Structural instability of atmospheric flows under perturbations of the mass balance and effect in transport calculations

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Abstract. Several methods to estimate the velocity field of atmospheric flows, have been proposed to the date for applications such as emergency response systems, transport calculations and for budget studies of all kinds. These applications require a wind field that satisfies the conservation of mass but, in general, estimated wind fields do not satisfy exactly the continuity equation. An approach to reduce the effect of using a divergent wind field as input in the transport-diffusion equations, was proposed in the literature. In this work, a linear local analysis of a wind field, is used to show analytically that the perturbation of a large-scale nondivergent flow can yield a divergent flow with a substantially different structure. The effects of these structural changes in transport calculations are illustrated by means of analytic solutions of the transport equation.

1. Introduction
Several methods to estimate trajectory models for long-range atmospheric transport calculations, have been proposed [1]. However, conservation of mass is not always exactly satisfied [2,3]. Although several authors have pointed out that the use of a wind field that does not satisfy exactly the continuity equation, can introduce significant errors in transport calculations of chemical species [3,4], the accuracy with which the continuity equation is satisfied, is not always reported in works that propose methods for estimating wind fields for transport calculations. Since large scale atmospheric flows are nearly nondivergent, it is generally accepted that a mass-balanced wind field has to satisfy the continuity equation in its simplest form $\nabla \cdot \mathbf{v} = 0$. Simple methods applied to wind field analysis can yield a divergence of order $10^{-5}$ s$^{-1}$. In this work we show that a divergence of this order can change the structure of a large-scale nondivergent flow.

A proposed method to reduce the effect of using a divergent field in transport calculations, consists in subtracting the value of $\nabla \cdot \mathbf{v}$ at each grid point where the transport equations are solved with standard spatial-discretization methods [4]. The results of this work show that this procedure can yield results with a significant error because the structure of a nondivergent wind field can be different from that of a divergent one with a divergence of order $10^{-5}$ s$^{-1}$. 
2. Types of mass-balanced flows and their perturbations

The structure of an atmospheric flow $\mathbf{v}=\mathbf{u}^0+i\mathbf{v}^0$ in the vicinity of an arbitrary point $(x_0,y_0)$ can be studied by means of the linear terms of its Taylor series. Let us consider a Cartesian system with its origin at $(x_0,y_0)$, then we have

$$ u = M_{11}x + M_{12}y + u_{00}, \quad v = M_{21}x + M_{22}y + v $$

where the matrix $\mathbf{M}=[M_{ij}]$ is the velocity gradient at the origin. In terms of the parameters

$$ \delta = \nabla \cdot \mathbf{v}/2, \quad \omega = \mathbf{k} \cdot \nabla \times \mathbf{v}/2, \quad a = (M_{11} - M_{22})/2, \quad b = (M_{12} + M_{21})/2 $$

we have

$$ u = (\delta + a)x + (b - \omega)y + u_{00}, \quad v = (b + \omega)x + (\delta - a)y + v $$

Hence the velocity field $\mathbf{v}$ can be written as $\mathbf{v}^0 + \mathbf{u}^0$ where $\mathbf{v}^0$ and $\mathbf{u}^0=\delta\,(x\,i+y\,j)$ are the nondivergent and divergent components of $\mathbf{v}^0$. Since large scale atmospheric flows are nearly nondivergent, $\mathbf{v}^0$ will be considered an ideal mass-balanced flow, and $\mathbf{u}^0$ will quantify the perturbation of the mass balance of $\mathbf{v}^0$. Accordingly, the mass-unbalanced flow $\mathbf{v}^0$ with $\delta \neq 0$ and the mass balanced one $\mathbf{v}^0$ will be referred to as a divergent flow (DF) and a nondivergent flow (NDF), respectively.

The discriminant of equation $\det(M - \lambda I) = 0$ and the eigenvalues of $\mathbf{M}$ are given by

$$ \Delta = \alpha^2 + \beta^2 - \omega^2, \quad \lambda_1^2 = \delta + \sqrt{\Delta}, \quad \lambda_2^2 = \delta - \sqrt{\Delta} \quad (4) $$

