8 FIGURE CAPTIONS

Fig. 1. Percent difference between (1) SO_2 concentration at 1000m for June 1988 as calculated by including all sulphur sources at the northern hemisphere and (2) the sum of the SO_2 concentration at 1000m calculated with only the North Amercian emissions and all other sources excluding the North American sources.

Fig. 2. Same as Fig. 1, but for SO_4.

Fig. 3. Same as Fig. 1, but for total deposition (wet+dry) of sulphur.

Fig. 4. Percent difference between (1) SO_2 concentration at 1000m for June 1988

as calculated by including all sulphur sources at the northern hemisphere and (2) the sum of the SO_2 concentration at 1000m calculated with only the DMS emissions in the North Atlantic and all other sources excluding the North Atlantic sources.

Fig. 5. Same as Fig.4, but for total deposition (wet+dry) of sulphur.

Fig. 6. Averaged calculated SO_2 concentration (ug/m^3) at 1000m for June 1988 including all sources.

Fig. 7. Same as Fig. 6, but for SO_4.

Fig. 8. Initial distribution for a) the cone test and b) the square wave. Distribution after one rotation of the cone using c) the BOS and d) the PSS and for the square wave using e) the BOS and f) the PSS. The step-function in the corner of the grid is used to scale the graphics and is not related to the numerical experiments.

Fig. 9. Square wave passing the boundaries along the diagonal using a) the PSS with damping near the boundaries, b) the PSS without damping and c) the BOS.

Fig. 10. a) Initial distribution of the isolated puff experiments, b) the distribution after 100 time iterations along the x axis with the BOS, c) same as b), but for the PSS, d) same as b), but along the diagonal and e) same as b), but along the diagonal for the PSS. The step-function in the corner of the grid is used to scale the graphics and is not related to the numerical experiments.

Fig. 11. Same as Fig. 10, but with a constant source in x=y=5.

Fig. 12. Exact solution for the experiment with transport along the diagonal and continous source for a) the flux method and b) the pseudospectral method.

Table 1.

	MAX	MIN	AMAX	AMIN	RSE	$\delta/\delta t(M)$	$\delta/\delta t(M)^2$
Cone BOS	0.85	0	0.99	0	3.6	0	-1.32
Cone PSS	0.98	-0.015	1.00	-0.019	0.93	0	-0.0005
Square wave BOS	1.19	0	1.33	0	39.14	0	-22.71
Square wave PSS	1.28	-0.16	1.33	-0.22	19.52	-0.28	-1.42

Table 2.

	MAX	MIN	AMAX	AMIN
PSS with damping	1.48	-0.39	1.48	-0.39
PSS without damping	1.32	-0.21	1.34	-0.21
BOS	1.18	0	1.29	0

Table 3.

	MAX	MIN	AMAX	AMIN	RSE	$\delta/\delta t(M)$	$\delta/\delta t(M)^2$
BOS parallel	0.30	0	0.82	0	1.45	0	-0.80
PSS parallel	0.94	-0.25	1.00	-0.26	1.28	0.18	-0.006
BOS diagonal	0.10	0	0.77	0	1.83	0	-0.95
PSS diagonal	0.90	-0.18	1.00	-0.19	4.27	0.34	-0.11

Table 4.

	MAX	MIN	AMAX	AMIN	RSE	$\delta/\delta t(M)$	$\delta/\delta t(M)^2$
BOS parallel	1.12	0	1.15	0	1.27	0	-0.54
PSS parallel	1.72	-0.35	1.72	-0.35	6.78	2.02	6.24
BOS diagonal	1.04	0	1.10	0	14.23	0	-8.85
PSS diagonal	1.44	-0.26	1.48	-0.30	25.92	3.03	-0.082

Fig. 1

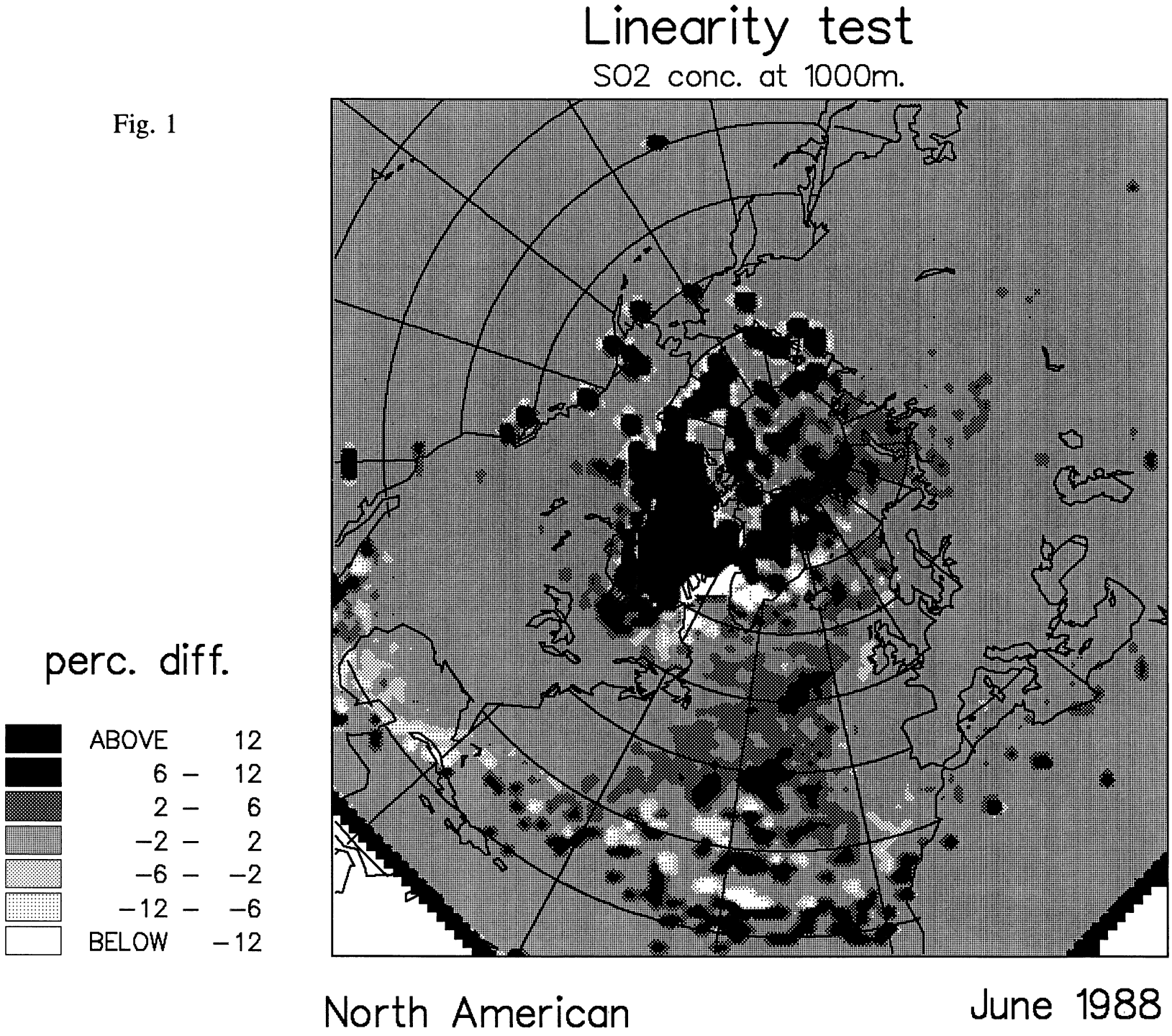

Linearity test
SO2 conc. at 1000m.
perc. diff.
ABOVE 12
6 – 12
2 – 6
–2 – 2
–6 – –2
–12 – –6
BELOW –12
North American
June 1988

Fig. 2

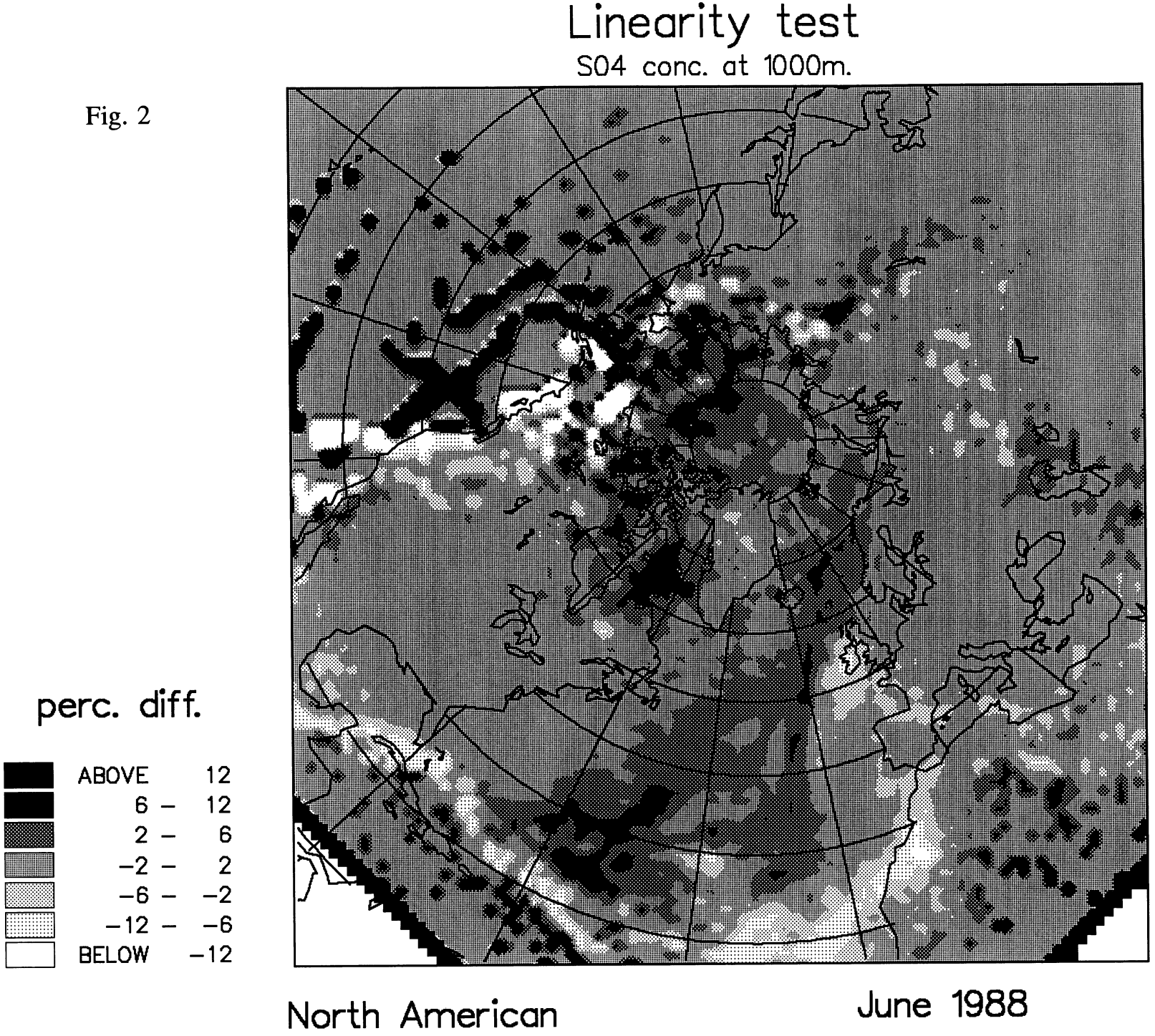

Linearity test
S04 conc. at 1000m.
perc. diff.
ABOVE 12
6 – 12
2 – 6
–2 – 2
–6 – –2
–12 – –6
BELOW –12
North American
June 1988

