A variational modification algorithm for three-dimensional mass flux non-divergence

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SUMMARY

The diagnosed three-dimensional (3D) wind field should strictly satisfy the continuity equation; however, because of analysis, interpolation, and numerical errors this requirement is not met in practice. The resulting noise divergence is of the order of $10^{-6}$ s$^{-1}$. Its impact upon energy budgets is fatal. In order to remove the noise divergence it is suggested that a 3D minimum mean-square modifying field is added to the diagnosed wind under the constraint that the modified wind strictly satisfies mass continuity. It is shown that the solution of the resulting variational problem, namely the modifying wind field, has the property of conserving the 3D vorticity of the diagnosed wind field.

In this paper the theory proposed for modification of the diagnosed wind field is rigorously developed for the first time for both the continuous and the discrete situation. The discrete problem—its solution being referred to as variational modification algorithm (VMA)—is approached by converting the diagnosed wind field into mass fluxes across the faces of finite boxes; the modifying mass flux components are obtained as differences of a potential function being the solution of a 3D Poisson equation which—owing to consideration of mass fluxes—is free of coordinate increments. A fast direct algorithm to solve this equation through decoupling coordinate directions is presented and compared with a fast Fourier algorithm.

The VMA is applied to the wind field over Europe, as routinely analysed by the European Centre for Medium-range Weather Forecasts (ECMWF), for the specific case of the strong rain episode over central Europe on 1 August 1991. The wind is converted into mass flux components across the faces of boxes (100 km)$^2 \times 100 \text{ hPa}$ in size. The modification of the mass flux enforced by the VMA is about 7 per cent of the analysed mass flux, and 6 per cent of the initialized mass flux; this similarity suggests that the original 3D noise divergence is not in the ECMWF data (analysed or initialized), but is generated by the interpolation procedure from the ECMWF model coordinates to pressure levels. Investigation of analysed and initialized mass fluxes before and after application of the VMA reveals that the modification of the mass flux field through the initialization procedure at the ECMWF is considerably larger than the modification required to enforce non-divergence through application of the VMA.

The impact of the modification upon the imbalance of the heat budgets in the atmosphere over Europe is investigated by a diagnostic model. It is found that the VMA reduces the root-mean-square values of the sensible-heat imbalance from 518 (337) down to 66 (35) W m$^{-2}$ for analysed (initialized) input data. The reduction is less dramatic for the latent-heat imbalance (about 30 per cent).

The effectiveness of the VMA as well as its generalization to arbitrary coordinate systems and variable resolution are briefly discussed.

1. INTRODUCTION

Budgeting has been a diagnostic tool in meteorology ever since observations in the free atmosphere became available in the 1940s. First examples of comprehensive atmospheric budgets of heat and momentum include the classical studies of Priestley (1949) and Riehl et al. (1951). The climatological viewpoint dominated in this early work (e.g. Palmén and Newton 1969). Today, modern budget studies are able to resolve considerably higher time and length scales than these early studies owing to an increase in the density of observations. From the climatological global scale (e.g. Trenberth 1991; 1 month/2.8 degrees) over the meso-beta scale (e.g. Dörninger et al. 1992; 1 day/100 km), and the urban micro-alpha scale (e.g. Moussiopoulos et al. 1988; 1 hour/1 km), down to the micro-gamma scale of individual convective elements (e.g. Graf and Schumann 1991; 10 minutes/100 m), the budgeting approach has become a familiar method for investigating meteorological phenomena of increasing complexity with improving accuracy.

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A notorious stumbling-block in budgeting is the mass conservation law. The diagnosed data, namely the data obtained from the raw observations by application of an analysis/assimilation procedure, are, in general, contaminated with errors due to observational inaccuracy, lack of representativeness, and inaccurate interpolation procedures. These errors are in many cases quite small. For example, the three-dimensional (3D) noise divergence carried by the diagnosed mass flux fields available for the computations in this study—these mass fluxes were obtained by interpolation of the analyses made by the European Centre for Medium-range Weather Forecasts (ECMWF) as stored in the Meteorological Archive and Retrieval System (MARS) to the grid used here (see sections 3 and 4)—is of the order of $10^{-6}$ s$^{-1}$ (see, also, Trenberth (1991) as well as the discussion of Fig. 5 later). This noise divergence is small indeed; however, it leads to mass flux fields that are useless for diagnostic purposes, like the diagnostic study of the heat budget.

In order to illustrate the negative impact of these errors in the wind field on budget calculations, the following estimate is considered for a simple one-dimensional (1D) case assuming the use of pressure coordinates. Consider the horizontal wind field, $u(x)$, in the x-direction; $T$ denotes temperature (see Fig. 1). If the data are perfect, continuity implies:

$$ u_2 - u_1 = 0 $$  \hspace{1cm} (1.1)

and the heat flux divergence $\mathcal{D}$ is perfect:

$$ T_2 u_2 - T_1 u_1 = \mathcal{D}. $$  \hspace{1cm} (1.2)

However, for imperfect data, Eq. (1.1) is replaced by:

$$ (u_2 + \Delta u_2) - (u_1 + \Delta u_1) = \Delta u $$  \hspace{1cm} (1.3)

where $\Delta u$ represents the erroneous divergence that is implied through the diagnosed mass flux field containing the errors $\Delta u_2$ and $\Delta u_1$. Likewise, in the case of imperfect data, the diagnosed estimate of the heat flux divergence comprises the true signal $\mathcal{D}$ plus an erroneous heat flux divergence. This may be seen by introducing temperature errors $\Delta T_1$ and $\Delta T_2$ into (1.2), and simplifying the result by neglecting nonlinear terms:

$$ (T_2 + \Delta T_2)(u_2 + \Delta u_2) - (T_1 + \Delta T_1)(u_1 + \Delta u_1) $$

$$ = (T_2 u_2 - T_1 u_1) + (T_2 \Delta u_2 - T_1 \Delta u_1) + (u_2 \Delta T_2 - u_1 \Delta T_1). $$  \hspace{1cm} (1.4)

The numbers shown above have units of K m s$^{-1}$ and are obtained by assuming a relative error of 1% and 10% for $T$ and $u$ respectively:

$$ T = 250 \text{ K} \quad \Delta T = 2.5 \text{ K} $$

$$ T_1 = T - 2\Delta T \quad T_2 = T + 2\Delta T $$

$$ u = 25 \text{ m s}^{-1} \quad \Delta u = 2.5 \text{ m s}^{-1} $$

$$ u_1 = u \quad u_2 = u. $$  \hspace{1cm} (1.5)

Thus the perfect gradient of $T$ from $x_1$ to $x_2$ is assumed to be $4\Delta T = 10$ K, which is a conservative estimate for temperature gradients in the atmosphere over a horizontal distance of, say, 2500 km. These assumptions justify the approximations $T_2 \Delta u_2 - T_1 \Delta u_1 = T \Delta u$ and $u_2 \Delta T_2 - u_1 \Delta T_1 = u(\Delta T_2 - \Delta T_1) \approx u \Delta T$ made in Eq. (1.4).

This example demonstrates that the error of $\mathcal{D}$ is potentially larger than the signal, governed by the error of $u$, and not governed by the error of $T$. The reason for the two
latter statements is that the relative wind error is usually larger than the relative temperature error. This simple estimate demonstrates further that adjusting the diagnosed wind field for $\Delta u = 0$ enforces two conditions at once, namely mass conservation, and minimization of the error of the heat flux divergence. Similar results are obtained if budgets of moisture or tracers are considered. Note, further, that the argument presented is not restricted to one dimension, but applies also in three dimensions.

The problem illustrated does not disappear if the advective form (e.g. Nitta 1977; Luo and Yanai 1983, 1984) of the heat equation is used instead of the flux form. In that case the continuity equation must be satisfied as a separate requirement, whereas it is implicitly assumed to be correct when the equations are written in flux form. In addition, use of the advective form may be considered to be disadvantageous in diagnostic studies in the sense that the Gaussian theorem cannot any longer be used for finite volumes.

Referring back to Eq. (1.4), it appears possible to minimize the impact of $\Delta u$ on the estimation of $\Theta$ by substituting for $T$ a temperature deviation $T - T_0$, where $T_0$ is an externally specified global constant. Although this trick appears helpful and does, in fact, reduce the error component $T \Delta u$ by about one order of magnitude (e.g. Hantel 1976), it does not really solve the problem.

It is the purpose of this paper to present a general methodology to solve the problem in the sense that it allows one to modify a given diagnosed wind field such that it becomes strictly non-divergent. (With reference to the continuity equation in pressure coordinates a wind field strictly satisfying mass continuity is also denoted as strictly non-divergent.) The methodology presented starts with a given 3D mass flux field—to be denoted as diagnosed mass flux field—which is not strictly non-divergent. All questions concerning the origin, significance, or quality of the diagnosed mass flux field, or those concerning the actual source of the noise divergence, shall be considered irrelevant. In addition to the specification of the diagnosed 3D mass flux field over a given domain, the a priori assumption is made that the domain average of its divergence vanishes. The notion of divergence is used here in the sense of a divergence integrated over finite mass boxes by making use of the Gaussian theorem. This implies that the divergence is the difference of respective mass flux components. In other words, details about the properties of the boxes of integration, like their shape or size, for which the individual mass flux components are representative are not specified (see also section 3).
Specifically, the question addressed is: How can the noise divergence be unambiguously removed from the diagnosed mass flux field? The following answer is proposed: Choose a modifying mass flux field and add it to the diagnosed field, thereby generating the modified mass flux field. The following three properties are required to be satisfied by the modifying field: it shall (i) exactly remove the diagnosed noise divergence, (ii) be specified at the boundaries of the domain, and (iii) be minimum in a root-mean-square (r.m.s.) sense (see section 2). It is demonstrated in sections 2 and 3 that there exists a unique solution with desirable meteorological properties. Even though the problem stated has long been recognized and has been partially solved in previous studies (see below), a fully coherent and complete theory for both the discrete and the continuous situation has been lacking; it is presented here for the first time.

The question formulated above was, to the knowledge of the authors, first investigated by Hacker (1981). Since the approach taken by Hacker (1981) resembles some of the properties of the general methodology presented here, his solution to the problem is outlined below for a simple example in terms of four basic steps (see Fig. 2). In Fig. 2 four adjacent two-dimensional (2D) atmospheric boxes are considered that are arranged in two layers (upper and lower) and two columns (northern and southern). This arrangement also serves as a skeleton version of the more general set-up described in sections

Figure 2. Conceptual example for variational modification of a diagnosed mass flux field to enforce strict nondivergence. Suggested interpretation of coordinates: horizontal = y, vertical = z. (a) Diagnosed horizontal and vertical mass flux components (units arbitrary) across faces of two hypothetical adjacent atmospheric columns each divided vertically into two boxes. Numbers in circles: diagnosed mass flux divergence. (b) Same as (a), but with modifying fluxes a, b, c, and d across inner faces. Modifying fluxes are to be determined such that the modified divergence vanishes in all four boxes under the constraint that a, b, c, and d are minimum in an r.m.s. sense. (c) Result of executing (b). The modified mass flux field is non-divergent for all four boxes. Further, the circulation around the centre of the array (8 units) is the same as in (a). (d) Result of subtracting 12 flux units in the upper and 3 units in the lower layer. This leaves all divergences unchanged but reduces shear in the vertical direction. Consequently, the circulation around the centre of the array is changed down to −1 unit. Notation of arrows is such that positive values go in the arrow direction, while negative values go opposite. (e) Nomenclature for expressing modifying mass fluxes with mass flux potential. Potential χ is defined for each box. For example: \( a = \chi_a - \chi_b \), \( b = \chi_a - \chi_b \), etc. The values of χ in boxes are the field values to be determined. The values outside the array are the boundary values. (f) Result of determining potential and modifying mass fluxes. It is equivalent to the results shown in panel (c).
2 and 3. The upper surface of the upper layer is assumed to be impermeable, as is the lower boundary of the lower layer. The northern and southern boundaries are assumed to be permeable with the constraint that the entire array is non-divergent (see also the preceding paragraphs; if this is not the case in practice it has to be enforced at the beginning).
(i) Diagnosed fluxes (Fig. 2(a)). The diagnosed fluxes are not exactly consistent (i.e. non-divergent), but show some noise divergence; for example, \( 15 - 12 + 0 - 0 = 3 \) units remain in the upper northern box.