For a NDF $\mathbf{v}^0$ the eigenvalues $\lambda_1 = \sqrt{\Delta}$, $\lambda_2 = -\sqrt{\Delta}$, imply that $\mathbf{v}^0$ has one of the following structures. Case (NDF-a): For $\Delta > 0$ the eigenvalues are real and have different signs, $\mathbf{v}^0$ has a hyperbolic structure whose principal directions are given by the eigenvectors of $\mathbf{M}$. Case (NDF-b): For $\Delta < 0$ the eigenvalues are imaginary and $\mathbf{v}^0$ has an elliptic structure. Case (NDF-c): For $\Delta = 0$ there is one (real) eigenvalue, $\mathbf{v}^0$ has a linear structure since the trajectory of each fluid particle is a straight-line and the eigenvector of $\mathbf{M}$ yields the unique principal direction. A DF $\mathbf{v}^0$ admits the same structures but the eigenvalue expression (4) implies that $\mathbf{v}^0$ can have additional structures. Case (DF-a): For $\delta \neq 0$ and $\Delta^0 > 0$ there are three types of flows: (i) For $|\delta| < \Delta^0$ the flow $\mathbf{v}^0$ is hyperbolic. (ii) For $\delta = \Delta^0$ one eigenvalue $\lambda_j$ is zero and another $\lambda_k$ has the sign of $\delta$. The principal axis associated to $\lambda_j$ consists of equilibrium points which are sources for $\delta > 0$ and sinks for $\delta < 0$. (iii) For $|\delta| > \Delta^0$ the eigenvalues have the sign of $\delta$ and $\mathbf{v}^0$ has a parabolic structure, the trajectories behave like parabolas that converge toward the origin for $\delta > 0$ and diverge for $\delta < 0$. Case (DF-b). For $\delta \neq 0$ and $\Delta^0 < 0$ the DF $\mathbf{v}^0$ is similar to the corresponding elliptic NDF, the trajectories are spirals that converge toward the origin for $\delta > 0$ and diverge for $\delta < 0$.

Cases (DF-a)-i), (DF-a)-ii), show that the perturbation $\mathbf{u}^0$ of a NDF $\mathbf{v}^0$ can yield a DF $\mathbf{v}^0$ with a different structure. To determine the structural differences between $\mathbf{v}^0$ and $\mathbf{v}^0$ with characteristic values of large scale atmospheric flows, we can define the characteristic value of a variable $f(x,y)$ in a region $R=\{0 \leq x \leq L, 0 \leq y \leq L\}$ with length scale $L$, by its mean value (denoted by $\bar{f}$) on $R$. According to equation (3) the relation between mean values $\bar{u}$, $\bar{v}$, $\bar{x}$, $\bar{y}$ and the parameters (2) is

$$ \bar{u} = (\delta + a)\bar{x} + (b - \omega)\bar{y} + u_{00}, \quad \bar{v} = (b + \omega)\bar{x} + (\delta - a)\bar{y} + v $$

with $\bar{x} = \bar{y} = L/2$. By simplicity we set $u = \bar{u} = v = 0$. These expressions yield $a$, $b$, in terms of $\delta$, $\omega$, and the mean values, namely,

$$ a = (\alpha + 2\alpha\omega)/2\bar{x}, \quad b = (\beta - 2\delta)/2\bar{x} \quad (6) $$

where we set $\alpha = \bar{u} - \bar{v}$, $\beta = \bar{u} + \bar{v}$. Since the last relations imply that there is a one-to-one relation between the pairs $\{\bar{u},\bar{v}\}$, $\{a,\beta\}$, the latter will used in our study. The discriminants of $\mathbf{v}^0$, $\mathbf{v}^0$, are

$$ \Delta = (\alpha^2 + \beta^2 + 4\alpha\bar{x}\omega)/4\bar{x}^2, \quad \Delta^0 = \Delta + q(\delta, \beta, \bar{x}) \quad (7) $$

where we set $q(\delta, \beta, \bar{x}) = \delta(\delta - \beta/\bar{x})$. As is shown below, the characteristic values for large scale atmospheric flows $\delta$, $\omega \sim 10^{-3}$ s$^{-1}$, $\alpha, \beta \sim 10$ ms$^{-1}$, $L=10^3$ km ($\bar{x}=5\times10^3$ m), of large scale atmospheric flows can yield fields $\mathbf{v}^0$, $\mathbf{v}^0$ with different structure.

To analyze the effect of a mass imbalance in transport calculations we consider the transport equation
\[ \partial_t \delta^\parallel + \nabla \cdot (c \parallel \delta^\parallel) = -k \parallel \delta. \]

Superscript \( \delta \) indicates that \( c^\parallel \) is solution of equation (8) with a field \( \delta^\parallel \) having divergence \(2\delta^\parallel \).