Fig. 3

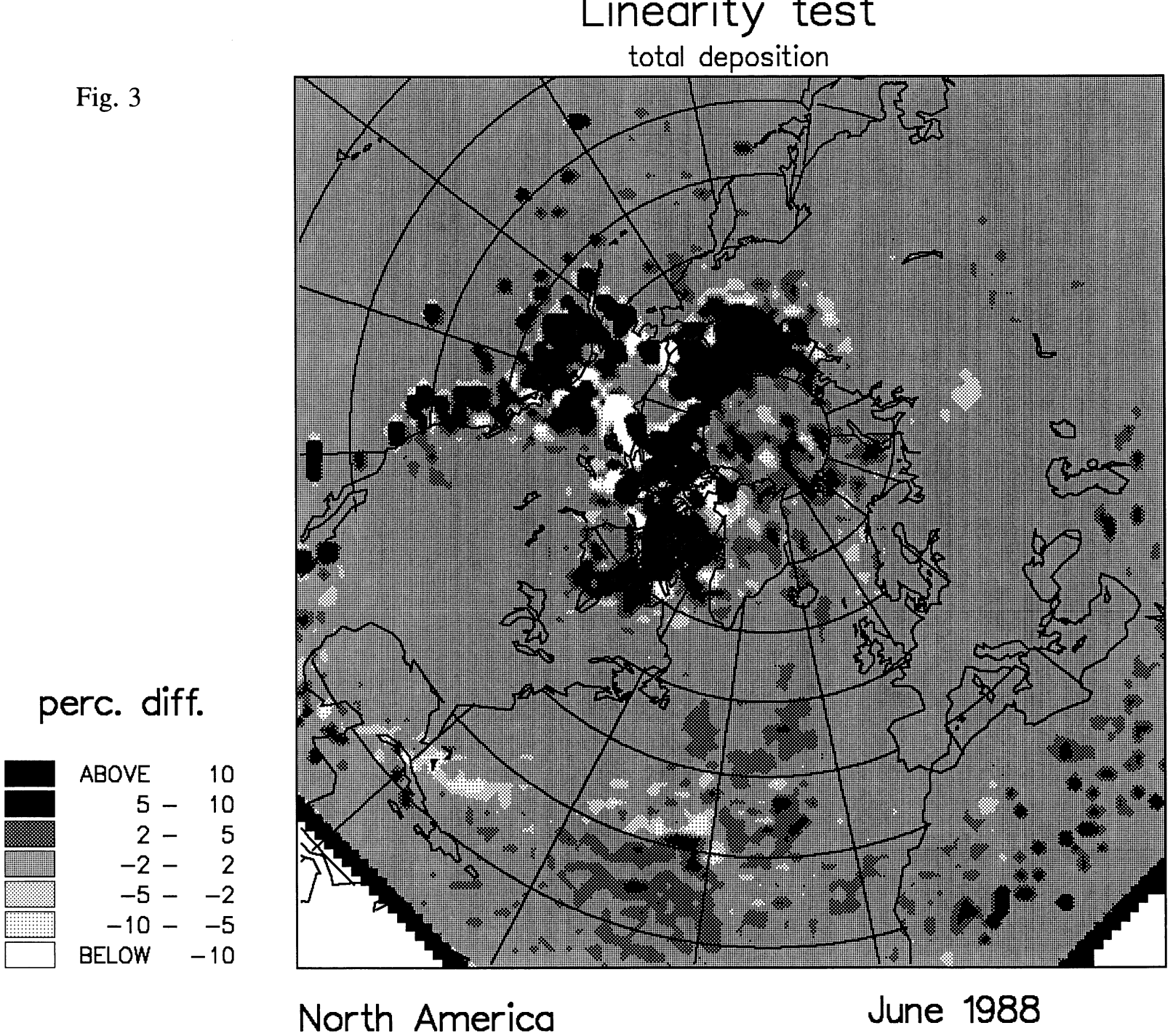

Linearity test
total deposition
perc. diff.
ABOVE 10
5 – 10
2 – 5
–2 – 2
–5 – –2
–10 – –5
BELOW –10
North America
June 1988

Fig. 4

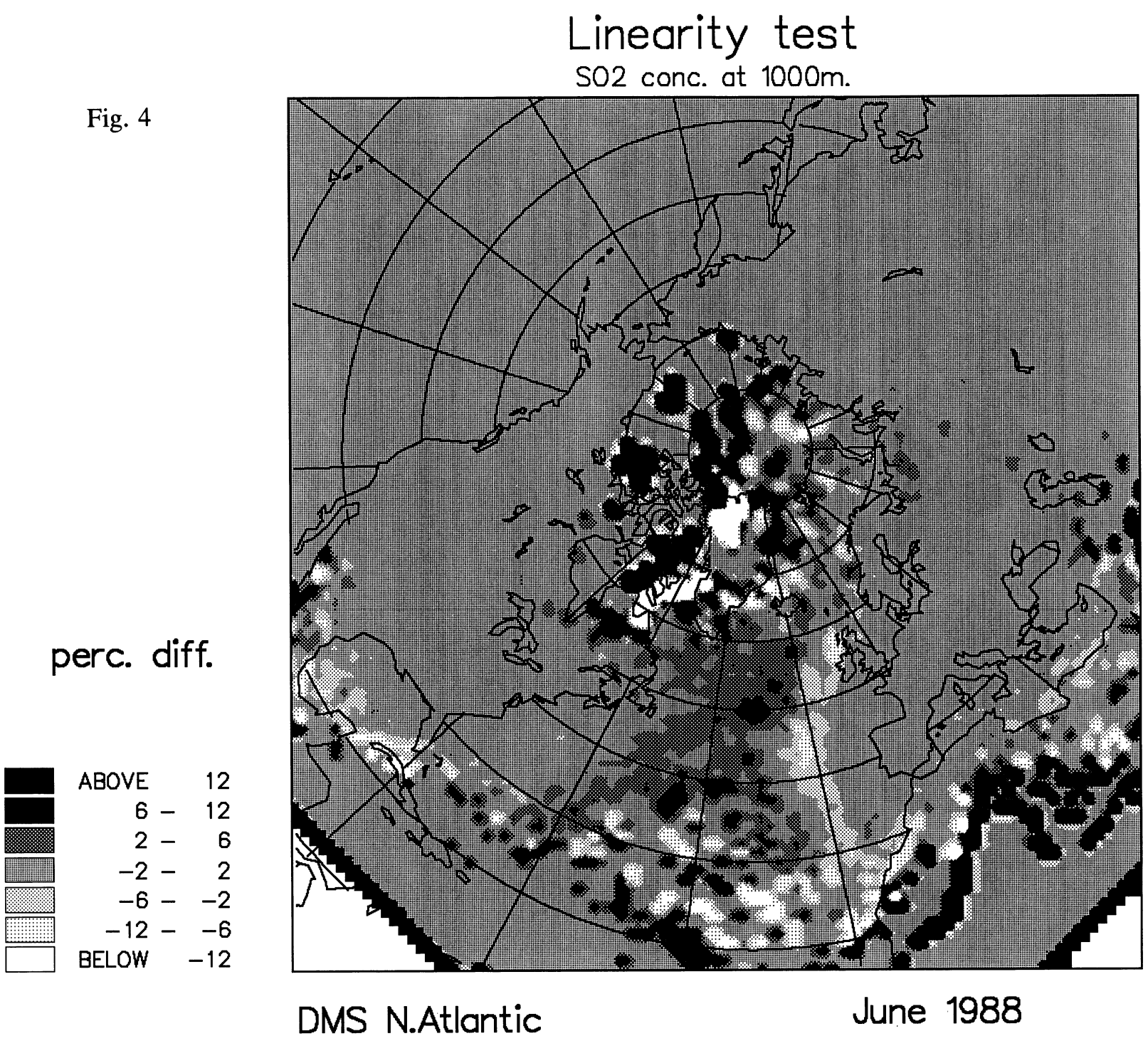

Linearity test
SO2 conc. at 1000m.
perc. diff.
ABOVE 12
6 – 12
2 – 6
–2 – 2
–6 – –2
–12 – –6
BELOW –12
DMS N.Atlantic
June 1988

Fig. 5

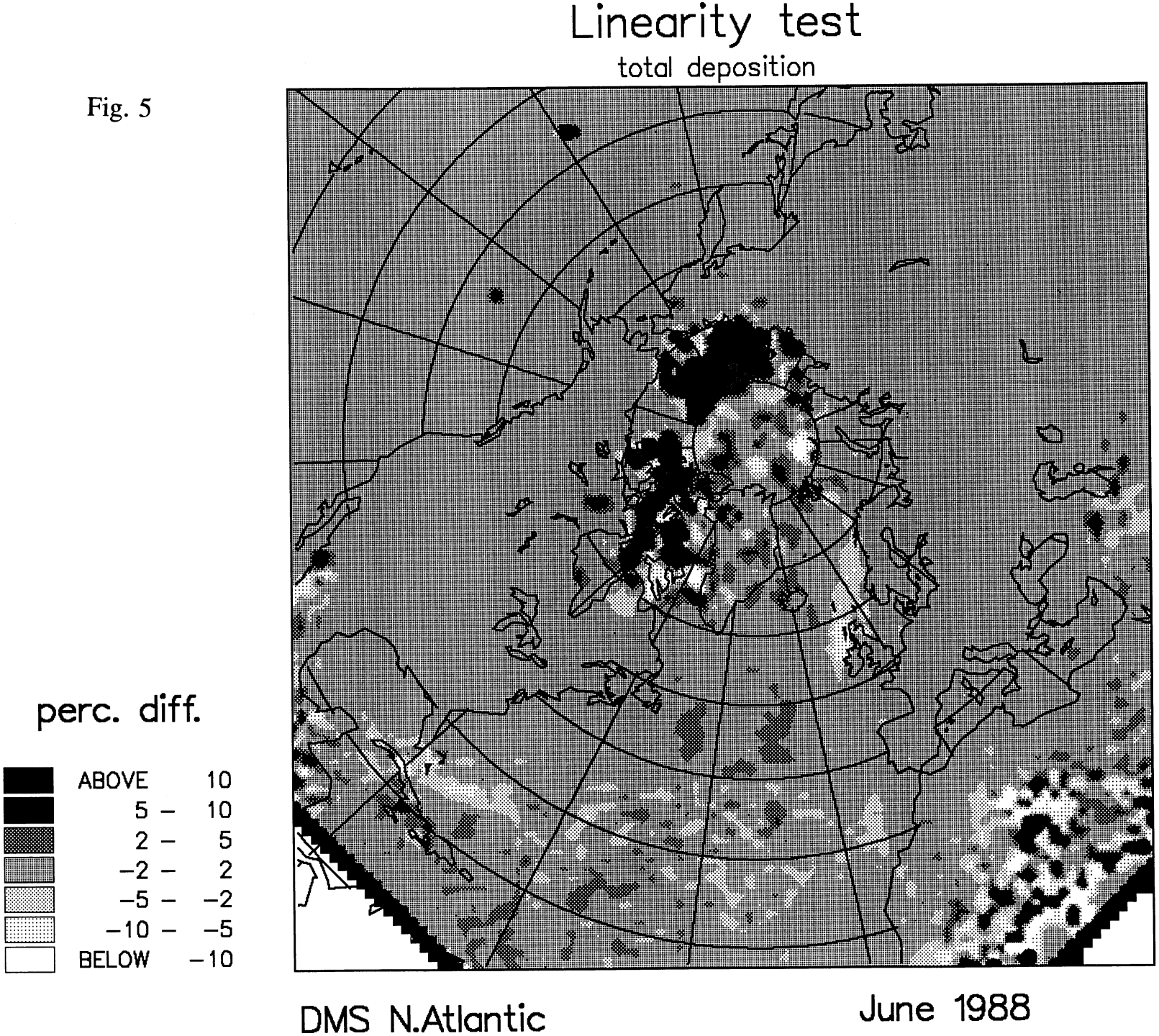
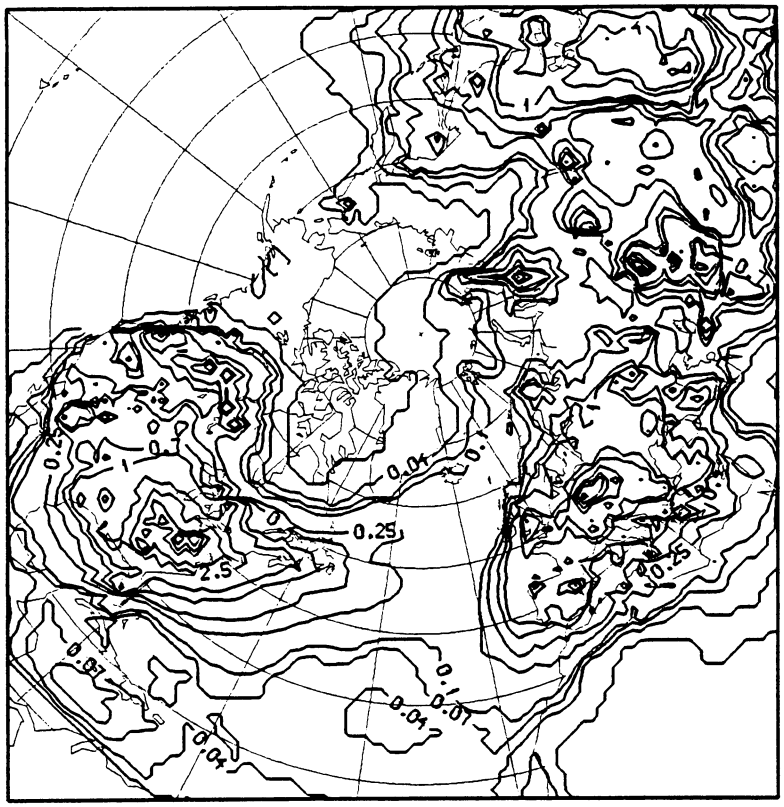
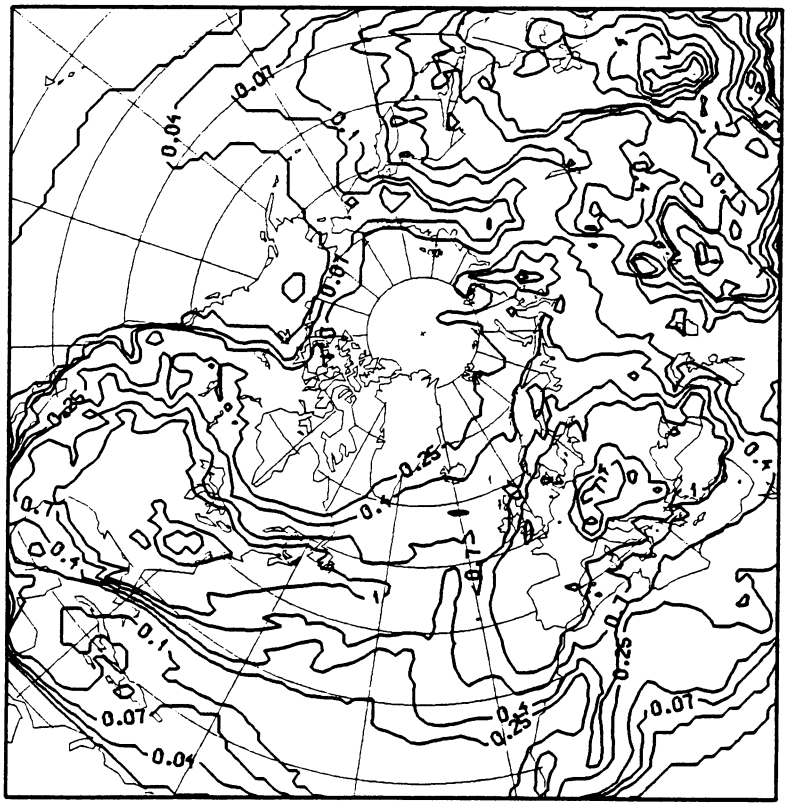