(ii) Modifying fluxes (Fig. 2(b)). Upon introducing the modifying mass fluxes \( a, b, c, \text{ and } d \) into the mass budget, the following conditions must be satisfied to enforce non-divergence:

\[
\begin{align*}
(15) - (12 + a) + (0) - (0 + b) &= 0 \\
(0) - (5 + c) + (0 + b) - (0) &= 0 \\
(5 + c) - (5) + (1 + d) - (0) &= 0 \\
(12 + a) - (10) + (0) - (1 + d) &= 0.
\end{align*}
\] (1.6)

However, these modifications cannot be calculated unambiguously from (1.6) because the pertinent determinant vanishes. The reason is that one of the four equations in (1.6) is redundant. For example, adding the first three yields the fourth.

(iii) Minimum modification. In order to deal with the redundancy in step (ii), Hacker (1981) introduces the condition:

\[
\frac{1}{2} (a^2 + b^2 + c^2 + d^2) = \text{minimum}
\] (1.7)

which is satisfied if the first variation of the left-hand side vanishes:

\[
a \delta a + b \delta b + c \delta c + d \delta d = 0.
\] (1.8)

The first variation of system (1.6):

\[
\begin{align*}
- \delta a - \delta b &= 0 \\
- \delta c + \delta b &= 0 \\
\delta c + \delta d &= 0 \\
\delta a - \delta d &= 0
\end{align*}
\] (1.9)

may be used to eliminate in Eq. (1.8) all variations of the modifying mass fluxes except one. For example, expressing all variations in (1.8), in terms of \( \delta a \), leads to:

\[
(a - b - c + d) \delta a = 0
\] (1.10)

which is equivalent to:

\[
a - b - c + d = 0.
\] (1.11)

Use of Eq. (1.11), together with three equations arbitrarily selected from the system (1.6), yields the following non-singular system for the modifications:

\[
\begin{pmatrix}
-1 & -1 & 0 & 0 \\
0 & 1 & -1 & 0 \\
0 & 0 & 1 & 0 \\
1 & -1 & -1 & 1
\end{pmatrix}
\begin{pmatrix}
a \\
b \\
c \\
d
\end{pmatrix}
=
\begin{pmatrix}
-3 \\
5 \\
-1 \\
0
\end{pmatrix}.
\] (1.12)

The column vector on the right-hand side in Eq. (1.12) contains as elements the negative box divergences of Fig. 2(a), except, of course, for the last element. The solution of (1.12) is (see Figs. 2(c) and 2(d)):

\[
a = 0, \quad b = 3, \quad c = -2, \quad d = 1.
\] (1.13)
The modified mass fluxes shown in Fig. 2(c) are strictly non-divergent. Further, enforcement of condition (1.7) has not changed the circulation, as may be checked by comparing the circulations in panels (a) and (c). Thus, in more meteorological terms, the modification performed keeps the diagnosed vorticity constant, which is equivalent to condition (1.11).

(iv) Circulation modification (Fig. 2(d)). The circulation of the mass flux field is changed by subtracting a total of 9 units of shear circulation (12 units in the upper and 3 units in the lower layer). Naturally, the fluxes obtained thereby are still non-divergent. In addition, these fluxes would be the result of enforcing non-divergence if the circulation were modified in that way in panel (a) before performing steps (ii) and (iii).

The result suggested by steps (i)–(iv) in the example considered has been generalized by Hacker (1981) in an investigation of the mass and heat budget of the northern atmosphere divided into an array of $4 \times 4 \times 12$ boxes of equal mass. This generalization, named integral correction technique, describes a modification algorithm of an externally specified 3D mass flux field such that every single box is individually non-divergent after the modification, while the modifying circulations between adjacent boxes are zero. Hacker (1981) demonstrated that the integral correction technique yielded a meteorologically reasonable solution for the modifying mass flux field.

Hantel and Haase (1983) compared the integral correction technique with two other modification techniques (one of them equivalent to the reduction of the transported field by one global constant as discussed above). They applied these techniques in the context of the zonal heat budget of the northern atmosphere and showed that the integral correction technique gave the best results. However, neither Hacker (1981) nor Hantel and Haase (1983) proved that enforcing non-divergence subject to (1.7) leaves the circulation unchanged, except for the simple example of Fig. 2.

However, Hantel and Haase (1983) proved this result for the continuous case in a preliminary manner. They showed that the noise divergence of the diagnosed wind field can be removed in a minimum r.m.s. sense by adding a uniquely defined irrotational vector field with opposite divergence that is the gradient of a velocity potential (see also Hantel 1986). Independently, Moussiopoulos and Flassak (1986) suggested, for the continuous case, that minimizing the modification can be achieved by requiring vorticity conservation.

Hantel (1986) applied the continuous result (without proof) to the discrete mass flux case. In the context of Fig. 2 his approach can be described by continuing steps (i)–(iv) with the two following steps:

(v) Mass flux potential. The unknown modifying mass fluxes $a$, $b$, $c$, and $d$ are expressed in terms of differences of a potential $\chi$ as (see Fig. 2(c)):

$$\chi_a - \chi_d = a; \quad \chi_a - \chi_b = b; \quad \chi_b - \chi_c = c; \quad \chi_c - \chi_e = d. \quad (1.14)$$

By inserting Eq. (1.14) into (1.12) the corresponding algebraic system for the $\chi$'s is obtained as:

$$\begin{pmatrix} -2 & 1 & 0 & 1 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \chi_a \\ \chi_b \\ \chi_c \\ \chi_d \end{pmatrix} = \begin{pmatrix} -3 \\ -5 \\ 1 \\ 0 \end{pmatrix}. \quad (1.15)$$
This replacement of the modifying fluxes by differences of a potential may be compared with the following procedure. In each box of Fig. 2(e) the 2D discrete Laplacian applied to \( \chi \) is set equal to the negative diagnosed divergence in this box. According to this procedure, the following equation:

\[
\chi_a + \chi_b + \chi_d - 4\chi_a = -3
\]

(1.16)

is obtained, for example, for the upper northern box by incorporating staggered Neumann boundary conditions; this is schematically indicated in Fig. 2(e). This procedure does indeed lead to the same set of equations for the \( \chi \)'s as given by Eq. (1.15), except for the last one. The last line of (1.15) expresses the condition that one of the \( \chi \)'s, or, equivalently, the mean potential, is arbitrary.

(vi) **Solution.** The solution for the potential \( \chi \), and the corresponding modifying fluxes, are shown in Fig. 2(f). The mean potential is set to zero. As expected, the results given in panel (f) agree with the results of step (iii).

The above discussion of previous approaches to the problem of enforcing non-divergence shows clearly the need to present a coherent, straightforward, and theoretically satisfactory methodology capable of solving the problem. It is the purpose of this paper to present such a methodology and to indicate its potential benefits in the context of high-resolution budgeting studies.

In section 2 a rigorous variational derivation is presented for the enforcement of non-divergence in the continuous situation. In section 3, which is the core of this study, an equivalent, and closely related, methodology is presented for the box-integrated discrete case. It is shown that the modifying fluxes are simply expressed as the differences of the Lagrange multipliers appearing in a minimum mean-square condition. The resulting modifying algorithm is denoted as variational modification algorithm (VMA). In section 4 the benefits of making the diagnosed mass flux non-divergent by application of the VMA are illustrated in the context of latent- and sensible-heat budgets in columns over Europe for the rain-storm episode of 1 August 1991. Some conclusions and implications of this work for future budgeting studies are discussed in section 5. The appendices are devoted to some relevant numerical details. Appendix A describes a fast Poisson solver based on a 3D reduction method denoted as decoupling method. Appendix B compares the performance of the decoupling method with a Poisson solver based on the fast-Fourier-transform method.

2. **THE CONTINUOUS PROBLEM: VARIATIONAL WIND FIELD MODIFICATION**

This section describes a variational algorithm proposed to remove any spurious noise divergences from the wind field. This modifying algorithm has been described by Hantel and Haase (1983), Hantel (1986), and Moussiopoulos and Flasak (1986). However, the presentation in these references is theoretically unsatisfactory. Both Hantel and Haase (1983) and Hantel (1986) do not consider a variational problem by starting with a functional, but rather use Helmholtz's theorem to decompose the wind field and to show that the rotational part of the modification has to vanish in order to satisfy a minimal requirement. The argument by Moussiopoulos and Flasak (1986) is limited in generality because these authors express the modifying wind field *a priori* as the gradient of a function that is also used as a Lagrange multiplier in the functional to be minimized (see appendix A in Moussiopoulos and Flasak (1986)).

The derivation presented here starts with an externally specified, diagnosed 3D wind field \( \mathbf{v}_d = (u^d, v^d, w^d) \), where \( w^d \) is the observed vertical velocity in pressure coordinates; \( \alpha \) is a pressure-independent factor of units (length)/(pressure) designed to ensure that
all three velocity components have the same unit. This diagnosed wind field \( \mathbf{v}^d \) does not, in general, satisfy the continuity equation, written here in pressure coordinates. This deficit may be expressed as:

\[
\nabla \cdot \mathbf{v}^d + D = 0 \tag{2.1}
\]

where \( \nabla \cdot \mathbf{v}^d \) is the divergence of \( \mathbf{v}^d \) in pressure coordinates, and

\[
\nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial p} \right).
\]

It is assumed \textit{a priori} that the volume integral of the noise divergence \( D \) vanishes:

\[
\int_V D \, dV = 0 \tag{2.2}
\]

which implies that the diagnosed net flux across the boundaries of the computational volume \( V \) (i.e. the domain) is zero. If the volume integral of the noise divergence \( D \) does not vanish \textit{a priori}, it must be removed before application of the procedure developed below. This initial step simply requires the modification of the diagnosed net flux across the boundaries of the computational volume by a constant.

In order to obtain a non-divergent wind field \( \mathbf{v} \), namely:

\[
\nabla \cdot \mathbf{v} = 0 \tag{2.3}
\]

a modification \( \mathbf{v}^m \) of the diagnosed wind is considered in the following form:

\[
\mathbf{v} = \mathbf{v}^d + \mathbf{v}^m. \tag{2.4}
\]

The modified, strictly non-divergent, wind field \( \mathbf{v} \), or, equivalently, the modification \( \mathbf{v}^m \), is specified through the following three conditions:

(i) \( \mathbf{v} \) satisfies (2.3) \( \iff \nabla \cdot \mathbf{v}^m - D = 0 \) by Eqs. (2.1) and (2.4).

(ii) \( \mathbf{v}^m \) is specified \textit{a priori} at the boundaries of the domain.

(iii) The domain-integrated squared modification is a minimum.

It is obvious that the first two conditions are not sufficient to determine \( \mathbf{v}^m \); it is only the divergent component of \( \mathbf{v}^m \) that can be determined from conditions (i) and (ii). Condition (iii) is shown to be central for specifying the rotational component of \( \mathbf{v}^m \).

Consideration of condition (iii) under the constraint (i) leads to the formulation of a variational problem through specification of the functional:

\[
\mathcal{F} (\mathbf{v}^m, \chi) = \int_V \left\{ \frac{1}{2} (\mathbf{v}^m)^2 + \chi (\nabla \cdot \mathbf{v}^m - D) \right\} \, dV \tag{2.5}
\]

where \( \chi \) is a Lagrange multiplier introduced to enforce the strong constraint (i), and use of the factor one-half implies the constrained minimization of the modifying kinetic energy. It is noted in this context that it is conceivable that non-divergence can be imposed through the approach presented here by assigning different weights to the individual modifying wind components in the first term of \( \mathcal{F} \). The choice of such different weights must be based on \textit{a priori} knowledge of the accuracy of the diagnosed wind components, and may serve to control the magnitude of the modifications obtained. However, in this case it is no longer the modifying kinetic energy that is minimized subject to constraint (i).