A scale analysis shows that the diffusion term can be neglected for large scale flows. Replacing \( \nabla \cdot \delta^\parallel = 2\delta \) into equation (8) it takes the form

\[ \partial_t \delta^\parallel + \nabla \cdot (\delta^\parallel \nabla \delta^\parallel) = -k \delta^\parallel - 2\delta \delta^\parallel. \]

We see that the perturbation term \( \Delta^\parallel \) in a DF \( \delta^\parallel = \delta^0 + \Delta^\parallel \) generates a fictitious reaction term \(-2\delta \delta^\parallel \). Since characteristic values of \( k \) are of order \(10^{-12}\text{s}^{-1} \), a divergence \(|\delta| \) of order \(10^{-2}\text{s}^{-1}\) yields unrealistic solutions \( \delta^\parallel \). The solution proposed in the literature [3,4] to reduce the effect of using a DF \( \delta^\parallel \) is to subtract the term \( \delta^\parallel \nabla \delta^\parallel \) on the left hand side of equation (8). This is equivalent to solving the equation

\[ \partial_t \delta^\parallel + \nabla \cdot (\delta^\parallel \nabla \delta^\parallel) = -k \delta^\parallel \]

Transport calculations reported below were made by solving equation (10) analytically with the characteristics method and \( c = \exp\left[\frac{-((x - x_0)^2 - (y - y_0)^2)}{\sigma^2}\right] \), \( \sigma = 0.5\text{km} \) at \( t = 0 \). For brevity, we shall consider some cases where the structure of a DF \( \delta^\parallel \) differs from that of the NDF \( \delta^0 \).

Let us consider cases where an hyperbolic NDF \( \delta^0 \) becomes an elliptic DF \( \delta^\parallel \). A condition to go from \( \Delta^0 > 0 \) to \( \Delta^\parallel < 0 \), is \( q = \delta (\beta - \beta / \bar{x}) < 0 \). Since the minimum value of \( q \) is \(-\beta^2/4 \bar{x}^2 \) at \( \delta_m = \beta / 2 \bar{x} \), condition \( \beta < 0 \) is sufficient to guarantee the existence of an interval of \( \delta \) values with which \( q < 0 \). We have the following cases:

(a) Let \( \alpha \) be fixed and \( \beta \) variable. For \( \delta = \delta_m, \delta^\parallel = \alpha (\alpha + 4 \bar{x} \alpha) \) has the minimum value \(-\alpha^2 \) at \( \alpha = -2 \bar{x} \omega \). Therefore, for \( \omega, \beta \neq 0, \delta \) such that \( \Delta^0 > 0 \), there is a set of values of \( \delta, \alpha, \beta \), for which \( \Delta^\parallel < 0 \), and the hyperbolic NDF \( \delta^0 \) becomes an elliptic DF \( \delta^\parallel \). For instance, let \( \omega=10^{-5}\text{s}^{-1}, \beta = \pm 11\text{ms}^{-1}, L=10^{-1}\text{km}, \alpha = -2 \bar{x} \omega = -10^{-1}\text{ms}^{-1}, \delta = \delta_m \), then \( \Delta^0 > 0, \Delta^\parallel = -\omega^2 \) and, by continuity, \( \Delta^\parallel < 0 \) holds for \( \delta \) near \( \delta_m \).

(b) Consider fixed \( \alpha, \beta \neq 0 \), and variable \( \delta, \omega \). According to equation (7) the critical values

\[ \delta_c = \frac{-\alpha^2 + \beta^2}{4 \bar{x} \alpha}, \quad \delta^\parallel = \delta_c - q \bar{x} / \alpha \]

are the unique ones where \( \Delta^0 \) and \( \Delta^\parallel \) change their sign. The sets \( E_{\alpha\beta} = \{ \omega : \Delta^0 < 0 \} \), \( H_{\alpha\beta} = \{ \omega : \Delta^0 > 0 \} \), are \( \omega \) values where a NDF \( \delta^0 \) is elliptic and hyperbolic, respectively. Let \( E^\parallel_{\alpha\beta} \) and \( H^\parallel_{\alpha\beta} \) be the corresponding sets of a DF \( \delta^\parallel \) with the same \( \alpha, \beta, \delta \neq 0 \). Consider \( \delta, \beta \), such that \( q < 0 \) and \( \alpha = 0 \). This yields \( \delta_c < \omega^\parallel, H^\parallel_{\alpha\beta} = (\omega^\parallel, \infty) \), \( E^\parallel_{\alpha\beta} = (-\infty, \omega^\parallel) \), and the intersection \( I^\parallel_{\alpha\beta} = (\omega^\parallel, \omega^\parallel) \) is \( \omega \) values with which an hyperbolic NDF \( \delta^\parallel \) becomes and elliptic DF \( \delta^\parallel \). Example 1: Consider \( \delta=10^{-8}\text{s}^{-1}, \beta=10\text{ms}^{-1}, L=10^{-1}\text{km}, \) which yield \( q = -10^{-10}\text{s}^{-2} \), and let \( \alpha=1\text{ms}^{-1} \), then \( \omega^\parallel = -0.05 \times 10^{-5}\text{s}^{-1}, \omega^\parallel = -5.05 \times 10^{-5}\text{s}^{-1} \), and any \( \omega \) in \( I^\parallel_{\alpha\beta} \) yields an hyperbolic NDF \( \delta^\parallel \) that becomes an elliptic DF \( \delta^\parallel \). Figures 1, 2, show \( \delta^0, \delta^\parallel \), with \( \omega = -10^{-5}\text{s}^{-1} \) and the corresponding solutions of equation (10) by means of the movement of the iso-line with \( c=0.75 \) at \( t=0 \). For \( \alpha < 0 \) and \( \delta, \beta \), such that \( q < 0 \), we get \( \omega^\parallel < \omega^\parallel \) and the sets \( H^\parallel_{\alpha\beta} = (-\infty, \omega^\parallel), E^\parallel_{\alpha\beta} = (\omega^\parallel, \infty) \), whose intersection \( I^\parallel_{\alpha\beta} = (\omega^\parallel, \omega^\parallel) \) are \( \omega \) values with which an hyperbolic NDF \( \delta^\parallel \) becomes an elliptic DF \( \delta^\parallel \).