Linearity test
total deposition
perc. diff.
ABOVE 10
5 – 10
2 – 5
–2 – 2
–5 – –2
–10 – –5
BELOW –10
DMS N.Atlantic
June 1988

Fig. 6



AVERAGED SO2 CONCENTRATION (UG/M3) 1000 M. 06 1988 ALL SOURCES

Fig. 7



AVERAGED SO4 CONCENTRATION (UG/M3) 1000 M. 06 1988 ALL SOURCES

Fig. 8a

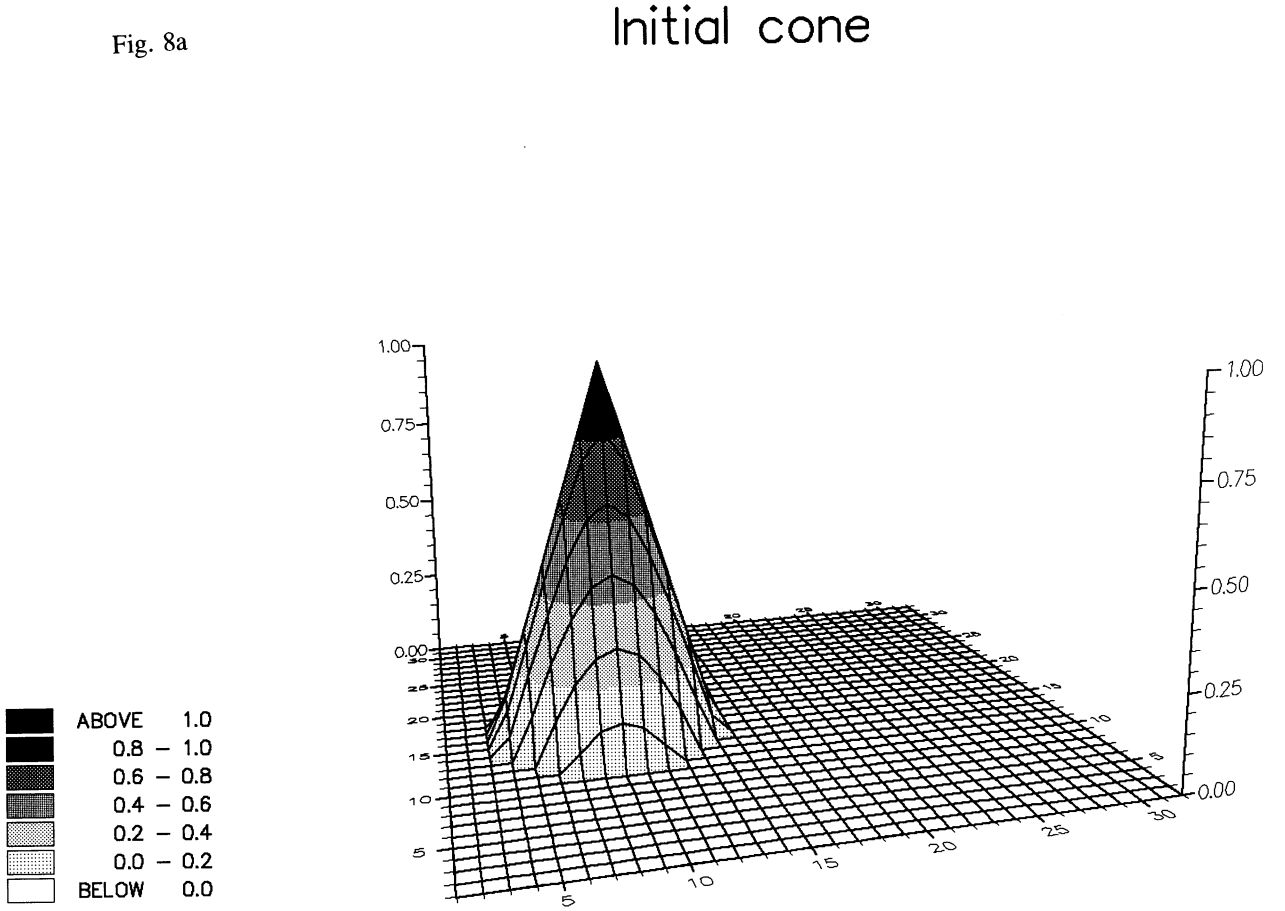

Initial cone
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.00
0.75
0.50
0.25
0.00
5
10
15
20
25
30

Fig. 8b

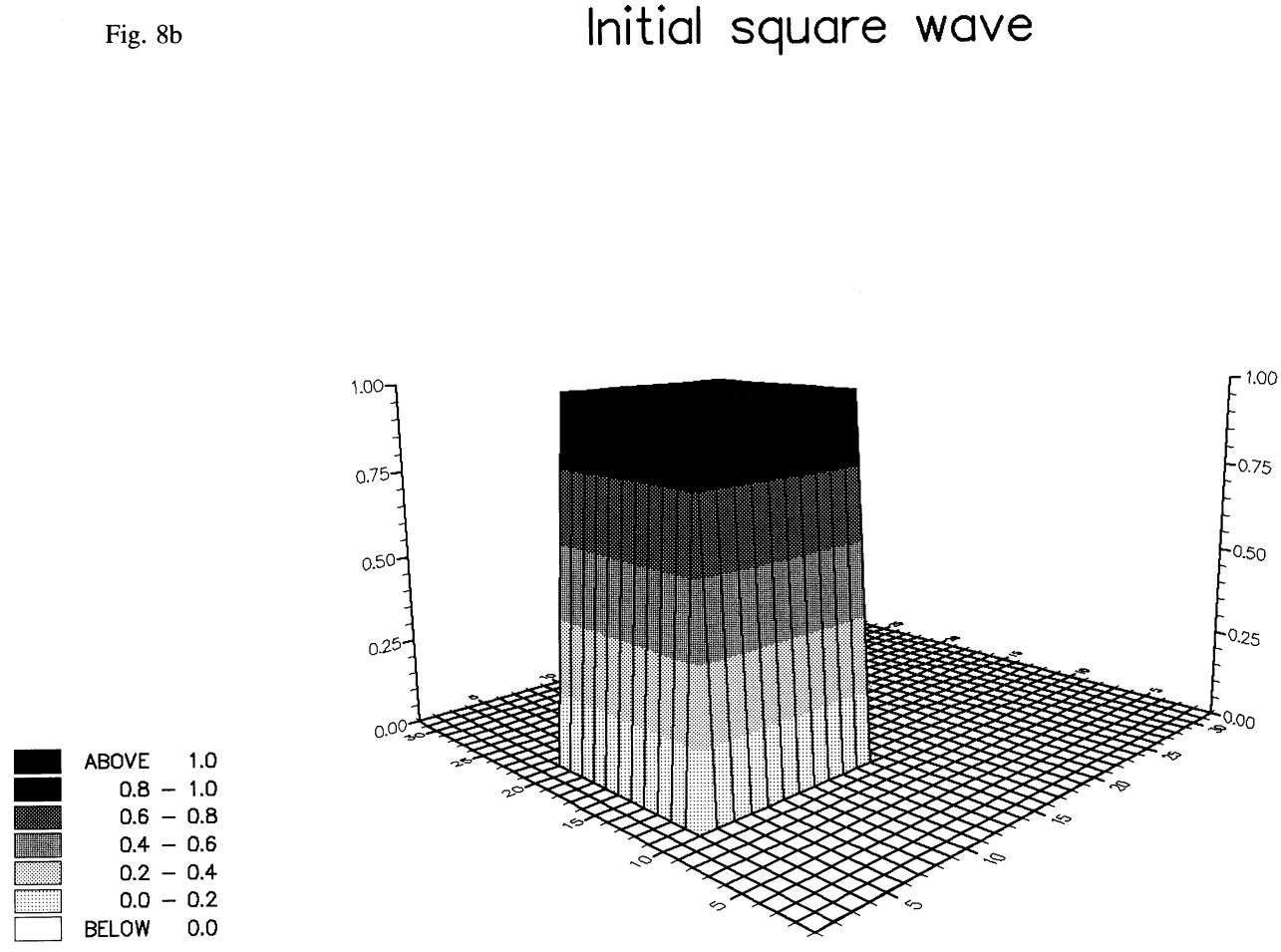

Initial square wave
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.00
0.75
0.50
0.25
0.00
5
10
15
20
25
30