In order to satisfy (i) and (iii) simultaneously, the functions \( \mathbf{v}^m \) and \( \chi \) must be chosen such that the functional \( \mathcal{F} \) takes on a minimum value. This may be achieved by considering the first variation of \( \mathcal{F} \) as:
\[
\delta \mathcal{F} = \int_V \{ \mathbf{v}^m \cdot \delta \mathbf{v}^m + \chi \nabla \cdot \delta \mathbf{v}^m + (\nabla \cdot \mathbf{v}^m - D) \delta \chi \} \, dV
\]

which may be rewritten as:

\[
\delta \mathcal{F} = \int_V \{ (\mathbf{v}^m - \nabla \chi) \cdot \delta \mathbf{v}^m + (\nabla \cdot \mathbf{v}^m - D) \delta \chi \} \, dV
\]

after the middle term in (2.6) has been integrated by parts and (ii) has been used in the form that the first variation of \( \mathbf{v}^m \) vanishes at the boundaries of the domain. From Eq. (2.7) it is seen that in order for the first variation of \( \mathcal{F} \) to vanish (which is a necessary condition for \( \mathcal{F} \) to attain an extremum), subject to the independence of the two variations in the integrand, the following two conditions must be satisfied by the modifying wind field:

\[
\mathbf{v}^m - \nabla \chi = 0 \quad (2.8)
\]

\[
\nabla \cdot \mathbf{v}^m - D = 0 \quad (2.9)
\]

which may be combined into the single Poisson equation:

\[
\nabla^2 \chi = D. \quad (2.10)
\]

Equation (2.10) must be satisfied throughout the computational domain subject to boundary conditions appropriately derived from condition (ii). Since condition (ii) has been used in the above derivation in the form that \( \mathbf{v}^m \) is constant at the boundaries, which by Eq. (2.8) implies that \( \nabla \chi = \) constant, the boundary conditions for \( \chi \) in Eq. (2.10) are recognized as Neumann boundary conditions.

A number of remarks are appropriate here. The modifying wind is irrotational, which is implied by Eq. (2.8). Thus, by (2.4), the vorticity of the diagnosed wind field is unchanged, and the modification applies only to the divergent part of the diagnosed wind. This result reproduces the suggestions of Moussiopoulos and Flasik (1986) and Hantel (1986). It is especially desirable in view of the fact that the rotational part of the wind is known with better relative accuracy than its divergent part (see, for example, Sardeshmanek and Hoskins 1987; Trenberth 1991).

Second, integrating Eq. (2.9) over the computational domain, in connection with the boundary condition \( \mathbf{v}^m = \) constant, implies that the integral of \( \mathbf{v}^m \) over the boundary surface must be zero, which is consistent with assumption (2.2).

Third, we note that the factor \( \alpha \) is simply used to ensure correct physical units in the continuous problem; \( \alpha \) may also be interpreted as a weighting factor of the vertical velocity in the first term of the functional \( \mathcal{F} \). It is emphasized that within the discrete problem (see next section) there is no need for a similar step, because the mass-integrated form of the continuity equation is used.

Finally, without loss of generality, the modifying wind field at the boundaries may be set to zero.

3. THE DISCRETE PROBLEM: VARIATIONAL MASS FLUX MODIFICATION

This section is devoted to the detailed description of the VMA, which is the general technique proposed to enforce strict non-divergence in the discrete situation, as exemplified in section 1. The derivation of the VMA follows closely the developments outlined in the previous section. Further, at the end of this section, some remarks are made concerning the numerical implementation of the VMA.
The discrete problem is formulated for an orthogonal coordinate system consisting of the horizontal coordinates $\lambda$ (longitude) and $\mu = \sin \phi$ ($\phi$ is latitude), and of the vertical coordinate $p$ (pressure). This coordinate system is chosen to ensure that a finite volume element of given increments in these coordinates possesses the same mass, independent of its location within the computational domain. This property of the coordinate system chosen is highly advantageous for carrying out subsequent budget calculations.

In order to arrive at an integral expression to be minimized analogous to (2.5), the continuity equation for the diagnosed wind (see also Eq. (2.1)) is considered in the form of a mass integral over one computational box identified by the indices $i, j, k$:

$$
\frac{\Delta p}{g} \frac{1}{\Delta \lambda \Delta \mu \Delta p} \int_{\lambda_i}^{\lambda_{i+1}} \int_{\mu_j}^{\mu_{j+1}} \int_{p_k}^{p_{k+1}} \left( \frac{\partial \hat{u}^d(\lambda, \mu, p)}{\partial \lambda} + \frac{\partial \hat{v}^d(\lambda, \mu, p)}{\partial \mu} + \frac{\partial \omega^d(\lambda, \mu, p)}{\partial p} + D(\lambda, \mu, p) \right) d\lambda \ d\mu \ dp = 0
$$

(3.1)

where $\hat{u}^d$, $\hat{v}^d$, and $\omega^d$ are the diagnosed velocity components in this coordinate system. The factor $\Delta p/g$ causes the terms in the equation to have the dimension of a mass flux density (i.e. kg m$^{-2}$ s$^{-1}$); $\Delta p$ is the pressure increment of one layer, and $g$ is gravitational acceleration. Using the Gaussian divergence theorem, Eq. (3.1) can be rewritten as:

$$
\frac{\Delta p}{g} \frac{1}{\Delta \lambda \Delta \mu \Delta p} \left[ \int_{\lambda_i}^{\lambda_{i+1}} \int_{\mu_j}^{\mu_{j+1}} \int_{p_k}^{p_{k+1}} \left( \hat{u}^d(\lambda, \mu, p) - \hat{v}^d(\lambda, \mu, p) \right) d\mu \ dp + \right.
$$

$$
\left. + \int_{\lambda_i}^{\lambda_{i+1}} \int_{\mu_j}^{\mu_{j+1}} \int_{p_k}^{p_{k+1}} \left( \hat{u}^d(\lambda, \mu, p) - \hat{v}^d(\lambda, \mu, p) \right) d\lambda \ dp + \right.
$$

$$
\left. + \int_{\lambda_i}^{\lambda_{i+1}} \int_{\mu_j}^{\mu_{j+1}} \int_{p_k}^{p_{k+1}} \left( \omega^d(\lambda, \mu, p) - \omega^d(\lambda, \mu, p) \right) d\lambda \ d\mu \ dp \right] = 0.
$$

(3.2)

At this point abbreviations are introduced for the mass flux density components according to the following notation:

$$
U_{i,j,k}^d = \frac{\Delta p}{g} \frac{1}{\Delta \lambda \Delta \mu \Delta p} \int_{\lambda_i}^{\lambda_{i+1}} \int_{\mu_j}^{\mu_{j+1}} \int_{p_k}^{p_{k+1}} \hat{u}^d(\lambda, \mu, p) d\mu \ dp
$$

(3.3)

which is the zonal component of the diagnosed mass flux at the $\lambda$-position $\lambda_i$ appropriately integrated over $\mu$ and $p$. Using analogous notation for the other components, Eq. (3.2) is rewritten as:

$$
U_{i,j,k}^d - U_{i+1,j,k}^d + V_{i,j+1,k}^d - V_{i,j,k}^d + W_{i,j,k+1}^d - W_{i,j,k}^d + \overline{D}_{i,j,k} = 0.
$$

(3.4)

The quantity $\overline{D}_{i,j,k}$ is the box-averaged noise divergence $D$ multiplied by $\Delta p/g$; for the sake of simplicity, $\overline{D}_{i,j,k}$ is referred to as box divergence.

Equation (3.4) is the integrated analogue of the continuity equation (2.1). The computational volume is divided into $I \cdot J \cdot K$ boxes (corresponding to $I$, $J$, and $K$ intervals in $\lambda$, $\mu$, and $p$ directions, respectively). The indices in Eq. (3.4) enumerate individual boxes and, therefore,

$$
i = 1, \ldots, I; \quad j = 1, \ldots, J; \quad k = 1, \ldots, K.
$$

(3.5)
Since, through the application of the Gaussian theorem, the fluxes \( U^d \), \( V^d \), and \( W^d \) are defined on the faces of individual boxes, the number of flux components in the direction of a particular coordinate is one plus the number of boxes in that coordinate direction, in accord with the indices in Eq. (3.4). This concept is illustrated for the 2D case in Fig. 3.

![Diagram showing fluxes and divergences](image)

**Figure 3.** Two-dimensional illustration of location of divergences, fluxes, and \( \chi \)-values. Fluxes \( U \) (in \( \lambda \)-direction, index \( i \)) and \( V \) (in \( \mu \)-direction, index \( j \)) are specified on boundaries between adjacent boxes, and indexed as shown; first index gives the value of \( i \), second index the value of \( j \). The noise divergence \( \bar{D}_{i,j} \) of an individual box is attributed to the centre of the box (since it is an area integral); likewise, the potential function \( \chi_{i,j} \) is attributed to the centre of the box. Diagnosed fluxes may cross the boundary of the domain (hatched), but modifying fluxes vanish at boundaries owing to boundary condition. For further details see section 3.

Further, in analogy to the continuous description (see Eq. (2.2)), it is assumed \textit{a priori} that the noise divergence vanishes when summed over the entire domain:

\[
\sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} \bar{D}_{i,j,k} = 0. \tag{3.6}
\]

Through (3.4), this assumption requires that the diagnosed net flux over the boundaries is zero (see also the example in section 1).

In order to obtain modified mass fluxes \((U, V, W)\) that satisfy exactly the continuity equation in box-integrated form, namely:

\[
U_{i+1,j,k} - U_{i,j,k} + V_{i,j+1,k} - V_{i,j,k} + W_{i,j,k+1} - W_{i,j,k} = 0 \tag{3.7}
\]

(compare with Eq. (2.3)) the modified mass fluxes are—in analogy to section 2—written as the sum of diagnosed and modifying mass fluxes:

\[
(U, V, W) = (U, V, W)^d + (U, V, W)^m. \tag{3.8}
\]
Equations (3.7) and (3.8), together with (3.4), imply that the modifying mass fluxes have to satisfy the following equation:

$$U_{i+1,j,k}^m - U_{i,j,k}^m + V_{i,j+1,k}^m - V_{i,j,k}^m + W_{i,j,k+1}^m - W_{i,j,k}^m - \overline{D}_{i,j,k} = 0 \quad (3.9)$$

which is the discrete analogue of condition (i) in section 2. The range of indices in (3.7) and (3.9) is given by (3.5).

Although Eqs. (3.4) and (3.9) look formally symmetric their physical significance is quite different. Equation (3.4) serves to determine the box divergences $\overline{D}_{i,j,k}$ from the diagnosed mass fluxes $U_{i,j,k}^m$, $V_{i,j,k}^m$, and $W_{i,j,k}^m$. The result is a set of $I \cdot J \cdot K$ divergences which, however, are linearly dependent owing to assumption (3.6); only $(I \cdot J \cdot K) - 1$ box divergences are independent. Equation (3.9), on the other hand, is a linear set of equations to be satisfied by the unknown modifying flux components $U_{i,j,k}^m$, $V_{i,j,k}^m$, and $W_{i,j,k}^m$.

In complete analogy to the developments in section 2, the modifying mass fluxes are specified through the following three conditions:

(i) The modifying fluxes $(U, V, W)^m$ in the interior of the domain satisfy Eq. (3.9).

(ii) The modifying fluxes are specified \textit{a priori} at the boundaries of the computational domain. Specifically, they are prescribed as:

$$U_{1,j,k}^m = 0; \quad U_{I+1,j,k}^m = 0; \quad j = 1, \ldots, J; \quad k = 1, \ldots, K; \quad (3.10)$$

$$V_{i,1,k}^m = 0; \quad V_{i,J+1,k}^m = 0; \quad i = 1, \ldots, I; \quad k = 1, \ldots, K; \quad (3.11)$$

$$W_{i,j,1}^m = 0; \quad W_{i,j,K+1}^m = 0; \quad i = 1, \ldots, I; \quad j = 1, \ldots, J. \quad (3.12)$$

Note that this choice for the boundary conditions is a particularly simple form consistent with requirement (3.6).