Let us consider cases where an elliptic NDF \( \delta^0 \) becomes an hyperbolic DF \( \delta^\parallel \). A condition to go from \( \Delta^0 < 0 \) to \( \Delta^\parallel > 0 \) is \( q > 0 \), this occurs with \(|\delta| > |\beta| / \bar{x} \). Let \( \alpha > 0 \), then \( \omega^\parallel < \omega^\parallel \), \( E^\parallel_{\alpha\beta} = (-\infty, \omega^\parallel), H^\parallel_{\alpha\beta} = (\omega^\parallel, \infty) \), and the set \( I^\parallel_{\alpha\beta} = (\omega^\parallel, \omega^\parallel) \) are \( \omega \) values with which an elliptic NDF \( \delta^\parallel \) becomes and hyperbolic DF \( \delta^\parallel \). Example 2: Consider \( \alpha=10\text{ms}^{-1}, L=10^{-1}\text{km}, \) then \( \omega^\parallel = -10^{-5}\text{s}^{-1} \), for \( \delta = 10^{-5}\text{s}^{-1} \), we have \( \omega^\parallel = 3 \times 10^{-10}\text{s}^{-2}, \omega^\parallel = -2.5 \times 10^{-5}\text{s}^{-1} \), and any \( \omega \) in \( I^\parallel_{\alpha\beta} \) yield a NDF \( \delta^\parallel \) and a hyperbolic DF \( \delta^\parallel \). Figures 3 and 4 show the fields \( \delta^0, \delta^\parallel \), with \( \omega = -1.5 \times 10^{-5}\text{s}^{-1} \) and the effect in the solution of equation (10). In a similar manner, for \( \alpha < 0 \) and \( \beta, \delta \), such that \( q > 0 \), we have \( \omega^\parallel < \omega^\parallel \), \( E^\parallel_{\alpha\beta} = (\omega^\parallel, \infty) \), \( H^\parallel_{\alpha\beta} = (-\infty, \omega^\parallel) \), and the \( \omega \) values in the interval \( (\omega^\parallel, \omega^\parallel) \) yield an elliptic NDF \( \delta^0 \) whose perturbation \( \delta^\parallel \) is hyperbolic.
3. Summary and concluding remarks

Standard methods to estimate the wind field from observational data yield, in general, a field $\mathbf{v}^0 = \mathbf{v} + \mathbf{u}^\delta$ with a nonzero divergent component $\mathbf{u}^\delta$ [2,3]. The procedure suggested in the literature to make transport calculations with a DF $\mathbf{v}^\delta$ (subtracting the value of the divergence at each grid point in the transport equation [3,4]), does not consider that a perturbation of a mass-balanced flow $\mathbf{v}^0$ can yield a divergent flow $\mathbf{v}^\delta$ with a significantly different structure. Thus, the use of a DF $\mathbf{v}^\delta$ in transport calculations can yield trajectories that diverge from those given by a mass-balanced flow $\mathbf{v}^0$. According to Kitada [3], simple data assimilation methods yield a DF $\mathbf{v}^\delta$ with $\nabla \cdot \mathbf{v}^\delta$ of order $10^{-5} \text{s}^{-1}$, but the examples reported in [5] show that variational methods conceived to minimize the divergence [6], can yield fields with $\nabla \cdot \mathbf{v}^\delta$ of order $10^{-3} \text{s}^{-1}$. In these cases, the use of $\mathbf{v}^\delta$ in transport calculations can yield results with errors larger than those reported above. A more complete study of the effects of perturbing the mass-balance of a wind field in the flow structure and transport calculations will be given in a forthcoming work.
4. References
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5. Acknowledgments
One of us (R. M.) wants to thank to Conacyt for a scholarship 588339