Fig. 8c

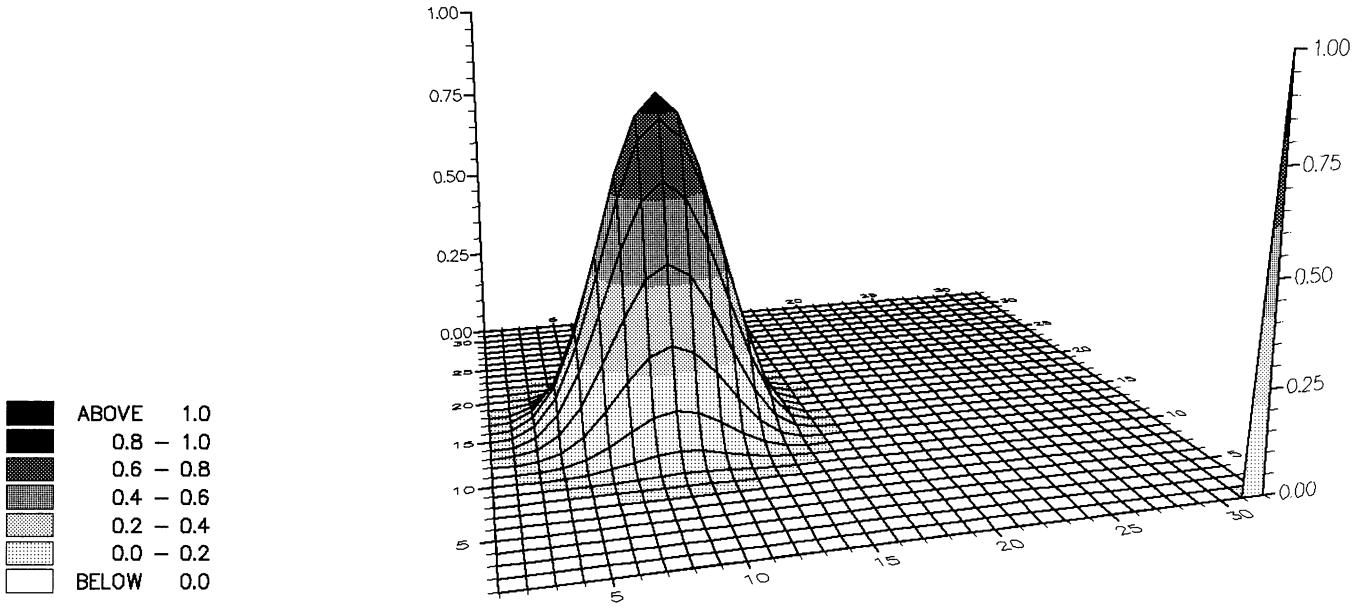

1 rotation with the BOS
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.00
0.75
0.50
0.25
0.00
5
10
15
20
25
30

Fig. 8d

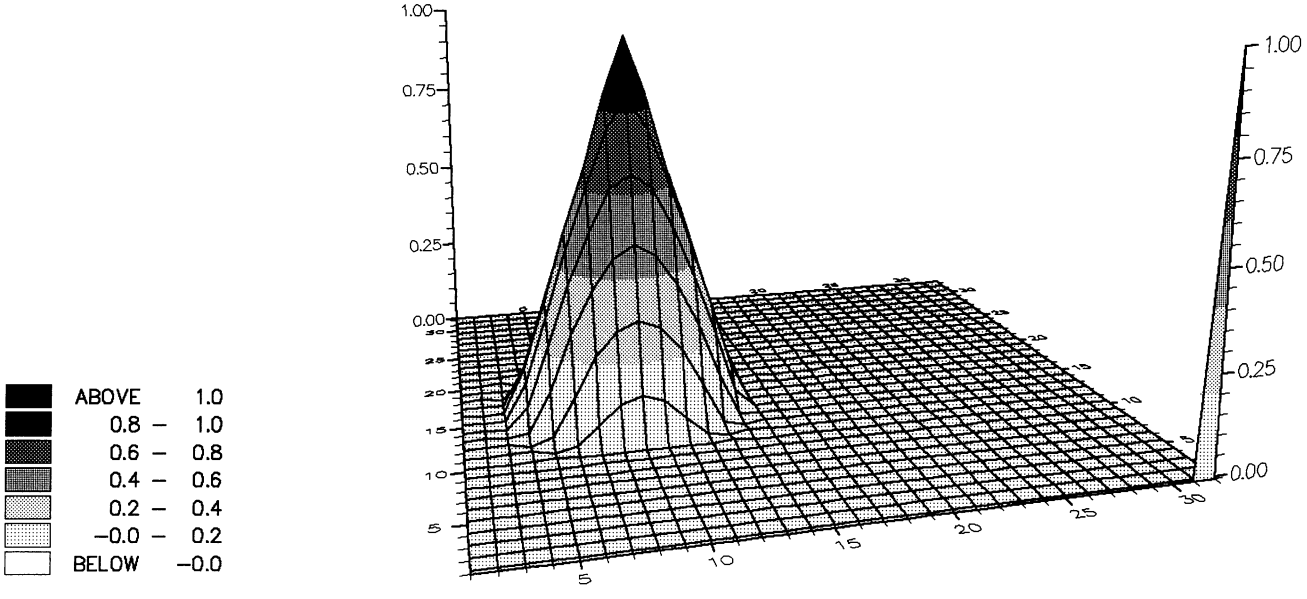

1 rotation with the PSS
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
–0.0 – 0.2
BELOW –0.0
1.00
0.75
0.50
0.25
0.00
5
10
15
20
25
30

Fig. 8e

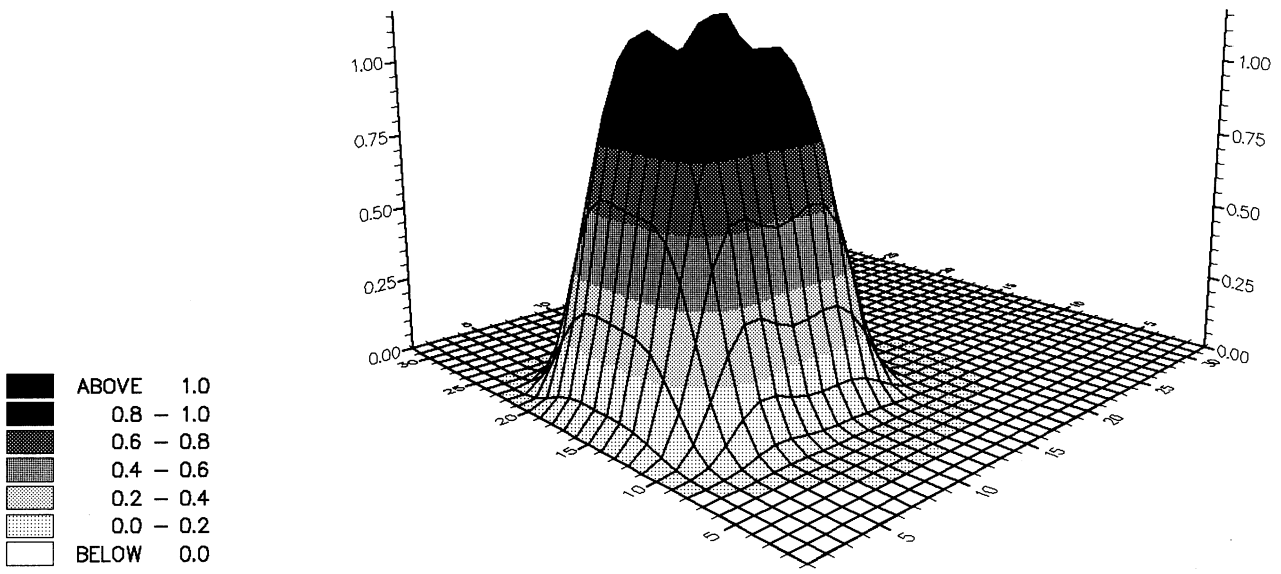

1 rotation with the BOS
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.00
0.75
0.50
0.25
0.00

Fig. 8f

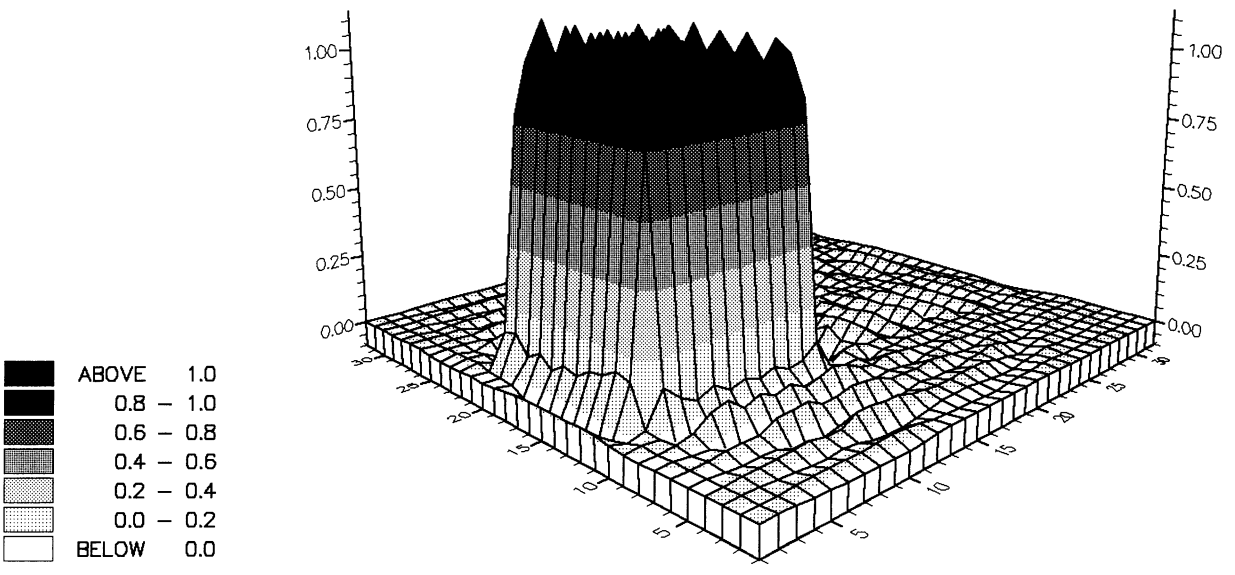

1 rotation with the PSS
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.00
0.75
0.50
0.25
0.00