(iii) The mean-square modification within the interior of the domain is a minimum.

In the discrete situation it is advantageous to distinguish explicitly between inner fluxes (i.e. fluxes within the computational volume) and boundary fluxes (i.e. fluxes crossing the boundary of the computational volume). As in the continuous situation the boundary fluxes are prescribed by a total of $2 \times (J \cdot K + I \cdot K + I \cdot J)$ equations (i.e. Eqs. (3.10)–(3.12)). As a consequence, only the inner fluxes are to be determined by conditions (i) and (iii), supplemented by condition (ii). Further, as in the continuous case, conditions (i) and (ii) are not sufficient to determine the modifying mass flux field, and condition (iii) must be considered in addition (see also the example in section 1). Formally, this may be understood by noting that the total number of inner fluxes, namely $(I - 1) \cdot J \cdot K + I \cdot (J - 1) \cdot K + I \cdot J \cdot (K - 1)$, is almost three times as many as the number of equations described by (3.9).

As in the continuous case, consideration of condition (iii) under the constraint (i) leads to a minimization problem through the specification of the following cost function:

$$F = \sum_{i=1}^{I+1} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{1}{2} (U_{i,j,k}^m)^2 + \sum_{i=1}^{I+1} \sum_{j=1}^{J} \sum_{k=1}^{K} \frac{1}{2} (V_{i,j,k}^m)^2 + \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K+1} \frac{1}{2} (W_{i,j,k}^m)^2 +$$

$$+ \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} X_{i,j,k} (U_{i+1,j,k}^m - U_{i,j,k}^m + V_{i,j+1,k}^m - V_{i,j,k}^m + W_{i,j,k+1}^m - W_{i,j,k}^m - \overline{D}_{i,j,k}). \quad (3.13)$$

The summation indices in Eq. (3.13) are chosen such that both boundary and inner fluxes are included in the cost function $F$. However, the former are not independent arguments
of $F$, like the inner fluxes and the Lagrange multipliers $\chi$, but must be considered as specified parameters due to Eqs. (3.10)--(3.12).

Concerning the indices appearing in (3.13) the following remark is made. Since the quantity $\overline{D}_{i,j,k}$ represents the divergence of the box with corner indices $(i, j, k)$, it appears appropriate to think of this quantity as being located in the centre of the box. Naturally then, the $\chi$'s may also be attributed to the centres of the boxes, whereas the modifying mass flux components refer to appropriate faces of the box (see also Fig. 3). This arrangement is a staggered grid.

Minimization of $F$ amounts to minimizing the total squared modification subject to the strong constraint (3.9). Necessary conditions for obtaining a minimum of $F$ are obtained by differentiating $F$ with respect to its arguments and setting the result equal to zero. Differentiation with respect to the Lagrange multipliers reproduces (3.9) with the range of indices given in (3.5), whereas differentiation of $F$ with respect to the inner fluxes results in:

$$U_{i,j,k}^m + \chi_{i-1,j,k} - \chi_{i,j,k} = 0, \quad i = 2, \ldots, I; \quad j = 1, \ldots, J; \quad k = 1, \ldots, K;$$

$$V_{i,j,k}^m + \chi_{i,j-1,k} - \chi_{i,j,k} = 0, \quad i = 1, \ldots, I; \quad j = 2, \ldots, J; \quad k = 1, \ldots, K;$$

$$W_{i,j,k}^m + \chi_{i,j,k-1} - \chi_{i,j,k} = 0, \quad i = 1, \ldots, I; \quad j = 1, \ldots, J; \quad k = 2, \ldots, K.$$  \hspace{1cm} (3.14)  \hspace{1cm} (3.15)  \hspace{1cm} (3.16)

This result is equivalent to Eq. (2.8) in the sense that in the discrete case the modifying fluxes are obtained as the gradient of a scalar function, too.

Formally introducing $\chi$-values outside the boundaries of the domain, the result (3.14)--(3.16) may be extended for the boundary fluxes as:

$$U_{i,j,k}^m + \chi_{0,j,k} - \chi_{i,j,k} = 0; \quad U_{i+1,j,k}^m + \chi_{i,j,k} - \chi_{i+1,j,k} = 0; \quad i = 1, \ldots, I; \quad k = 1, \ldots, K;$$

$$V_{i,j,k}^m + \chi_{i,0,k} - \chi_{i,j,k} = 0; \quad V_{i,j+1,k}^m + \chi_{i,j,k} - \chi_{i,j+1,k} = 0; \quad i = 1, \ldots, I; \quad k = 1, \ldots, K;$$

$$W_{i,j,k}^m + \chi_{i,j,0} - \chi_{i,j,k} = 0; \quad W_{i,j,k+1}^m + \chi_{i,j,k} - \chi_{i,j,k+1} = 0; \quad i = 1, \ldots, I; \quad j = 1, \ldots, J.$$  \hspace{1cm} (3.17)  \hspace{1cm} (3.18)  \hspace{1cm} (3.19)

It is noted that (3.17)--(3.19) do not follow from the minimization requirement. These expressions simply represent physically meaningful definitions of additional $\chi$-values outside the domain, in terms of the specified boundary conditions for the modifying fluxes, based on an analogy with results derived from the minimization problem.

At this point, the inner fluxes, given by (3.14)--(3.16), together with the boundary fluxes, formally expressed through (3.17)--(3.19), are introduced into (3.9). This leads to:

$$\{(\chi_{i+1,j,k} - \chi_{i,j,k}) - (\chi_{i,j,k} - \chi_{i-1,j,k})\} + \{(\chi_{i,j+1,k} - \chi_{i,j,k}) - (\chi_{i,j,k} - \chi_{i,j-1,k})\} +$$

$$\{\chi_{i,j,k+1} - \chi_{i,j,k}\} - \overline{D}_{i,j,k} = 0$$  \hspace{1cm} (3.20)

with the range of indices given by (3.5), or:

$$\chi_{i+1,j,k} + \chi_{i-1,j,k} + \chi_{i,j+1,k} + \chi_{i,j-1,k} + \chi_{i,j,k+1} + \chi_{i,j,k-1} - 6\chi_{i,j,k} = \overline{D}_{i,j,k}.$$  \hspace{1cm} (3.21)

Equation (3.21) is a 3D Poisson equation to be solved for $\chi$; it is the discrete analogue to Eq. (2.10). The boundary conditions for (3.21) are obtained by combining Eqs. (3.10)--(3.12) with (3.17)--(3.19) as:
\[ \chi_{0,j,k} - \chi_{1,j,k} = 0; \quad \chi_{i,j,k} - \chi_{i+1,j,k} = 0; \quad j = 1, \ldots, J; \quad k = 1, \ldots, K; \]  \tag{3.22}

\[ \chi_{i,0,k} - \chi_{i,1,k} = 0; \quad \chi_{i,j,k} - \chi_{i,j+1,k} = 0; \quad i = 1, \ldots, I; \quad k = 1, \ldots, K; \]  \tag{3.23}

\[ \chi_{i,j,0} - \chi_{i,j,1} = 0; \quad \chi_{i,j,k} - \chi_{i,j,k+1} = 0; \quad i = 1, \ldots, I; \quad j = 1, \ldots, J. \]  \tag{3.24}

These equations represent staggered Neumann boundary conditions, which, again, is in close correspondence to the continuous situation.

The 3D Poisson equation (3.21) consists of \( I \cdot J \cdot K \) algebraic equations for the \( I \cdot J \cdot K \) unknown inner \( \chi \)-values. By its nature, Eq. (3.21) can be solved for \( \chi \) only up to an additive constant; this may be realized by adding (3.21) over all its indices, while observing the boundary conditions and condition (3.6). Thus, the inherent linear dependence of these equations requires the external specification of one of the unknowns; for example, the mean of \( \chi \) may be specified arbitrarily. This choice clearly has no impact upon the modifying mass fluxes.

It is noted that the modifying mass flux field is represented simply by applying a difference operator to the \( \chi \)-field (Eqs. (3.14)–(3.16)) in contrast to the differential operator (Eq. (2.8)) emerging in the continuous case. This fact implies that no information about size or shape of the boxes is required in the discrete case (see Eq. (3.21)). In other words, the result derived is independent of specifications concerning the grid. This information has been incorporated into the mass flux fields through the integration procedure (3.3). Mass fluxes (in units of kg s\(^{-1}\))—unlike mass flux densities—carry no explicit information about the space in which the mass transport actually occurs.

The task of solving (3.21) for given \( \bar{D}_{i,j,k} \) subject to (3.22)–(3.24) may be attacked through various approaches. There are at least three different algorithms available, namely: direct methods, expansion into eigenfunctions, and relaxation methods. All three methods have been investigated in the course of this study; a more detailed description is found in appendices A and B. Classical relaxation converges extremely slowly and will not be considered further. Expansion of the unknown \( \chi \) into eigenfunctions and solving for the coefficients in this expansion is not completely straightforward in this case owing to the non-cyclic boundary conditions. It is, however, made possible through proper relabelling of unknowns (see appendix B). Applying a direct method, which in essence amounts to a decoupling of coordinate directions through diagonalization of coefficient matrices, is particularly attractive in the present context. This method is described in detail in appendix A. Its performance compared with a Fourier decomposition algorithm is described in appendix B. Briefly, the Fourier decomposition algorithm is executing faster, but the decoupling method is conceptually more straightforward and may easily be extended to an arbitrary number of dimensions.

The description of the VMA derived above can be summarized as follows. Given the box-integrated noise divergences, the Poisson equation (3.21) is solved for the \( \chi \)-field with staggered Neumann boundary conditions (3.22)–(3.24); the solution is obtained with a fast standard method. The emerging \( \chi \)-field determines the modifying mass fluxes in the interior of the domain by (3.14)–(3.16). These, in turn, determine the modified mass fluxes by (3.8) that are exactly consistent with the box-integrated continuity equation (3.7).

4. Meteorological application of the variational modification algorithm

The VMA is illustrated in this section for the case of the heavy rain episode over central Europe on 1 August 1991, 00 GMT ± 6 h. All results shown in the figures of this section refer to this event, which has been the subject of a recent diagnostic study (see
The data used for the computations presented here are analysed (uninitialized) and initialized T106 analyses from the ECMWF MARS archive at 11 pressure levels (namely, $p = 1000, 850, 700, 500, 400, 300, 250, 200, 150, 100$ and $50$ hPa).

There are two basic points investigated here. First, the analysed wind field is considered by itself (section 4(a)); in this case the noise divergences in the analyses are determined and the modifications necessary to obtain mass flux fields that carry no 3D divergence are computed. Second, the impact of small noise divergences is considered in the context of diagnostic energy-budget calculations (section 4(b)); these are based on the diagnostic model described by Dorninger et al. (1992).

The area of investigation is central Europe and the coordinate system described in section 3 is used with elementary horizontal and vertical resolutions of approximately $50$ km and $50$ hPa respectively (Fig. 4). The integrations are carried out over diagnostic boxes consisting of eight elementary boxes; thus, the corresponding diagnostic box resolution is $(100$ km$)^2 \times 100$ hPa. It is emphasized that both the VMA and the budget calculations are carried out in exactly the same coordinate system, because the mass fluxes resulting from the VMA are strictly non-divergent only in this framework. In other words, the discretization scheme chosen to implement the VMA must subsequently be used for the budget calculations, in order not to lose the property of non-divergence.

The elementary time resolution is six hours. A weighted averaging procedure over three adjacent time points is used to obtain results at the diagnostic time span of twelve hours that is centred, in this case, at 00 GMT 1 August 1991.

![Diagram](https://example.com/diagram.png)

**Figure 4.** Grid used for mass flux calculations and diagnostic model. Zonal coordinate $\lambda$, positive towards east; meridional coordinate $\mu = \sin \phi$ (\(\phi\) as latitude), positive towards north; vertical coordinate pressure $p$, positive downwards. Dots denote grid points for specification of input data. **Elementary box** defines resolution of input fields. **Diagnostic box**, consisting of $2 \times 2 \times 2$ elementary boxes, defines mass volume for which box divergences and budgets are computed.

Given the spectrally MARS-archived fields (in particular, wind, humidity and temperature) at the above-mentioned pressure levels, grid-point values are obtained through the usual transformation from spectral into physical space. Then a linear interpolation is used to obtain a vertically uniform resolution of 50 hPa. This process of vertical interpolation (see also second box in Fig. 20) causes a problem for the vertical velocity at the lower boundary of the domain (1000 hPa in our computations). The archived data set of $\omega$ at 1000 hPa is generated at the ECMWF by vertical downward-integration of
the continuity equation, possibly followed by extrapolation below the ground (Arpe (1992), personal communication); this procedure leads to considerable noise in the vertical-velocity field at this level. Therefore, we do not employ in this study the archived \( \omega \) at 1000 hPa. Instead, we use the time tendency of the pressure at the ground derived from the mean-sea-level pressure analysis at the ECMWF; this \( \omega(p_g) \) is then attributed to the 1000 hPa pressure level. However, no modifications of this kind are being applied to the other meteorological fields.

Before discussing the results it is necessary to clarify terminology. We have stressed above that the box integration results in \textit{flux differences}, instead of the familiar \textit{flux density divergences}; this applies to budgets of all kinds, specifically to the mass and energy budgets. In the present application of the VMA, however, a regular grid is used (see section 3); this is not required by the theory but is advantageous for other reasons. Thus, for ease of comparison, all fluxes, both in horizontal and vertical directions, are divided by the area \( A = (100 \text{ km})^2 \). This procedure generates the units \( \text{kg m}^{-2}\text{s}^{-1} \). The resulting quantities are true mean flux densities in the vertical direction; in the horizontal direction, however, they represent pseudo-flux densities. Nevertheless, all flux components remain to be comparable.

Consequently, we refer to the box average of the continuous 3D divergence specified in Eq. (3.1) as '3D divergence'; it is equal to the total mass flux difference, obtained by integrating the divergence over the mass of the box, and dividing the result by \( A \), as given in Eq. (3.4). Further, the horizontal and vertical equivalents are referred to as '2D divergence' and '1D divergence', respectively. Thus, by this convention, 3D divergence is the sum of 2D divergence and 1D divergence.

(a) \textit{The impact of the VMA upon the mass flux field}

In order to examine whether mass is conserved when the ECMWF analyses archived on standard pressure surfaces are interpolated to our grid, we have computed the 3D divergence of the unmodified mass flux with analysed data. The result is shown in Fig. 5 for the layer 700–800 hPa. The r.m.s. value of the 3D noise divergence in this layer is \( 36 \times 10^{-4} \text{ kg m}^{-2}\text{s}^{-1} \) corresponding* to \( 36 \times 10^{-7} \text{ s}^{-1} \). The maximum 3D mass flux divergence in Fig. 5 is almost \( 200 \times 10^{-4} \text{ kg m}^{-2}\text{s}^{-1} \), centred over the Alps. Alexander and Schubert (1990) found that mountainous areas are especially sensitive to interpolation from model to pressure surfaces. However, large noise diversions are found also over the Mediterranean.

At first glance it may seem that the reason for the noise divergence is the fact that Fig. 5 is based upon \textit{analysed} fields. Figure 6 shows the vertical distribution of r.m.s. and mean values of the 3D divergence for every 100 hPa layer computed with analysed (i.e. uninitialized) and with \textit{initialized} data. The results are quite similar in both cases, with a tendency that the initialized data perform better in the lower layers than do the analysed data. In general, the 3D divergence is a maximum in the lower troposphere; the main reason is presumably the unbalanced boundary value of \( \omega \)—see above—which affects analysed and initialized data sets in a similar manner. However, this explanation only accounts for the noise divergence in the 900–1000 hPa layer, but not the higher layers. In summary, the results shown in Fig. 6 demonstrate that the initialized fields are contaminated with about the same noise divergence as are the analysed fields.

* Note: In the following, mass fluxes as well as mass flux divergences are always given in units of \( \text{kg m}^{-2}\text{s}^{-1} \) (see also previous subsection). For conversion purposes, \( 1 \times 10^{-4} \text{ kg m}^{-2}\text{s}^{-1} \) corresponds to \( 1 \times 10^{-7} \text{ s}^{-1} \) for our diagnostic boxes as specified in Fig. 4.
Figure 5. 3D divergence of unmodified mass flux in the layer 700–800 hPa for 1 August 1991, 00 GMT ± 6 h, in units of $10^{-4}$ kg m$^{-2}$ s$^{-1}$ with a contour interval of 25 units. Zero line, heavy solid; positive (negative) values solid (dashed). Statistics (mean value/r.m.s. value/square root of variance): 0/36/36 units. Input: analysed ECMWF data.

Figure 6. Vertical profile of r.m.s. values (squares) and mean values (circles) of unmodified 3D mass flux divergence, averaged horizontally over entire model domain for every 100 hPa layer. Input data from ECMWF: analysed (empty symbols), initialized (full symbols).
Trenberth (1991) argued that the interpolation routine which transforms from the ECMWF model grid to standard pressure surfaces may produce the most accurate values at the archived levels; however, according to Trenberth (1991), they are not representative for finite layers. The results plotted in Fig. 6 are valid for finite layers. Thus, it appears that the primary source of the 3D noise divergence of Figs. 5 and 6 does not lie in the analysed/initialized ECMWF data, but in the interpolation necessary to transform from model levels to standard pressure surfaces, and from these to our diagnostic grid (see also second box in Fig. 20).

Ideally, the 3D divergence in p-coordinates should vanish everywhere. This implies that 2D divergence and 1D divergence should balance each other exactly. Figure 7 shows the unmodified fields of 2D divergence and 1D divergence for the layer 700–800 hPa; it demonstrates that there is balance to a reasonable degree. The unbalanced component is, of course, the 3D noise divergence.

Figure 8 shows the modified 2D and 1D divergences. They are quite similar to their unmodified counterparts. For example, the maximum analysed 2D convergence over the Alps and Italy (about 150 units, Fig. 7(a)) has not been much changed by the modification (Fig. 8(a)). Since the field of 2D divergence carries relevant meteorological information it is important to note that the modification algorithm conserves the pattern of this field in most parts. Comparison of the diagnosed 1D divergence (Fig. 7(b)) with its modified equivalent (Fig. 8(b)) shows largely the same result. However, the divergences shown in Fig. 8 balance each other exactly (to numerical accuracy) which is a result of the application of the VMA. Figure 9 confirms this balance for every layer of the model domain (note that 2D and 1D divergences have the same r.m.s. values, and opposing means). Further, Fig. 9 shows that the modification is moderate for the 2D divergences (Fig. 9(a)) and, albeit larger, still reasonable for the 1D divergence (Fig. 9(b)).

By applying the VMA, an exactly balanced mass flux field is enforced. The modified 3D mass flux divergence is about $10^{-9}$ kg m$^{-2}$ s$^{-1}$ everywhere for both data sets (analysed and initialized, not shown) which is a reduction of the noise divergence by about six orders of magnitude. This reduction can be arbitrarily increased by using higher numerical precision.

Statistics of diagnosed, modified, and modifying divergence components are presented in the last three columns of Table 1. These statistics summarize the results obtained

<table>
<thead>
<tr>
<th></th>
<th>$V$</th>
<th>$W$</th>
<th>$UVW$</th>
<th>3D div.</th>
<th>2D div.</th>
<th>1D div.</th>
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</thead>
<tbody>
<tr>
<td><strong>Diagnosed (i.e. before VMA) mass flux and its divergence</strong></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Mean value</td>
<td>285 (284)</td>
<td>47 (44)</td>
<td>27 (15)</td>
<td>122 (117)</td>
<td>-2 (-2)</td>
<td>-5 (-3)</td>
</tr>
<tr>
<td>R.m.s. value</td>
<td>771 (776)</td>
<td>400 (394)</td>
<td>139 (99)</td>
<td>513 (511)</td>
<td>37 (32)</td>
<td>45 (39)</td>
</tr>
<tr>
<td><strong>Modified (i.e. after VMA) mass flux and its divergence</strong></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Mean value</td>
<td>280 (283)</td>
<td>33 (26)</td>
<td>20 (17)</td>
<td>113 (111)</td>
<td>0 (0)</td>
<td>-1 (-1)</td>
</tr>
<tr>
<td>R.m.s. value</td>
<td>765 (768)</td>
<td>400 (393)</td>
<td>118 (86)</td>
<td>509 (506)</td>
<td>0 (0)</td>
<td>50 (41)</td>
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<tr>
<td><strong>Modifying mass flux and its divergence</strong></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Mean value</td>
<td>-5 (-1)</td>
<td>-14 (-18)</td>
<td>-7 (2)</td>
<td>-8 (-6)</td>
<td>2 (2)</td>
<td>3 (2)</td>
</tr>
<tr>
<td>R.m.s. value</td>
<td>34 (29)</td>
<td>40 (36)</td>
<td>37 (27)</td>
<td>37 (31)</td>
<td>37 (32)</td>
<td>23 (18)</td>
</tr>
</tbody>
</table>

Fluxes and divergences are given in units of $10^{-9}$ kg m$^{-2}$ s$^{-1}$. $UVW$ denotes the component-wise mean of $U$, $V$, and $W$. 2D div. refers to horizontal divergence, 1D div. to vertical divergence, whereas 3D div. is the sum of both horizontal and vertical divergences (see also beginning of section 4). Note that all flux divergences are actually flux differences. Input: analysed (initialized) ECMWF data.
above. In particular, they show moderate changes in the r.m.s. values in the 2D and 1D divergence components, before and after application of the VMA. Further, it is evident that there is no large difference between the analysed and the initialized data. For example, the 3D noise divergence to be removed by the modifying divergence is 37 units for analysed data and 32 units for initialized data. This requires modifications of the 2D and 1D divergences which for initialized data are only slightly smaller than for analysed data.
The individual mass flux components are relatively less sensitive to the modification than is their divergence. Figure 10 exhibits the unmodified, analysed, zonal mass flux $U^d$ on individual vertical profiles over Europe. The figure shows a large-scale pattern of a westerly mass flux component with a high tropospheric jet south of the precipitation maximum observed on that day over a line connecting eastern France with the Slovak Republic, with maximum over Salzburg. Note the remarkable cyclonic shear of $U^d$ with maximum in the high troposphere. The application of VMA does not change this
pattern—the modified equivalent of Fig. 10 (pattern of $U$, not shown) cannot be distinguished from $U^d$. Figure 11 demonstrates the smallness of the differences through the vertical profile of statistics.

Figure 12 shows the unmodified, analysed, vertical mass flux $W^d$. Areas of upward (negative) $W^d$ correspond closely to the precipitation field (not shown). The pattern of the modified vertical mass flux $W$ (not shown) looks again quite similar to Fig. 12; however, it is reduced in absolute size. In other words, the analysed vertical mass flux
Figure 10. Vertical profiles of unmodified (i.e. diagnosed) zonal mass flux $U^M$ for an array of $32 \times 32$ diagnostic columns (only every second column is plotted) in units of $10^{-3}$ kg m$^{-2}$ s$^{-1}$; scale as indicated on top. Each column is drawn at the pertinent geographic location. Statistics: 29/77/71 units. Input: analysed ECMWF data.

Figure 11. As Fig. 6 except for r.m.s. values of unmodified (empty squares), modified (full squares), and modifying (empty circles) zonal mass flux. Input: analysed ECMWF data.
shows a tendency to be too big. Consequently the analysed 1D divergence must also tend to be too big; this has already been noted above.

An important point is demonstrated in Fig. 13. When looking into the zonal flux case of Fig. 11, the analysed profiles (drawn) and initialized profiles (not drawn) cannot be distinguished. In the vertical flux case of Fig. 13, they can be distinguished. The relative difference unmodified/modified (empty/full symbols) is about the same for analysed data (32%, right-most curves in Fig. 13) and initialized data (31%, left-most curves).