Fig. 9a

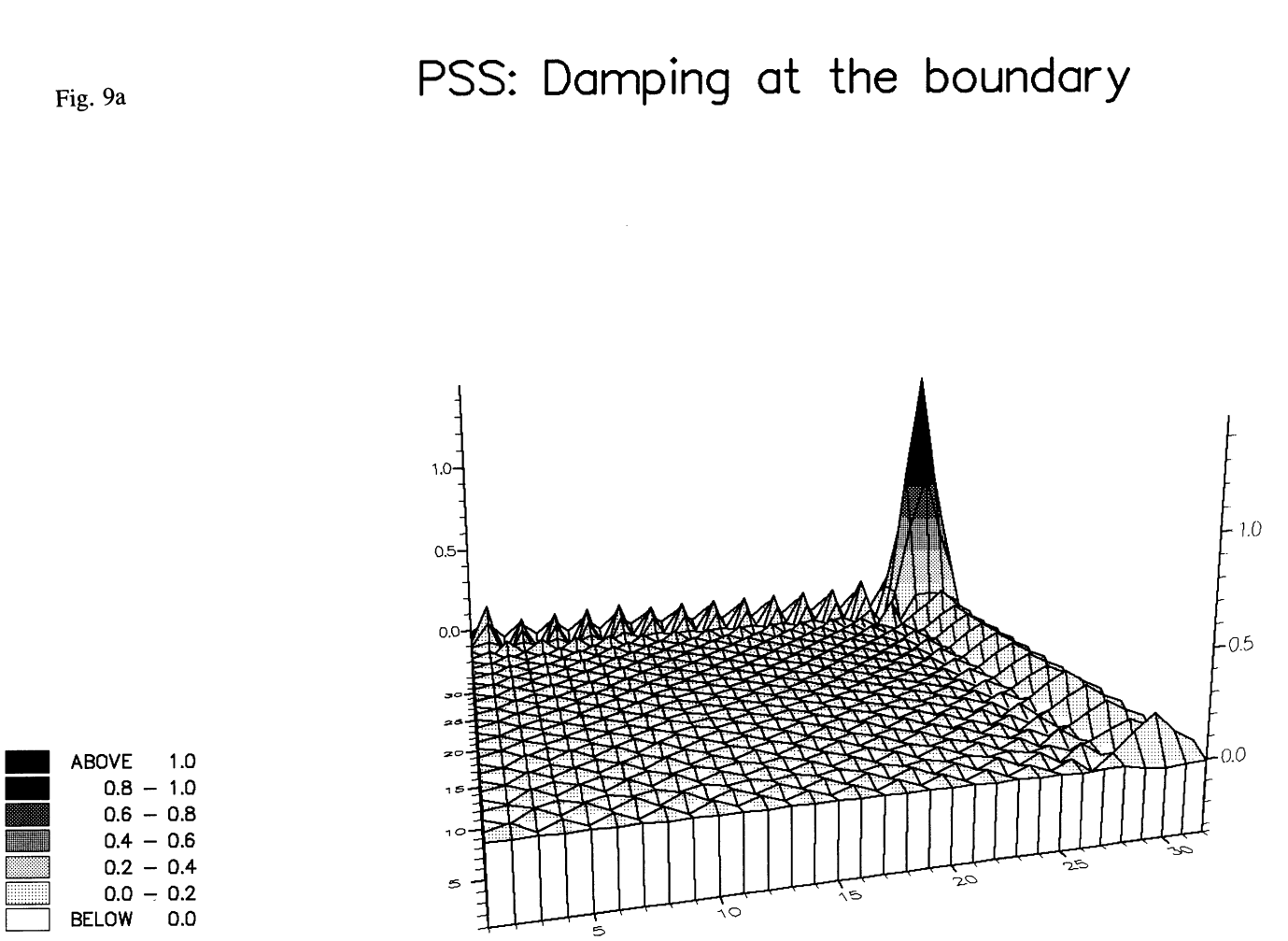

PSS: Damping at the boundary
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.0
0.5
0.0
5
10
15
20
25
30

Fig. 9b

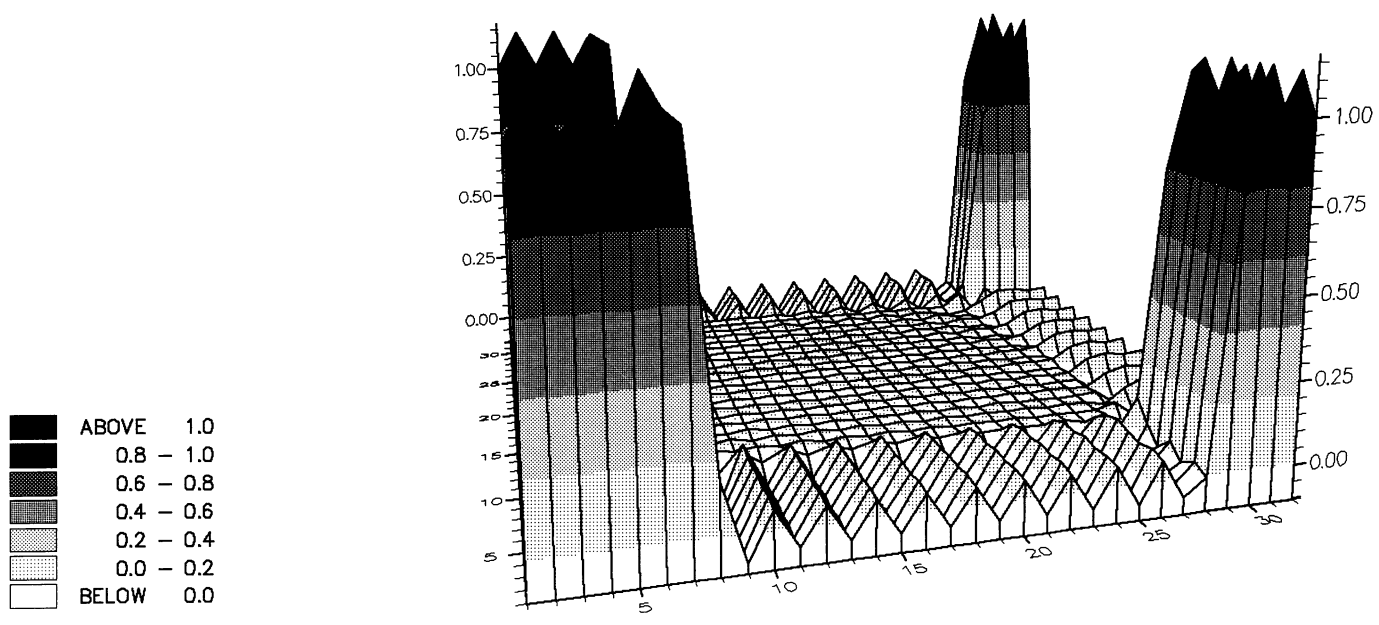

PSS: No damping at the boundary
ABOVE 1.0
0.8 – 1.0
0.6 – 0.8
0.4 – 0.6
0.2 – 0.4
0.0 – 0.2
BELOW 0.0
1.00
0.75
0.50
0.25
0.00
5
10
15
20
25
30

Fig. 9c

BOS: Boundary treatment

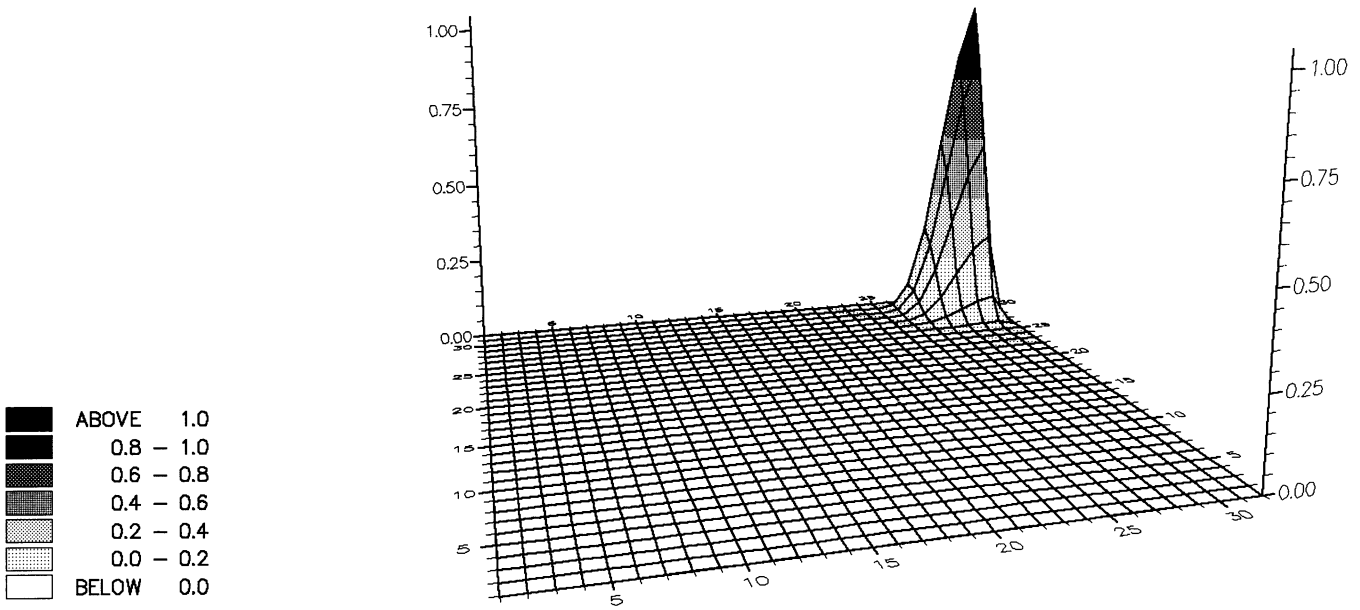


Fig. 10a

Initial isolated puff

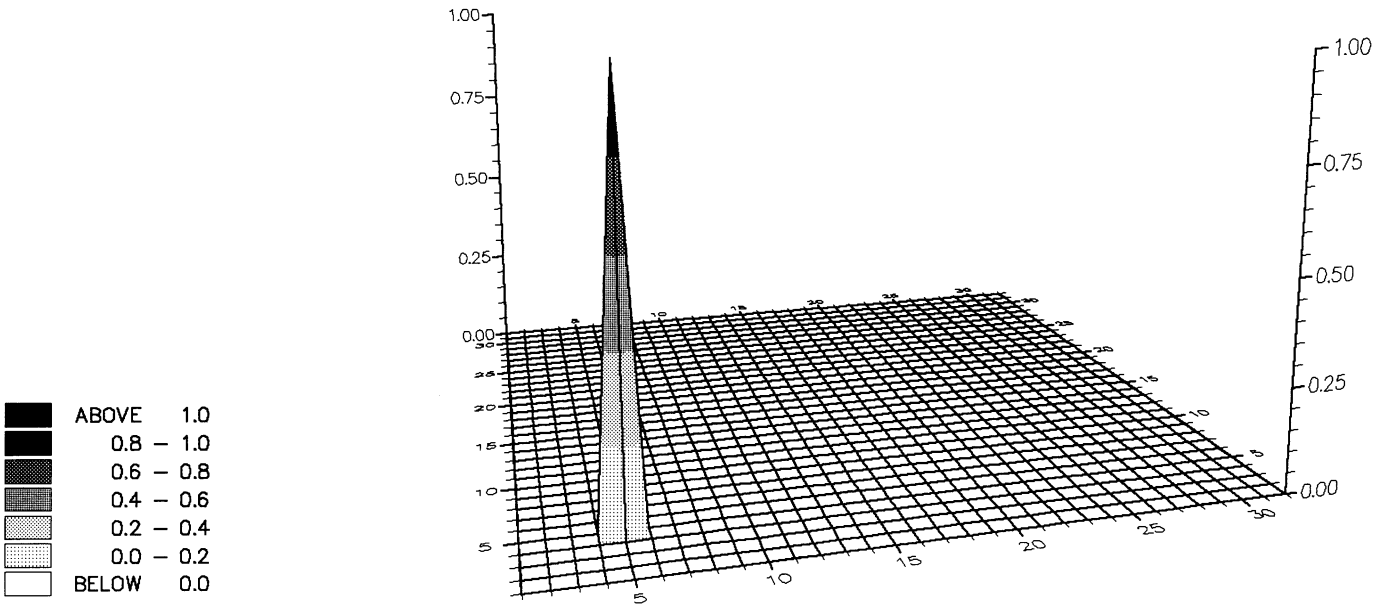


Fig. 10b

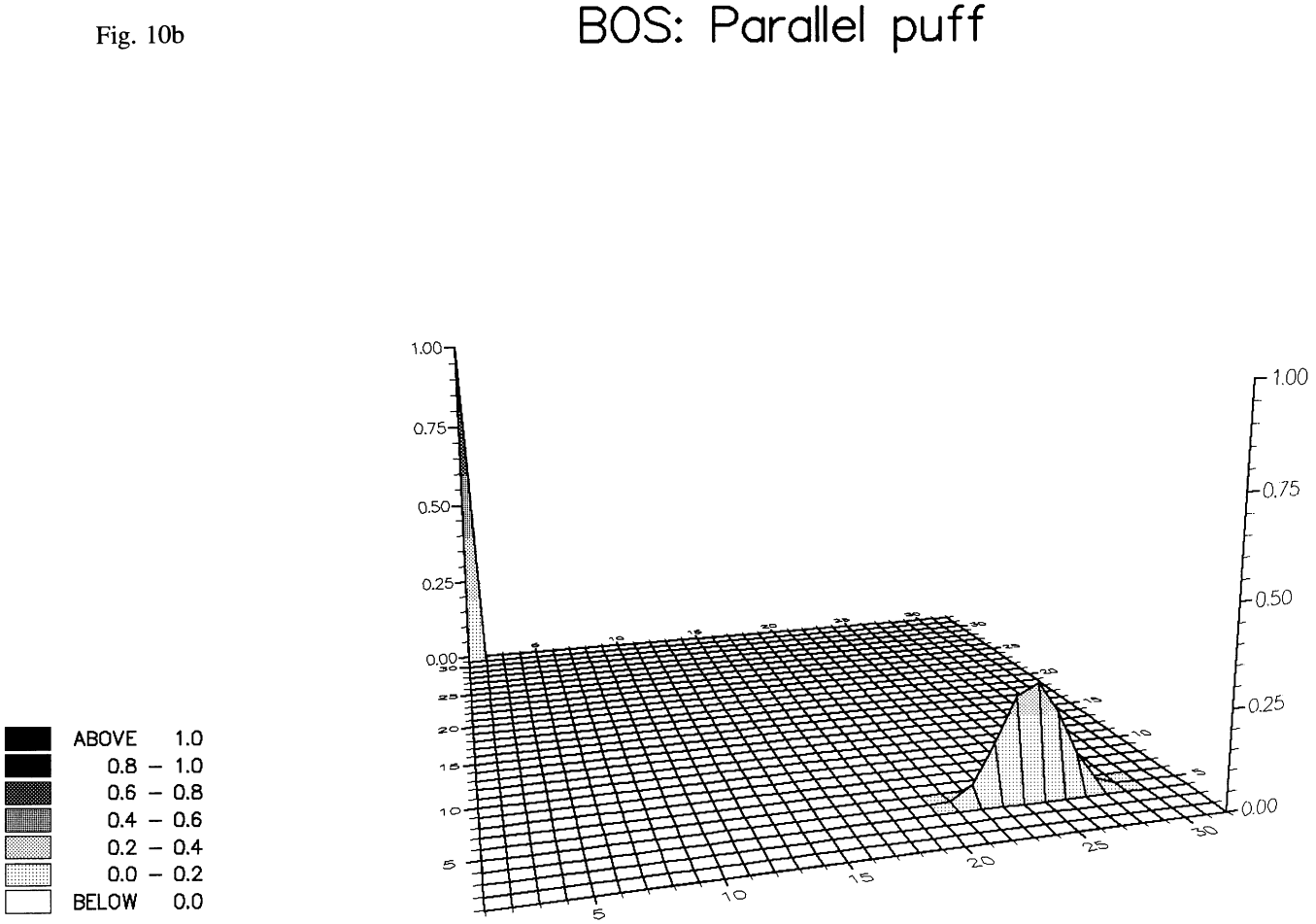


Fig. 10c