However, the relative difference analysed/initialized (squares/circles) is about twice as big as the difference unmodified/modified in Fig. 13 (approximately 70%); see also Table 1. These results indicate that the modification of the mass flux field through the initialization procedure at the ECMWF is considerably larger than the modification required to enforce non-divergence through application of the VMA. In making this comparison it is important to note that the purpose of the initialization procedure at the ECMWF is to reduce unrealistic surface-pressure tendencies, and, thereby, gravity waves, and not to remove noise divergences, since—within the coordinate system used for the ECMWF analysis—both analysed and initialized fields are free of noise divergences by construction (see also the discussion in section 5). Individual components of the 3D divergence are, however, changed during the process of initialization. The VMA, on the other hand, is specifically designed to remove noise divergences in an optimal way.

In order to demonstrate that the above result is not just an artificial effect generated by the statistics, the vertical mass flux is considered on a north–south section approximately at the longitude crossing Salzburg. Here we expect strongly negative mass fluxes in the centre of the rain maximum. The section of analysed $W$ (Fig. 14(a)) and modified $W$ (Fig. 14(b)) demonstrates that this is indeed the case; the upward mass flux is maximum.
between 46°N and 51°N (compare also, Dorninger et al. (1992)). The difference between \( W^d \) and \( W \) is minor. The same result is found if \( W^d \) and \( W \) are compared for initialized data (Fig. 15).

However, the difference between analysed and initialized data is more pronounced (compare, for example, Figs. 14(a) with 15(a)) than is the difference between analysed/initialized fields and the respective modified fields (compare Figs. 14(a), 14(b); Figs. 15(a), 15(b)). In other words, while it is the interpolation procedure to the diagnostic grid used here that causes the 3D noise divergence problem, the VMA is sufficient to remove this inconsistency with minimum effort, both for analysed and for initialized data.

A final point is seen by looking into Table 1. The absolute values of the modifying mass fluxes are about the same in all three directions, both for analysed and for initialized data. This is to be expected from the variational character of the VMA. However, the relative modification of \( W \) is much larger (31–32\%, see above) than the relative modification of \( V \) (9–10\%) or \( U \) (4\%); this is also to be expected when keeping in mind that the horizontal mass flux components carry a strong rotational component. The overall modification (\( UVW \) in Table 1) is 6–7\%. This figure is in accord with the results of Hantel (1987) who found a relative modification of about 5\% for a meteorologically different situation (ALPEX, 4–6 March 1982). A further coincidence is that the modifying \( UVW \) is practically equal to the diagnosed 3D divergence (Table 1; 37 units for analysed data, 32 units for initialized data); this is also in accord with Hantel (1987).

In closing the discussion of the impact of the VMA on the mass flux fields, we repeat that the results presented here are obtained with the formulation of the cost function (3.13) (see also (2.5)); that is, equal weights (namely unity) have been assigned to the modifying mass flux components in the formulation of the first term of the cost function. The use of different weights might lead to modifying mass fluxes with magnitudes differing from those stated above.
Figure 14. Meridional cross-section at 13.6°E of (a) unmodified (statistics: $-8/140/139$ units) and (b) modified (statistics: $-10/128/128$ units) vertical mass flux in units of $10^{-4} \text{ kg m}^{-2} \text{s}^{-1}$ with contour interval of 100 units. Zero line, heavy solid; positive (negative) values, solid (dashed). Input: analysed ECMWF data.
Figure 15. As Fig. 14 except for initialized ECMWF data taken as input. Statistics: (a) –28/122/118, (b) –19/110/109.
(b) The impact of the VMA upon the energy budgets

For the calculation of the energy budgets the diagnostic model DIAMOD is used (see Dorninger et al. 1992; Hantel et al. 1993). DIAMOD is based on the conservation equations for latent and sensible heat, written in pressure coordinates as:

$$\frac{\partial q}{\partial t} + L \nabla_2 \cdot q v_2 + L \frac{\partial q \omega}{\partial p} + gL \frac{\partial \bar{P}}{\partial p} + \text{(imb)}_q = 0 \quad (4.1)$$

$$c_p \frac{\partial T}{\partial t} + c_p \nabla_2 \cdot T v_2 + c_p \left( \frac{\partial}{\partial p} - \frac{\kappa}{P} \right) T \omega + g \frac{\partial R}{\partial p} +$$

$$+ c_p \left( \frac{\partial}{\partial p} - \frac{\kappa}{P} \right) \bar{T} \omega' - gL \frac{\partial \bar{P}}{\partial p} + \text{(imb)}_T = 0 \quad (4.2)$$

together with the mass continuity equation (2.3). The meaning of the symbols in Eqs. (4.1), (4.2) is standard: $q$ is specific humidity, $T$ is temperature, $L$ is the latent heat of condensation, $c_p$ is the specific heat of dry air at constant pressure, $\kappa$ is the ratio of the gas constant for dry air to $c_p$ (≈ 2/7). $L \bar{P}$ is the vertical rain flux, and $R$ is the net radiation flux (both in units of W m$^{-2}$). The horizontal gradient operator is denoted by $\nabla_2$, and $v_2$ is the horizontal wind vector. The terms in both equations have the dimensions W kg$^{-1}$.

The philosophy of DIAMOD is as follows (Hantel 1987; Dorninger et al. 1992): The budgets $b_q$ and $b_T$ in Eqs. (4.1) and (4.2) are specified from grid-scale analyses plus surface observations. The equations are then solved for the subgrid-scale signals $s_q$ and $s_T$. The imbalance terms, (imb)$_q$ and (imb)$_T$, are included to account for neglected quantities (e.g., horizontal divergences of subgrid-scale fluxes) and observational/representativeness errors (see below). The computed signals are meaningful only to the extent that the imbalances are small. Another feature of DIAMOD is the vertical integration of the signals and the separation of the subgrid-scale rain flux, $L \bar{P}$, moisture flux, $g^{-1} L q' \omega'$, and heat flux, $g^{-1} c_p \bar{T} \omega'$. However, details of these fluxes are not considered in this paper.

Figures 16(a) and 17(a) show the vertical profiles of the budgets $b_q$ and $b_T$ based upon analysed (i.e. uninitialized) data computed with unmodified mass fluxes (i.e. the VMA was not applied to enforce non-divergence before computation of the budgets). The vertical profiles are shown for 8 x 8 diagnostic columns over central Europe on 1 August 1991, 00 GMT ± 6 h; this day was characterized by heavy rainfall centred at Salzburg, Austria (see Dorninger et al. 1992). The pattern of $b_T$ (Fig. 17(a)) is seriously distorted; in most columns maximum values exceed 1000 W m$^{-2}$. It is obvious that the budget presented in Fig. 17(a) is unacceptable owing to the effect illustrated in the introduction, Eqs. (1.1) through (1.5). Specifically, there is no point in basing vertical integrals upon the profiles of Fig. 17(a).

The moisture budget $b_q$ computed with mass fluxes not modified by the VMA (Fig. 16(a)) is less seriously distorted than is the heat budget. However, the frequent peaks of $b_q$ in the lowest troposphere, sometimes exceeding 500 W m$^{-2}$, are unrealistic. It seems clear that they are caused by errors in $\partial \omega / \partial p$ in the boundary layer as discussed above (Fig. 9(b)).

The subjective impression that the budgets of Figs. 16(a) and 17(a), computed with unmodified mass fluxes, are 'distorted' or 'unacceptable' can be made more objective by
Figure 16. Vertical profiles of the moisture budget $b_q$ in units of W m$^{-2}$ for an array of 8 $\times$ 8 diagnostic columns over central Europe; scale as indicated on top. Input: analysed ECMWF data with (a) unmodified mass flux (statistics of $b_q$: -53/160/151 units), and (b) modified mass flux (statistics of $b_q$: -46/88/75 units).
Figure 17. As Fig. 16 except for heat budget $b_T$. Statistics of $b_T$: (a) -205/1798/1786, (b) 20/121/119.
considering the imbalances \((\text{imb})_q\) and \((\text{imb})_T\) shown in Figs. 18(a) and 19(a) respectively. For example, the r.m.s. value of \((\text{imb})_T\) is 518 W m\(^{-2}\) with individual values exceeding 1000 W m\(^{-2}\), which is unacceptable indeed. The r.m.s. value of \((\text{imb})_q\) is less dramatic, but yet too high (see Table 2).

<table>
<thead>
<tr>
<th>Data</th>
<th>(b_q)</th>
<th>(s_q)</th>
<th>((\text{imb})_q)</th>
<th>(b_T)</th>
<th>(s_T)</th>
<th>((\text{imb})_T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Without VMA</td>
<td>analysed</td>
<td>160</td>
<td>134</td>
<td>63</td>
<td>1798</td>
<td>1697</td>
</tr>
<tr>
<td></td>
<td>initialized</td>
<td>112</td>
<td>101</td>
<td>57</td>
<td>1219</td>
<td>1160</td>
</tr>
<tr>
<td>With VMA</td>
<td>analysed</td>
<td>88</td>
<td>84</td>
<td>46</td>
<td>121</td>
<td>111</td>
</tr>
<tr>
<td></td>
<td>initialized</td>
<td>87</td>
<td>83</td>
<td>42</td>
<td>87</td>
<td>95</td>
</tr>
</tbody>
</table>

Results are given for computations without and with application of the VMA, and analysed (i.e. uninitialized) and initialized ECMWF data, for 1 August 1991, 00 GMT ± 6 h. See text for explanation of column headings.

It is necessary at this point to describe in more detail the computation of the imbalances in DIAMOD. They consist of two components: the column vertical mean, and the vertical profile. The column means are determined by (4.1) and (4.2) (see also Hantel et al. 1993). The profiles, however, are specified externally by an error model. For the latter, the profile of \((\text{imb})_q\) is specified to decrease exponentially in the vertical, consistent with the equivalent decrease of moisture; the profile of \((\text{imb})_T\) is assumed to be vertically constant. These remarks imply that the mean imbalance is an objective measure of the degree to which analysed data are consistent with the budget equations.

Application of the VMA to the mass fluxes before the computation of the grid-scale budgets results in the fields shown in Figs. 16(b) through 19(b). In the moisture budget (Fig. 16(b)) the boundary-layer peaks of \(b_q\) have disappeared. This results in a clearer representation of the maximum precipitation area (Western Austria, south-eastern Germany; not shown), which is now characterized by maximum negative \(b_q\), as it should be from consideration of the budget equation (4.1). Just south of the Alps, where the rain abruptly stopped, the moisture budget is now almost negligible. Similarly, the sensible-heat budget \(b_T\) is improved when computed with mass fluxes modified by the VMA (Fig. 17(b)). In the region of the rain maximum, \(b_T\) is maximum and positive, as it should be.

These remarks, based upon meteorological evidence, are further supplemented by the fact that the VMA reduces the imbalances in the budget equations. In the case of \((\text{imb})_q\), the reduction is about 30% (Fig. 18(b) and Table 2); in the case of \((\text{imb})_T\) the reduction is almost one order of magnitude (Fig. 19(b) and Table 2). Reductions of this size are in accord with the results of Hantel (1987). The final imbalances are now tolerable and of the order of 46 W m\(^{-2}\) and 66 W m\(^{-2}\) (Table 2). Note that these results may be different in different meteorological situations.

The results obtained by using initialized ECMWF data (not shown except for the statistics in Table 2) are not qualitatively different from those shown in Figs. 16–19. For initialized, but unmodified, input data the pattern of \(b_T\) and, consequently, \(s_T\) is as unacceptable as in the uninitialized case. Again, application of the VMA solves the problem. Thus the difference between uninitialized and initialized data is of a quantitative nature, in the sense that all statistics are reduced by approximately 20–50% (see Table 2). However, it is noted that the statistics of the signals \(s_q\) and \(s_T\) computed from either
Figure 18. As Fig. 16 except for moisture imbalance \((\text{imb})_q\). Statistics of \((\text{imb})_q\): (a) 11/63/62, (b) 5/46/46.
Figure 19. As Fig. 16 except for heat imbalance $(\text{imb})_r$. Statistics of $(\text{imb})_r$: (a) 234/518/462, (b) 11/66/65.
analysed or initialized data, modified by the VMA, are rather similar (see Table 2, fields not shown).