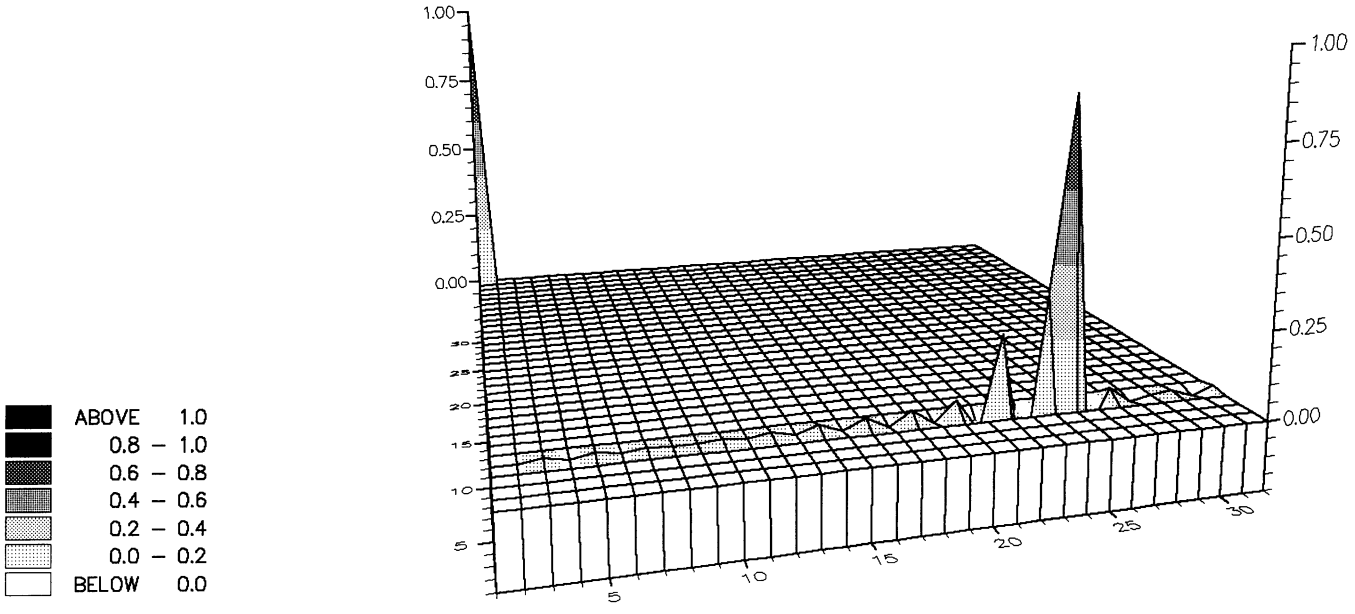


Fig. 10d

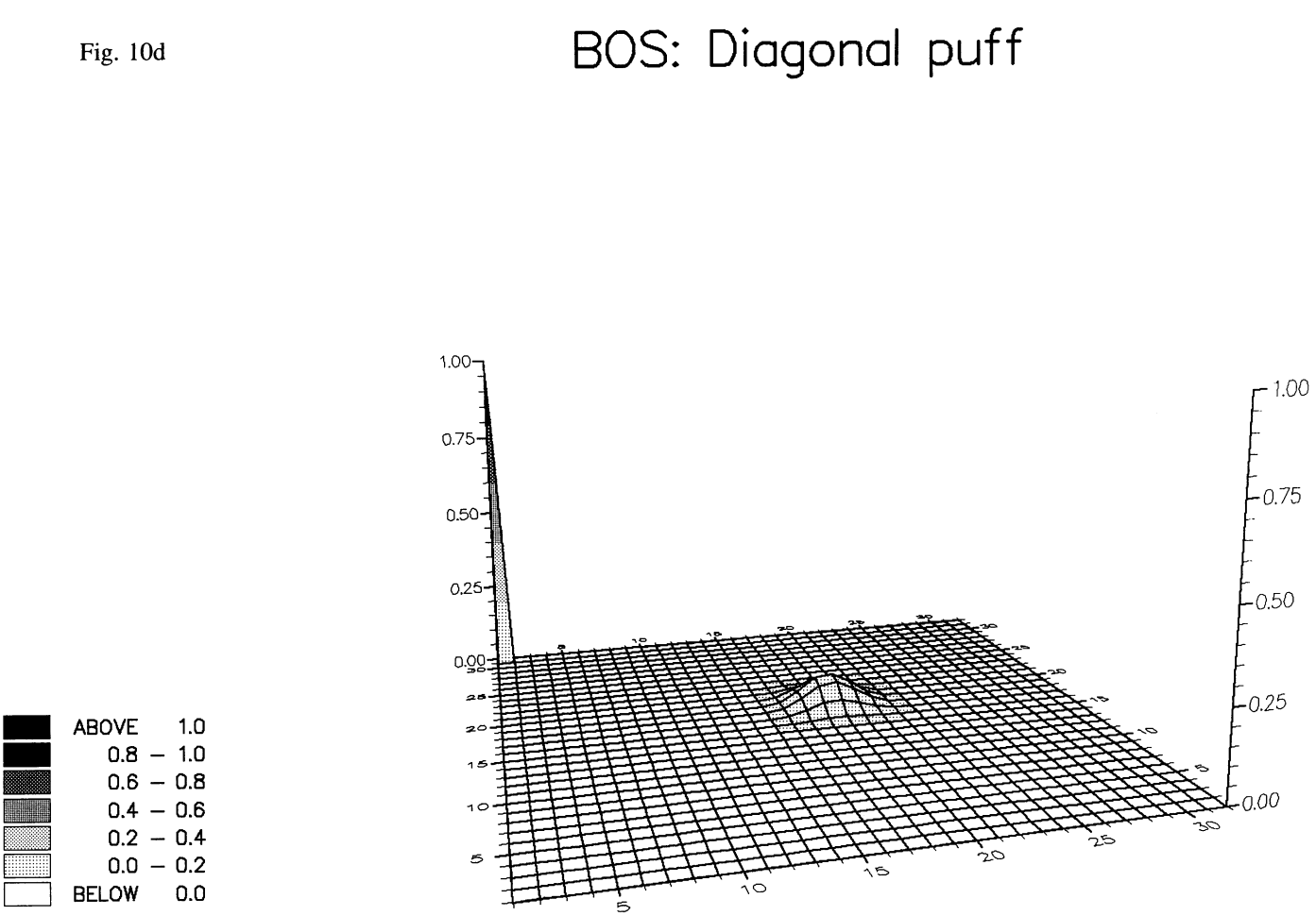


Fig. 10e

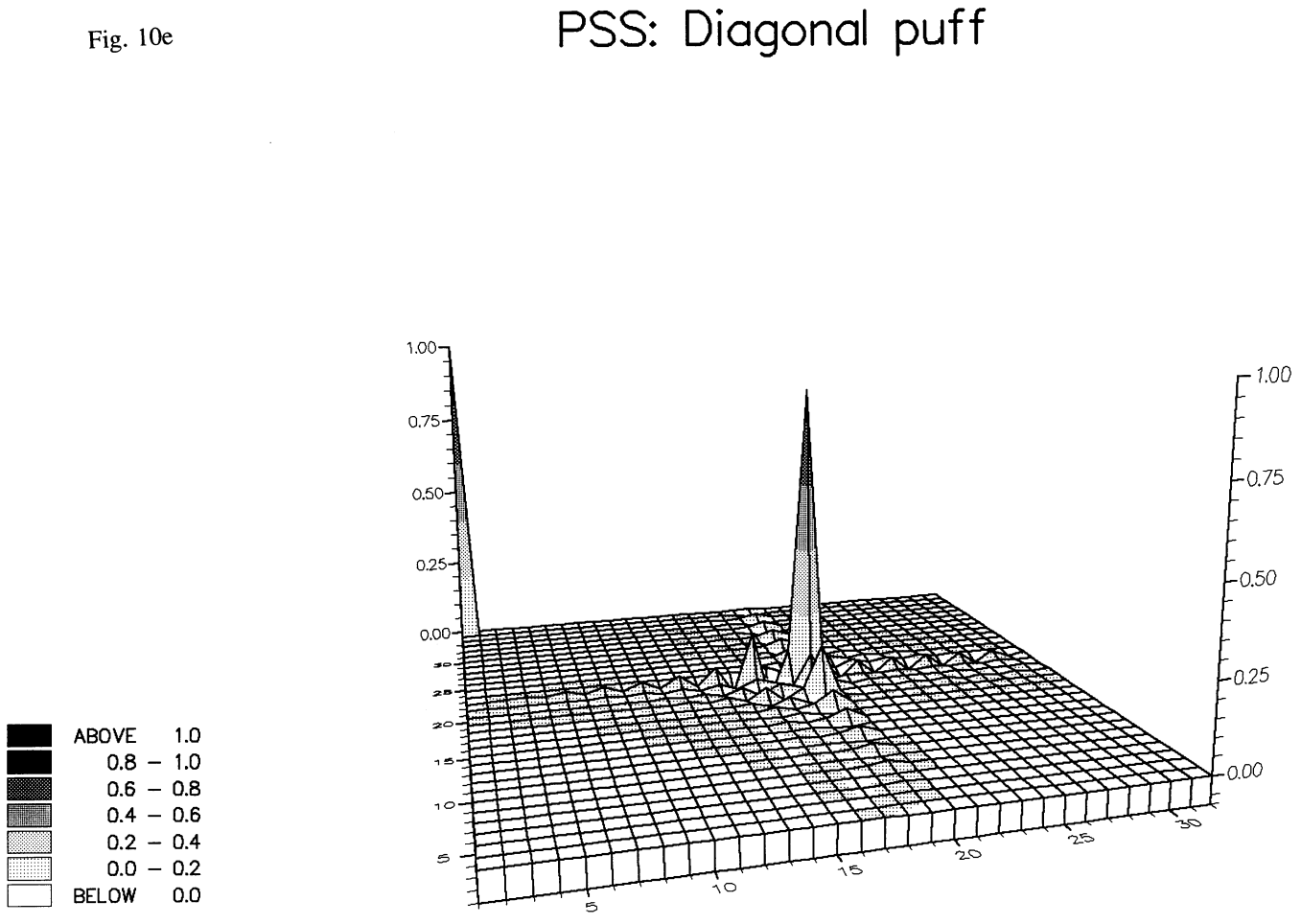


Fig. 11a

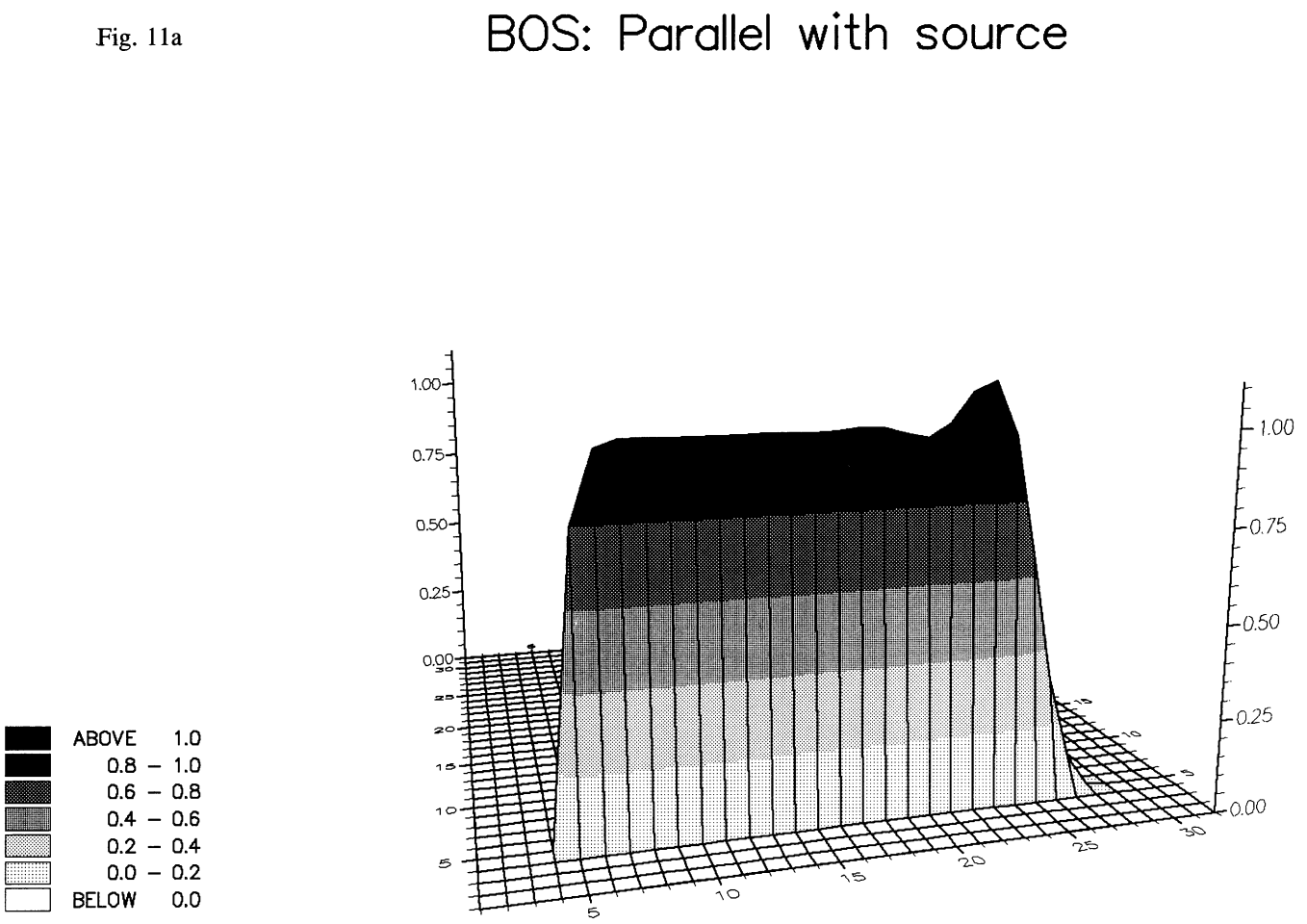


Fig. 11b

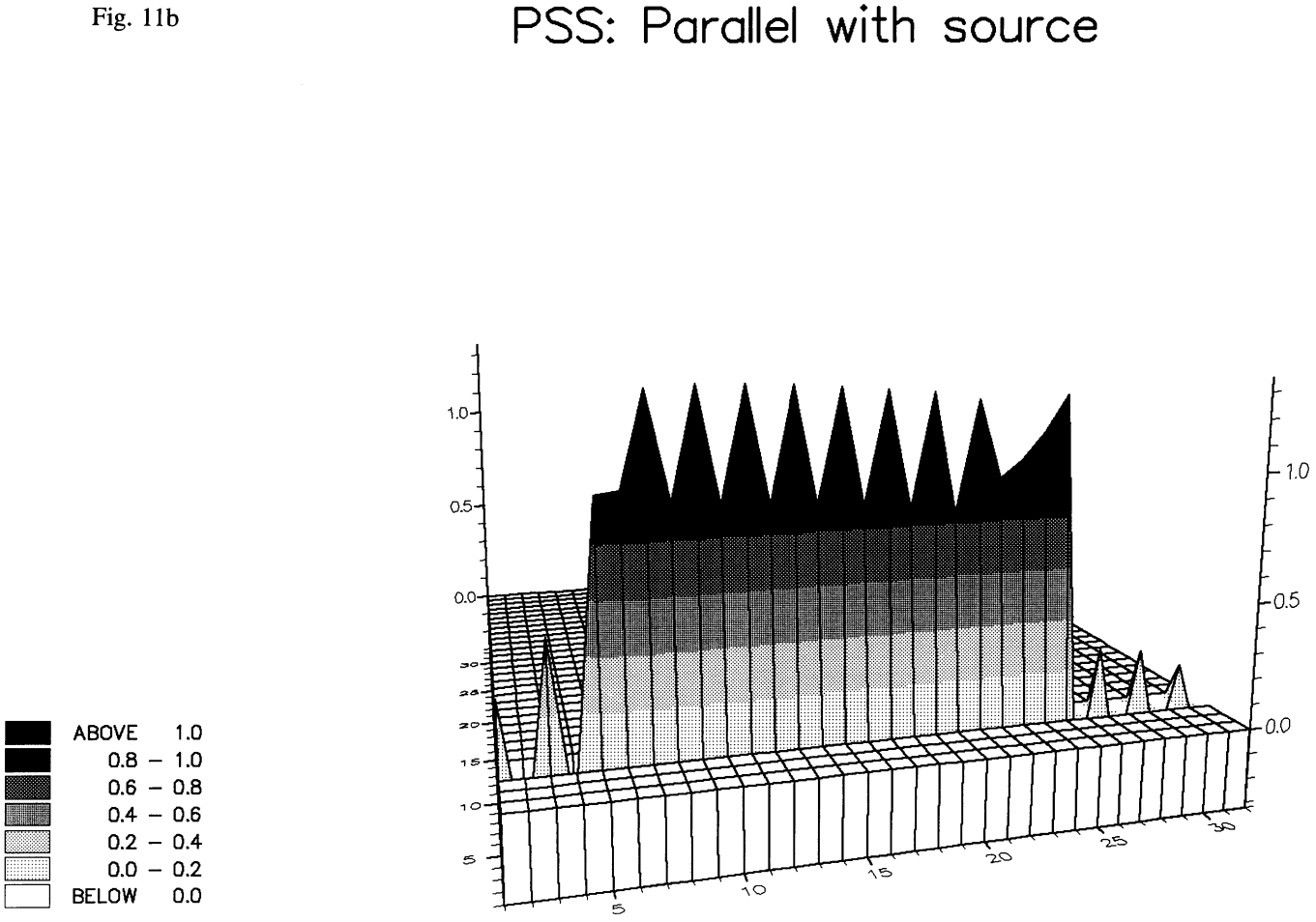