From the discussion of these results no clear preference can be given to either analysed or initialized data. It is clear that both require the application of the VMA before they can be used in diagnostic studies. However, there are indications that the initialized fields may be more consistent and also more valuable in a meteorological sense. First, the imbalances are smaller for the initialized fields (Table 2). In addition, the energy budgets computed from initialized analyses allow a realistic identification of the tropopause, which is not possible by the use of analysed data (Dörner 1992). Thus it appears that initialized analyses modified by the VMA are the best input data for the subsequent budget and flux-calculation routines of a diagnostic study.

5. DISCUSSION AND CONCLUSIONS

The purpose of this study has been to present the solution to the problem of how to deal with noise divergences of atmospheric mass fields. The primary motivation for this undertaking is the generally recognized necessity to use internally consistent mass flux fields in professional atmospheric budgeting studies. Specifically, the question is addressed of how to enforce strict non-divergence in pressure coordinates given a pre-specified, diagnosed, 3D wind field (or mass flux field in the discrete situation) with non-zero 3D divergence. The methodology proposed describes the computation of a 3D modifying field, with the property that the sum of the diagnosed and modifying fields results in a modified field that is indeed strictly non-divergent.

The solution to the problem outlined has been described in a rigorous form for both the continuous (section 2) and discrete (section 3) situation by consideration of a variational problem. It is found that the modifying field that is used to achieve strict non-divergence possesses two desirable properties: it is minimum in an r.m.s. sense, and it does not change the vorticity of the diagnosed field. In addition, the calculation of the modifying field—denoted as variational modification algorithm (VMA)—simply involves the solution of a Poisson equation subject to Neumann boundary conditions with the inhomogeneous term given by the noise divergence. A numerical algorithm is presented for the highly efficient implementation of the VMA (see appendices).

The theory proposed in this paper relates back to earlier work by Hacker (1981) and Hanzel and Haase (1983) (see also sections 1 and 2). However, the developments here are rigorously based on the variational method. Thus, in the continuous situation there is no need to employ Helmholtz's theorem for the a priori decomposition of the wind field into its divergent and rotational components as suggested by Hanzel (1986). This implies that the result of Hanzel (1986) is derived with a more general specification of the boundary conditions. The results relating to the discrete problem are presented here in a general and theoretically satisfactory form for the first time.

Diagnostic studies on a global scale (e.g. Hanzel and Haase 1983), or on a regional scale (Hanzel 1987; Döringer et al. 1992), or high-resolution diagnostics over complex terrain (e.g. Moussiopoulos and Flasak 1986), usually utilize data from an external database as basic input data, like the MARS system at the ECMWF.

The data that are entered into MARS are internally highly consistent products of an analysis/assimilation scheme (see first box in Fig. 20). However, in the course of the archiving process (involving transformation from model coordinates onto more standard coordinates, like standard pressure levels), as well as during the unavoidable process of transforming and interpolating the archived data onto a different diagnostic grid, inconsistencies (i.e. noise divergences) are inevitably introduced into the mass field (see
Figure 20. Flow chart from level of objective analysis (e.g. by ECMWF data-assimilation scheme (top box)) to level of evaluation for diagnostic purposes. The data link (second box) between analysis and diagnostic level comprises the post-processing stage that yields fields of diagnosed 3D wind as stored in grid-point form in, for example, the MARS archive of the ECMWF. Further processing (third box) in the present study requires integration of this grid-point wind over faces of diagnostic boxes (i.e. finite volumes of atmosphere). This yields diagnosed mass flux components as input for diagnostic budgets of heat and other quantities. Diagnosed mass flux is contaminated with spurious noise divergence largely because of interpolation and integration procedures. Variational modification algorithm (VMA) is used to make modified mass flux non-divergent everywhere in the domain. These non-divergent modified mass fluxes may be used for further diagnostic studies (bottom box).
second box in Fig. 20). For example, replacing the archived $\omega$-fields at 1000 hPa by the surface-pressure tendencies (see beginning of section 4) represents one source for such inconsistencies. The only way to avoid the introduction of these inconsistencies is to perform the budget calculations in the original coordinate system in which the mass flux field has originally been diagnosed and in which it is consistent. However, this can be impractical for a number of reasons. For example, the ECMWF data are more widely accessible on standard pressure levels than on the internal model levels. Also, the coordinate system chosen here offers the clear advantage of dealing with boxes of equal mass (see section 3).

The result of these processes is that the data available in standard situations for diagnostic purposes (i.e. the data to enter the third box in Fig. 20) exhibit spurious noise divergences even in the case of the high-quality wind fields like those routinely provided by the ECMWF. For the specific situation considered, the magnitude of these noise divergences is of the order of $10^{-6}$ s$^{-1}$ (see section 4(a)); however, this result is presumably independent of the specific meteorological situation.

From this result and the above considerations it may be tempting at this point to call for a different set of pressure surfaces in the MARS archive at the ECMWF in order to reduce interpolation errors. While steps in this direction would certainly be beneficial, they, in principle, cannot eliminate the interpolation problem, simply because in some studies a different diagnostic grid might be preferred. In this sense it will always be necessary to check a given mass flux field obtained from an arbitrary source, low quality or high quality, for internal mass consistency. If consistency is lacking, it must be enforced by the VMA or by an equivalent method.

The potential of the VMA to remove these noise divergences has been demonstrated in detail in section 4(a) (see also third box in Fig. 20). The 2D and 1D components of the 3D divergence of the mass flux field have been discussed separately. The rotational component of the mass flux field is absolutely much larger than its divergent part; however, the rotational part is not modified by the VMA. Further, the horizontal mass flux component is predominantly rotational, whereas the vertical component is both rotational and divergent. It has been found that the absolute modification of the divergent part is about the same in the horizontal and vertical directions. It follows that the relative modification tends to be larger in the vertical than in the horizontal mass flux component.

The patterns of the 2D and 1D mass flux divergences have been found to be relatively insensitive to the VMA. This suggests that the routinely analysed wind fields implicitly carry horizontal and vertical divergence distributions that are quite robust with respect to data interpolation from the analysis coordinate system to standard pressure levels. This implies that the ECMWF analyses of these important kinematic parameters deserve credence.

A further result of this study is that in an overall r.m.s. sense the modification necessary to enforce 3D non-divergence is 7% for uninitialized and 6% for initialized data; the percentages are with respect to the diagnosed mass flux and are valid for the specific situation considered. These figures are in accord with the results of Hantel (1987) who found a necessary modification of 5% for boxes of the same size as used here, but for daily averages. In addition, the detailed investigation of the uninitialized and initialized mass fluxes (in particular the vertical component) before and after application of the VMA has revealed that the modification of the mass flux field through the initialization procedure at the ECMWF is considerably larger than the modification required to enforce non-divergence through application of the VMA.

The beneficial impact of the VMA upon energy-budget calculations has been demonstrated in section 4(b) through the use of a sophisticated diagnostic model. The spurious
noise divergences of $10^{-6}$ s$^{-1}$ (see above) have been shown to lead to unacceptable budgets of latent and sensible heat, as well as to energy-budget errors of the order of 500 W m$^{-2}$. These results support the qualitative argument made at the beginning of section 1, and substantiate the imperative use of appropriate mass flux modification at the beginning of the diagnostic calculations (see bottom box in Fig. 20).

In the case of uninitialized data, application of the VMA has led to a reduction of the r.m.s. values of the sensible-heat-budget imbalance from an intolerable 518 W m$^{-2}$ down to a moderate 66 W m$^{-2}$, with a less dramatic reduction of approximately 30% of the latent-heat-budget imbalance. These values are of the same order of magnitude for initialized data. Smaller budget imbalances have led to the preliminary conclusion that initialized fields might be more useful for diagnostic studies.

It seems appropriate at this point to view the methodology presented in this paper in the perspective of the often-cited paper by O'Brien (1970) who discussed several solutions to the classical vertical-velocity problem. As a first step, O'Brien considered the situation that only the horizontal wind field (i.e. its divergence) is available in diagnosed form, while the vertical velocity $\omega$ is to be gained from the horizontal wind. The problem to be faced, of course, is that the continuity equation is a first-order differential equation for $\omega$ in $p$, to be solved—based on the 2D analysed divergence—subject to two boundary conditions (e.g. at the top and bottom of the atmosphere). In order to circumvent this unsolvable problem, O'Brien obtained—by differentiation of the continuity equation with respect to $p$—a second-order differential equation in $p$ which can be solved unambiguously for the vertical velocity. However, the principal limit of this approach is that the emerging $\omega$ does not necessarily satisfy the (undifferentiated form of the) continuity equation. O'Brien (1970) proceeds to propose several alternative approaches based on the variational method to diagnose the vertical velocity from modified horizontal divergences.

Meteorological data bases have changed since then to the extent that $\omega$ can now also be considered to be diagnosed, either through independent solution of the omega equation or through an internally consistent data-assimilation scheme. It is at this point where the methodology presented here is applicable: in the case that all wind (or mass flux) components, including $\omega$, have been independently diagnosed, the VMA is applicable and indeed extremely useful. In this sense we dare to say that the VMA is the final solution to the classical vertical-velocity problem. In addition, the VMA seems to be a most appropriate tool to enforce non-divergence for any given data set of mass fluxes, an imperative preliminary step to be performed before subsequent budget calculations.

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APPENDIX A

The decoupling method

The VMA is described in section 3. It was shown that the necessary modification is obtained by solving a 3D Poisson equation. This appendix is devoted to the detailed description of how to solve this Poisson equation.

The solution method presented here is denoted as decoupling method because it effectively amounts to decoupling the three dimensions from each other by a sequence of similarity transformations; this allows one to solve the transformed equations almost trivially. This method is applicable owing to the form of the discrete Laplacian and the special choice of boundary conditions. The idea of decoupling dimensions has been used in normal-mode initialization (e.g. Machenhauer 1977; Daley 1981) and is of particular advantage in the present context.

Consider the Poisson equation (3.21):

\[ \chi_{i+1,j,k} + \chi_{i-1,j,k} + \chi_{i,j+1,k} + \chi_{i,j-1,k} + \chi_{i,j,k+1} + \chi_{i,j,k-1} - 6\chi_{i,j,k} = \bar{D}_{i,j,k} \]  
(A.1)

with:

\[ i = 1, \ldots, I; \quad j = 1, \ldots, J; \quad k = 1, \ldots, K \]  
(A.2)

subject to the staggered Neumann boundary conditions (3.22)–(3.24).

As a first step (A.1) is rewritten as:

\[ a_{i+1,j} + a_{i-1,j} + a_{i,j+1} + a_{i,j-1} + A a_{i,j} - 6 a_{i,j} = x_{i,j} \]  
(A.3)

with the definitions of the vectors \( a \) and \( x \):

\[ a_{i,j} = (\chi_{i,j,1}, \chi_{i,j,2}, \ldots, \chi_{i,j,K})^T \]  
(A.4)

\[ x_{i,j} = (\bar{D}_{i,j,1}, \bar{D}_{i,j,2}, \ldots, \bar{D}_{i,j,K})^T \]  
(A.5)

and the symmetric \((K \times K)\) matrix \( A \):

\[
A = \begin{pmatrix}
1 & 1 & 0 & 0 & \ldots & 0 & 0 \\
1 & 0 & 1 & 0 & \ldots & 0 & 0 \\
0 & 1 & 0 & 1 & \ldots & 0 & 0 \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
& & & & & & \\
0 & 0 & \ldots & 1 & 0 & 1 & \ldots \\
0 & 0 & \ldots & 0 & 1 & 0 & 1 \\
0 & 0 & \ldots & 0 & 0 & 1 & 1 \\
\end{pmatrix}
\]  
(A.6)

The superscript \( T \) denotes the transpose. The boundary conditions in the \( k \)-direction are observed through the special form of \( A \). Since \( A \) is symmetric, it can be similarity-transformed as:

\[ A = X P X^T \]  
(A.7)

or, equivalently:

\[ P = X^T A X \]  
(A.8)
where both \( \mathbf{X} \) and \( \mathbf{P} \) are of the same dimension as \( \mathbf{A} \). The columns of the orthonormal matrix \( \mathbf{X} \) (i.e., \( \mathbf{X}^T \mathbf{X} \) is the unit matrix) are the normalized eigenvectors of \( \mathbf{A} \), whereas \( \mathbf{P} \) is a diagonal matrix whose elements are the eigenvalues of \( \mathbf{A} \), which are all real due to the symmetry of \( \mathbf{A} \).