Fig. 11c

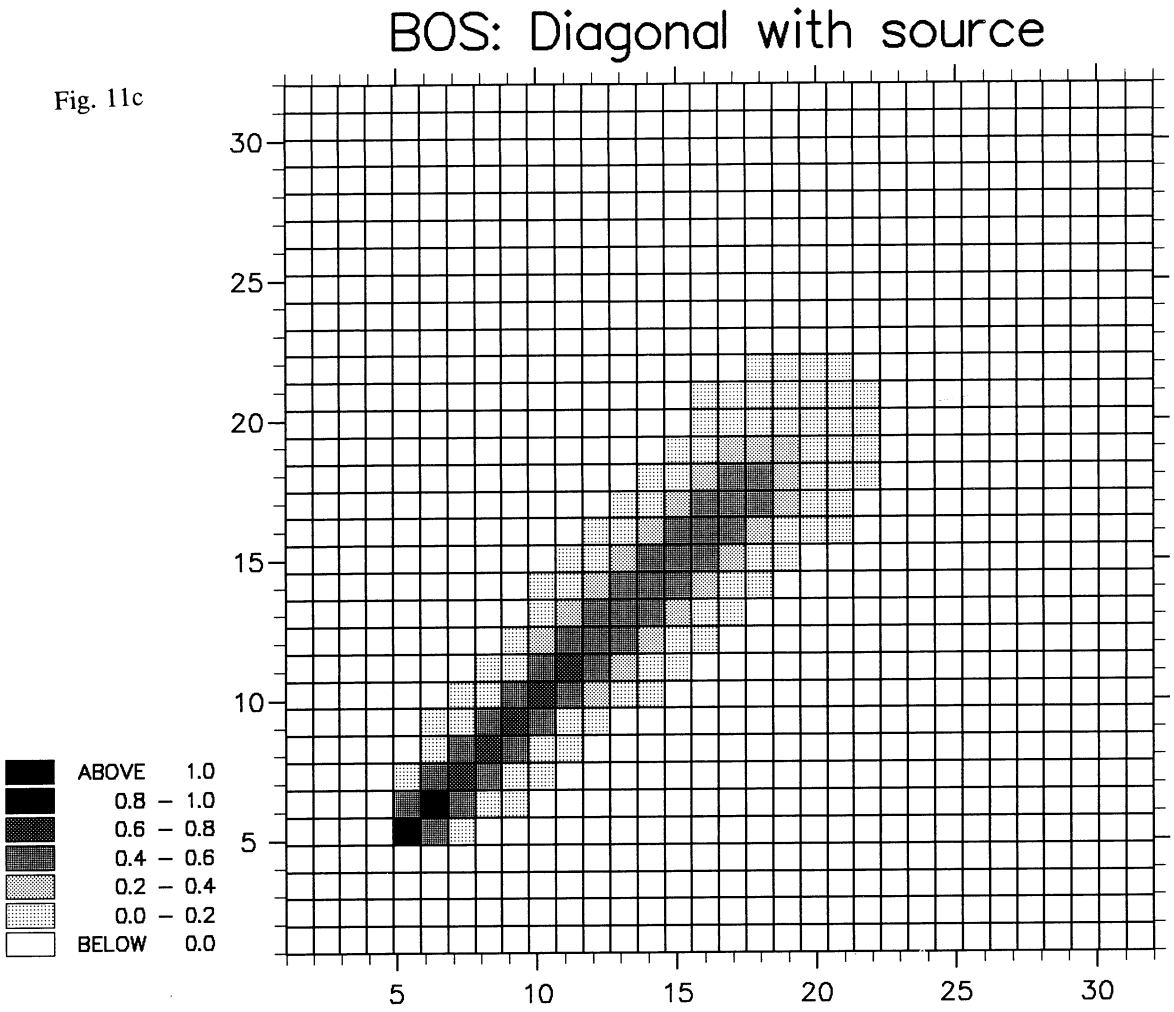


Fig. 11d

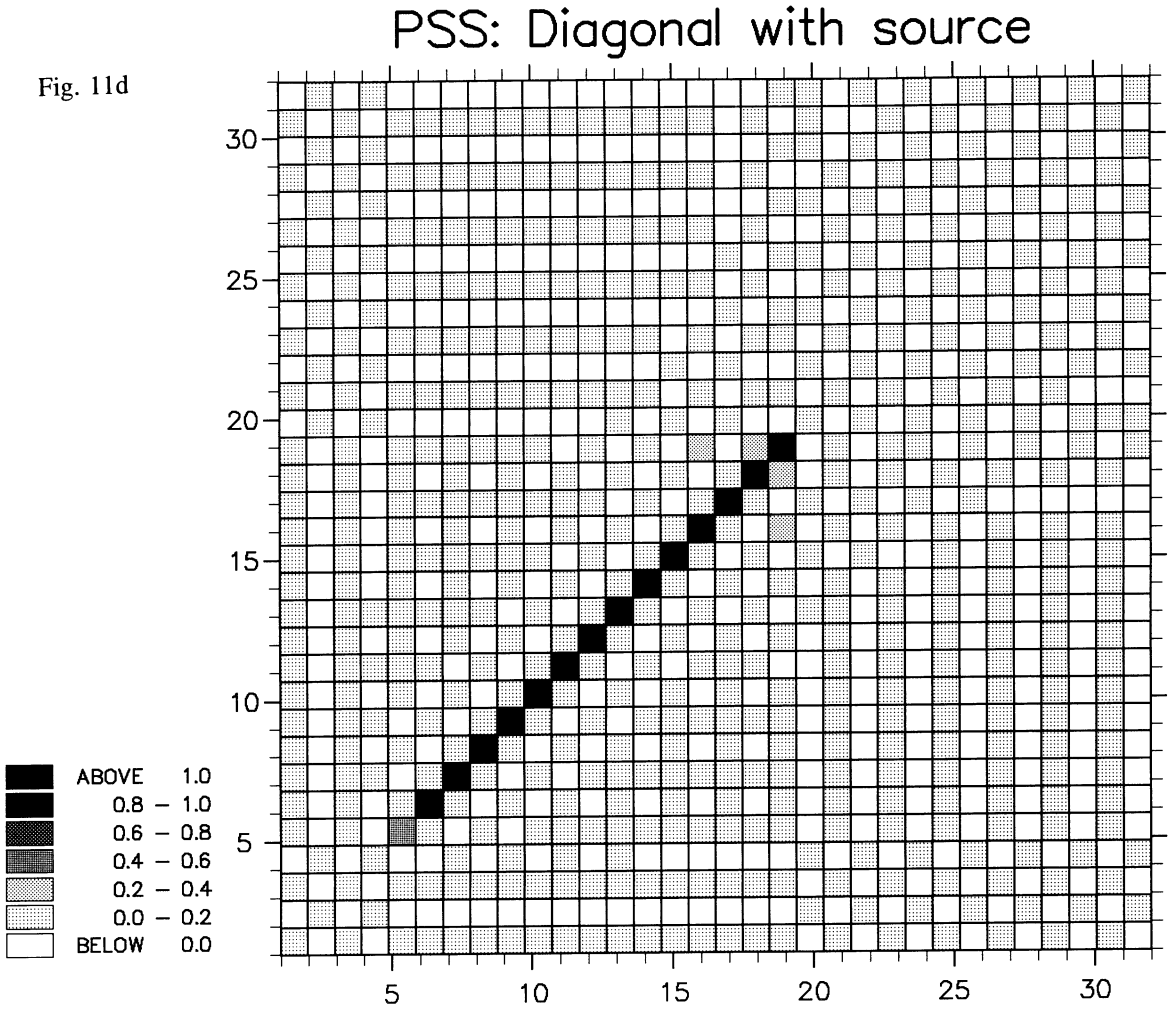


Fig. 12a

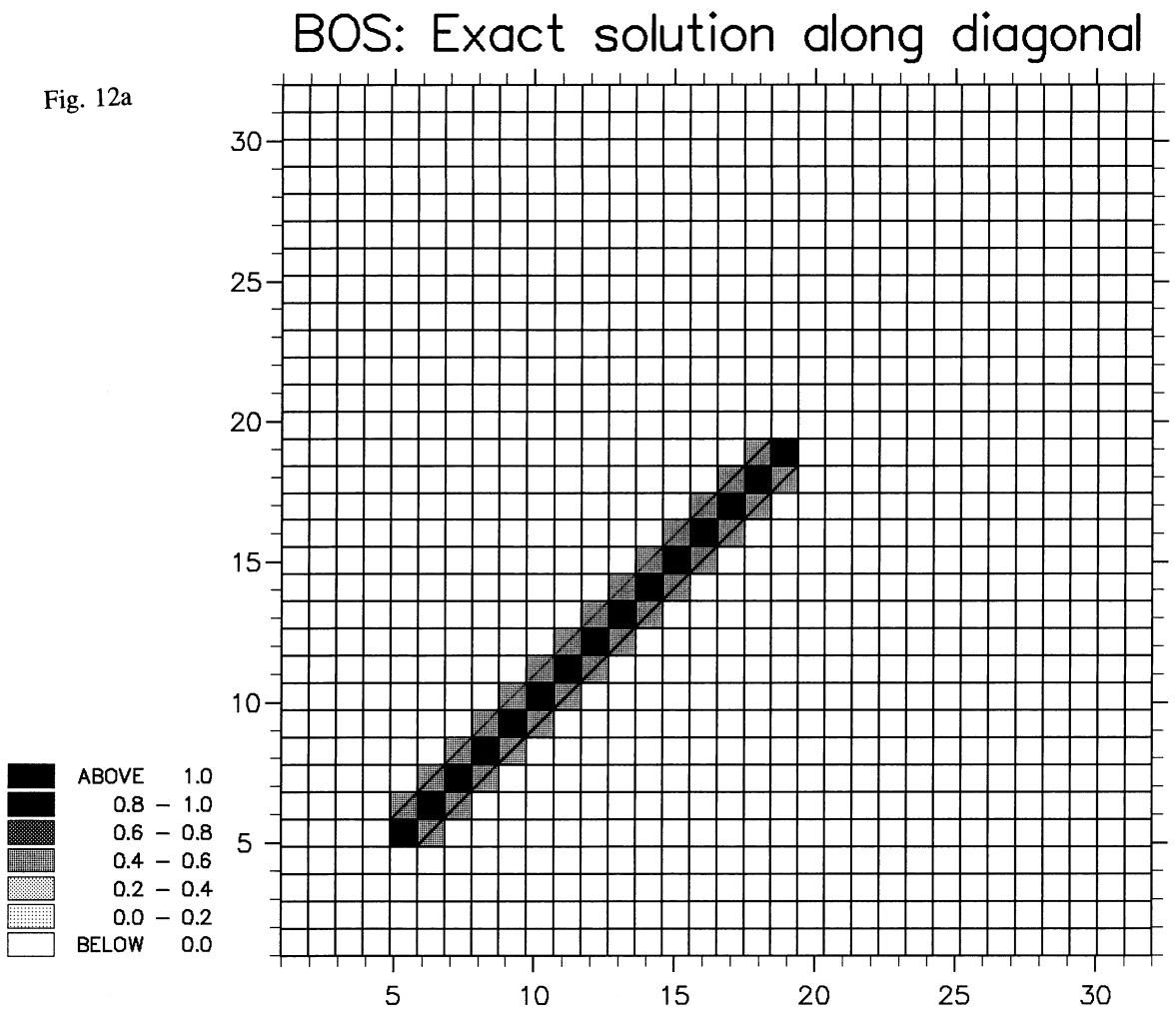
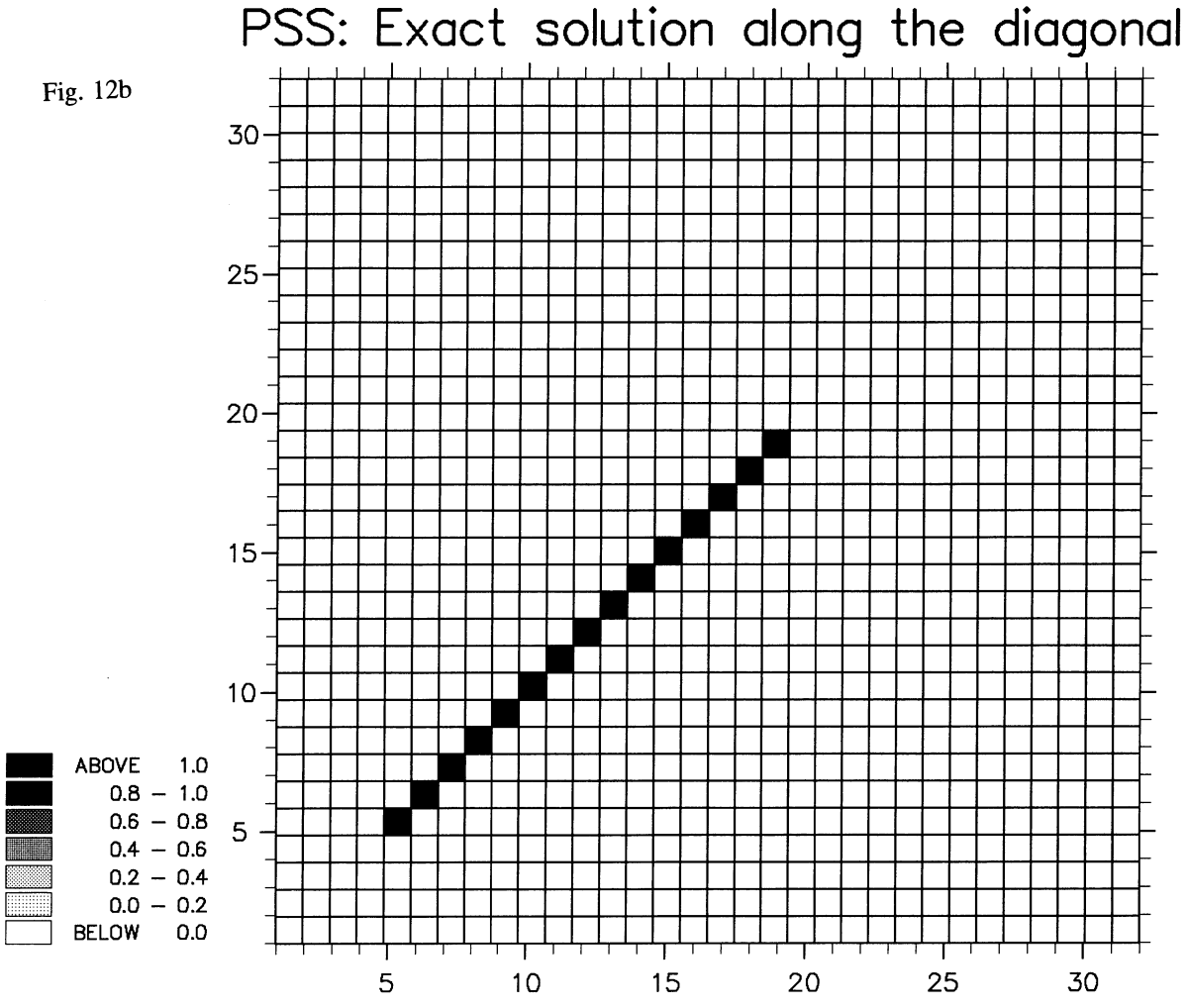



Fig. 12b