Premultiplication of (A.3) with \( \mathbf{X}^T \) results in:

\[
\bar{a}_{i+1,j} + \bar{a}_{i-1,j} + \bar{a}_{i,j+1} + \bar{a}_{i,j-1} + \mathbf{P} \bar{a}_{i,j} = \bar{x}_{i,j}
\]  

(A.9)

with the transformed vectors \( \bar{a} \) and \( \bar{x} \) defined as:

\[
\bar{a}_{i,j} = \mathbf{X}^T a_{i,j}
\]

(A.10)

\[
\bar{x}_{i,j} = \mathbf{X}^T x_{i,j}.
\]

(A.11)

Equation (A.9), being the result of the first step, represents \( K \) decoupled 2D problems, since \( \mathbf{P} \) is a diagonal matrix. This may be seen by rewriting (A.9) in component form as:

\[
\bar{a}_{i,k+1,j} + \bar{a}_{i,k-1,j} + \bar{a}_{i,k,j+1} + \bar{a}_{i,k,j-1} + (p^k - 6)\bar{a}_{i,k,j} = \bar{x}_{i,k,j} \quad k = 1, \ldots, K
\]

(A.12)

where \( p^k \) represents the \( k \)th diagonal element of \( \mathbf{P} \) and the superscript \( k \) is used to denote the \( k \)th element of the corresponding column vectors \( \bar{a} \) and \( \bar{x} \). Note that the form of Eq. (A.12) is entirely equivalent to (A.1) with the advantage that the \( k \)-dimension has been eliminated; or, more precisely, the superscript \( k \) does not appear in shifted form (i.e. \( k \pm 1 \)) any longer. Naturally, the second and the third step are completely analogous to the first, and are thus outlined only briefly.

As a second step, for fixed \( k \), Eq. (A.12) is rewritten as:

\[
\mathbf{b}_{i+1}^k + \mathbf{b}_{i-1}^k + \mathbf{B} \mathbf{b}_i^k + (p^k - 6)\mathbf{b}_i^k = \mathbf{y}_i^k
\]

(A.13)

with the definitions of the vectors \( \mathbf{b} \) and \( \mathbf{y} \):

\[
\mathbf{b}_i^k = (\bar{a}_{i,1}^k, \bar{a}_{i,2}^k, \ldots, \bar{a}_{i,J}^k)^T
\]

(A.14)

\[
\mathbf{y}_i^k = (\bar{x}_{i,1}^k, \bar{x}_{i,2}^k, \ldots, \bar{x}_{i,J}^k)^T
\]

(A.15)

and the symmetric \( (J \times J) \) matrix \( \mathbf{B} \) that is of the same form as \( \mathbf{A} \). Again the boundary conditions are appropriately incorporated through the definition of \( \mathbf{B} \). Completely similar to (A.7) through (A.11) one obtains:

\[
\mathbf{B} = YQY^T
\]

(A.16)

\[
\mathbf{Q} = Y^T \mathbf{B} Y
\]

(A.17)

\[
\tilde{\mathbf{b}}_{i+1}^k + \tilde{\mathbf{b}}_{i-1}^k + \mathbf{Q} \tilde{\mathbf{b}}_i^k + (p^k - 6)\tilde{\mathbf{b}}_i^k = \tilde{\mathbf{y}}_i^k
\]

(A.18)

with the definitions:

\[
\tilde{\mathbf{b}}_i^k = Y^T \mathbf{b}_i^k
\]

(A.19)

\[
\tilde{\mathbf{y}}_i^k = Y^T \mathbf{y}_i^k.
\]

(A.20)

Similar to (A.9), Eq. (A.18) is the result of the second step and represents \( K \cdot J \) decoupled 1D problems, because \( \mathbf{Q} \) is a diagonal matrix. This becomes clearer by rewriting (A.18) in the form:

\[
\tilde{\mathbf{b}}_{i+1}^{k,j} + \tilde{\mathbf{b}}_{i-1}^{k,j} + (p^k + q^j - 6)\tilde{\mathbf{b}}_i^{k,j} = \tilde{\mathbf{y}}_i^{k,j} \quad j = 1, \ldots, J; \quad k = 1, \ldots, K
\]

(A.21)

where \( q^j \) represents the \( j \)th diagonal element of \( \mathbf{Q} \) and, again, the superscript \( j \) is used to denote the \( j \)th element of the corresponding vectors. At this point the only remaining shifted index is \( i \), which is removed in the third step analogously to the foregoing.
In the third step, for fixed $k$ and $j$, Eq. (A.21) is expressed in the following form:

$$Ckij + (p^k + q^j - 6)e^{kij} = z^{kij}$$  
(A.22)

with the definitions of the vectors $e$ and $z$:

$$e^{kij} = (b_1^{kij}, b_2^{kij}, \ldots, b_{l}^{kij})^T$$  
(A.23)

$$z^{kij} = (y_1^{kij}, y_2^{kij}, \ldots, y_{l}^{kij})^T$$  
(A.24)

and the symmetric $(I \times I)$ matrix $C$ that is of the same form as $A$. Again the boundary conditions are appropriately incorporated through the definition of $C$. Similar to Eqs. (A.7) through (A.11) the similarity transformation results in:

$$C = ZRZ^T$$  
(A.25)

$$R = Z^TCZ$$  
(A.26)

$$Re^{kij} + (p^k + q^j - 6)e^{kij} = \tilde{z}^{kij}$$  
(A.27)

with:

$$\tilde{e}^{kij} = Z^Te^{kij}$$  
(A.28)

$$\tilde{z}^{kij} = Z^Tz^{kij}.$$  
(A.29)

Similar to Eqs. (A.9) and (A.18), Eq. (A.27) is the result of the third step and represents $K \cdot J \cdot I$ decoupled zero-dimensional problems, because $R$ is a diagonal matrix. This is seen more clearly if (A.27) is written for its components:

$$(p^k + q^j + r^l - 6)\tilde{z}^{k,j,i} = \tilde{z}^{k,j,i}$$  
(A.30)

where the range of the superscripts is given in (A.2) and $r^l$ represents the $l$th diagonal element of $R$.

At this point the basic issues of the decoupling method are clear. Given the right-hand side of Eq. (A.30)—which is obtained from $D_{l,j,k}$ by going through the three transformation steps (i.e. (A.11), (A.20), (A.29))—it is a trivial matter to compute $\tilde{z}^{k,j,i}$. Thereafter, the decoupling steps must be inverted in order to obtain $u_{l,j,k}$ from $\tilde{z}^{k,j,i}$, which is achieved by using Eqs. (A.28), (A.19), and (A.10).

A number of further remarks are appropriate. First, it is easy to see that the coefficient of $\tilde{z}^{k,j,i}$ in (A.30) vanishes exactly once, because the largest eigenvalue of $A$, $B$, and $C$ is exactly two and appears once for each matrix. This, in turn, implies that one unknown cannot be computed, but must be specified arbitrarily. This remark is in agreement with the fact that the solution of the Poisson equation (with staggered Neumann boundary conditions) is indeterminate up to an additive constant (see also end of section 3).

Second, it is clear that given the size of a certain problem (namely, $I$, $J$, and $K$) the necessary similarity transformations may be precomputed. These precomputed results are evidently advantageously used if the solution is repeatedly sought for different right-hand sides. This possibility to perform certain computations independently of the actual input data has similarities to the Fourier transform method. When measuring the computing times necessary to solve the Poisson equation with the decoupling method, the time needed for diagonalizing matrices has not been taken into account (see also appendix B).

Third, a technical point is mentioned. It is certainly possible to combine the three transformation steps by performing the matrix multiplications at once. This, however, is
highly inefficient and should be avoided; the efficient way is to proceed as outlined here, namely, to transform individual vectors while holding the remaining two indices constant.

Finally, it is obvious that the decoupling method is easily generalized to an arbitrary number of dimensions. In the present context, the decoupling method has been implemented for the 3D case in the DIRECTS routine which is available from the first author upon request.

**Appendix B**

*The decoupling method versus the Fourier transform method*

In contrast to the decoupling method (see appendix A), the more traditional approach to solve a Poisson (or Helmholtz) equation directly relies on the fast Fourier transform (FFT) (e.g. Temperton 1983; Adams et al. 1982; Boisvert 1987a, b; LeBail 1972; Schumann and Sweet 1988; Wilhelmson and Ericksen 1977). However, particular care and effort is necessary to implement boundary conditions other than cyclic in connection with the Fourier transform method correctly (e.g. Schumann and Sweet 1988). In fact this problem may make certain packages, which simply do not provide the desired boundary conditions, useless.

In order to compare the decoupling method described in appendix A with the Fourier transform method, a Fourier decomposition algorithm is required that allows one to specify the use of staggered Neumann boundary conditions. None of the Poisson solvers referenced above has proved to be appropriate for this task. However, the algorithm SHAFT3 described by Flasak and Moussiopoulos (1988) does supply the facility to choose staggered Neumann boundary conditions in all three coordinate directions.

The algorithm SHAFT3 does a Fourier decomposition in the horizontal coordinate directions and uses an elimination algorithm in the vertical direction. Due to the possibility of correctly specifying the boundary conditions we have compared our algorithm DIRECTS (see appendix A) with SHAFT3. We expect that the results are typical for the comparative behaviour of the decoupling and the Fourier transform method.

In Fig. B.1 the computing times necessary to solve the 3D Poisson equation by both DIRECTS and SHAFT3 are displayed. The computing times are given in seconds and have been obtained by running both algorithms on a Macintosh IIci. The dimension of the problem is indicated by \( N \) which means that the equation is solved on a cube of volume \( N^3 \) (i.e. \( I = J = K = N \)). For given \( N \), both algorithms allow one to perform certain computations that are independent of the actual numbers given in the right-hand side of the Poisson equation (like diagonalizing the coefficient matrices in DIRECTS). The time needed for these preparing computations (being of the order of 10% of the total computing time of DIRECTS and being negligible for SHAFT3) is not included in the computing times shown in Fig. B.1.

The results visible in Fig. B.1 are not surprising. DIRECTS operates close to an order \( N^3 \) process, whereas the computing time necessary for SHAFT3 is in accordance with the order of the amount of work necessary to perform an FFT. Thus, the Fourier transform method is clearly superior to the decoupling method with regard to computing time.

However, certain other aspects of both algorithms may be of interest, too. First, the storage requirements for both algorithms are approximately equal. Second, in the case that \( N \) is not the product of small primes, an FFT is not really efficient. In fact it can be
seen that SHAFT3 allows one to solve the problem only for certain values of $N$. From experiments with HW3CRT (Adams et al. 1982) which allows one to use an arbitrary value of $N$ and which also uses the Fourier transform method (it does not, however, allow for staggered Neumann boundary conditions), it is found (not shown) that the computing times of the Fourier transform method and the decoupling method become similar (within several ten per cent) for certain values of $N$ (e.g. 37) that are disadvantageous for an FFT.

The third remark applies to the complexity of the code necessary to solve a given problem. In this respect the decoupling method is clearly superior to the Fourier transform method. For example, the SHAFT3 routines consist of seven times more FORTRAN statements than the DIRECTS routines (236 versus 1760; this includes all auxiliary routines like FFT and diagonalization algorithms).

In view of these comments favourable for either algorithm, the user must decide which algorithm to employ, depending on the aspect considered. In a non-operational environment with no crucial time limits we have chosen the decoupling method because of its apparent brevity and clarity.
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