Boundary Conditions for the Psi Equations

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ABSTRACT

This paper examines admissible boundary conditions for the quasigeostrophic psi equations that govern ageostrophic motion. Both the essential (Dirichlet-type) and natural (Neumann-type) admissible boundary conditions are derived from the variational formulations of the psi equations. Different ways of extracting the admissible boundary values from observational data are proposed.

1. Introduction

The omega (ω) equation has proved very useful in diagnostic studies of synoptic-scale vertical motion (Sutcliffe 1947; Trenberth 1978; Hoskins et al. 1978; Hoskins and Pedder 1980; Barnes 1985; Durran and Snellman 1987; Sanders and Hoskins 1990; Keyser et al. 1992). When the ω equation is applied to a limited area, homogeneous boundary conditions (i.e., zero vertical velocity) traditionally are used, not only for lower and upper boundaries but also for the lateral boundaries. Although the mathematical problem of solving for vertical motion from the ω equation (which is elliptic) with homogeneous boundary conditions is well posed, the use of homogeneous boundary conditions may be physically inappropriate for a case where vertical motion is not negligible at the boundaries. In this case, nonhomogeneous boundary conditions need to be considered. This is the motivation of this study. Specifically, this paper examines nonhomogeneous boundary conditions for a more general type of diagnostic equations—the psi equations (Hoskins and Draghici 1977). The ω equation can be derived by taking the divergence of the psi equations and eliminating the horizontal ageostrophic wind; but the vertical velocity field obtained from the ω equation relates to the divergent part of the horizontal ageostrophic wind only. The rotational part of the horizontal ageostrophic wind can be obtained only from solution of more general types of diagnostic equations, such as the psi equations (Xu and Keyser 1993; Xu 1992b).

It was proposed by Xu and Keyser (1993) that the essential (Dirichlet-type) nonhomogeneous boundary conditions for the psi equations require knowledge of the boundary-normal ageostrophic wind, as is the case for the **C**-vector diagnostic equations of ageostrophic circulation (Xu 1992b). The mathematical rationale (admissibility) of the aforementioned boundary conditions for the **C**-vector formulations of ageostrophic circulation is clear (Xu 1992b), but it is not so obvious for the psi equations. Also, the natural (Neumann-type) boundary conditions for the psi equations have not been considered previously. These problems are the concerns of this study. In the next section, we review the psi equations with the essential boundary conditions. The admissible natural boundary conditions are derived from the variational formulation of the psi equations in section 3. All the derivations will be developed with the quasigeostrophic (QG) equations, though the results can be similarly applied to the counterpart semigeostrophic (SG) psi equations in geostrophic-coordinate space. Different ways of extracting the admissible boundary values from observational data are proposed in section 4. Our results are summarized in section 5.

2. Psi equations and essential boundary conditions

The adiabatic and frictionless quasigeostrophic (QG) equations on an f plane have the following form:

$$f^2 u = -(\partial_t + \mathbf{v}_g \cdot \nabla)\partial_x \varphi_g, \qquad (2.1a)$$

$$f^2 v = -(\partial_t + \mathbf{v}_g \cdot \nabla)\partial_y \varphi_g, \qquad (2.1b)$$

$$N^2 w = -(\partial_t + \mathbf{v}_g \cdot \nabla)\partial_z \varphi_g, \qquad (2.1c)$$

$$\nabla \cdot \mathbf{v} = 0, \qquad (2.1d)$$

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where $\mathbf{v} \equiv (u, v, w)$ is the ageostrophic wind, $\mathbf{v}_g \equiv (u_g, v_g, 0) \equiv \mathbf{k} \times \nabla \varphi_g / f$ is the geostrophic wind, $\nabla \equiv (\partial_x, \partial_y, \partial_z)$, and φ_g is the geopotential. Here $z \equiv [1 - (p/p_0)^\kappa] c_p \theta_0 / g$ is the pseudoheight coordinate introduced by Hoskins and Bretherton (1972) and θ_0 is a constant reference temperature, $N^2 \equiv \gamma \partial_z \theta_g$ is the square of the buoyancy frequency (defined locally), $\gamma \equiv g/\theta_0$, and $\theta_g \equiv \partial_z \varphi_g / \gamma$ is the potential temperature satisfying the thermal-wind relationship with the geostrophic wind $\mathbf{v}_g$. The definition of N^2 is more general than in the conventional QG case, where it is considered to be a function of z alone. The Coriolis parameter f and acceleration of gravity g are assumed to be constant.

By introducing the vector psi streamfunction $\mathbf{\Psi} \equiv (\psi_1, \psi_2)$:

$$-\partial_z \psi_1 \equiv u, \quad -\partial_z \psi_2 \equiv v, \quad \partial_x \psi_1 + \partial_y \psi_2 \equiv w, \quad (2.2)$$

the psi equations can be derived from $\partial_x(2.1\text{c}) - \partial_z(2.1\text{a})$ and $\partial_y(2.1\text{c}) - \partial_z(2.1\text{b})$:

$$\mathbf{D}\mathbf{\Psi} = 2\mathbf{Q}, \quad (2.3\text{a})$$

where

$$\mathbf{D} \equiv \begin{pmatrix} f^2\partial_z^2 + \partial_x N^2 \partial_x, & \partial_x N^2 \partial_y \\ \partial_y N^2 \partial_x, & f^2 \partial_z^2 + \partial_y N^2 \partial_y \end{pmatrix} \quad (2.3\text{b})$$

and $\mathbf{Q} \equiv (Q_1, Q_2)$ is the geostrophic forcing vector with

$$Q_1 \equiv \frac{-f\partial(u_g, v_g)}{\partial(x, z)} \text{ and } Q_2 \equiv \frac{-f\partial(u_g, v_g)}{\partial(y, z)}. \quad (2.3\text{c})$$

As shown by Xu and Keyser (1993), the complete solution $\mathbf{\Psi}$ for a three-dimensional ageostrophic circulation can be computed from (2.3a)–(2.3c) with the following essential (Dirichlet-type) nonhomogeneous boundary conditions:

$$\psi_1 \text{ given at } |x| = L_1, \quad (2.4\text{a})$$

$$\psi_2 \text{ given at } |y| = L_2, \quad (2.4\text{b})$$

$$\psi_1 \text{ and } \psi_2 \text{ given at } z = 0, H. \quad (2.4\text{c})$$

Clearly, (2.4a)–(2.4c) require knowledge of the boundary-normal ageostrophic wind and the boundary-parallel ageostrophic wind should not be simultaneously specified. Otherwise, the boundary conditions will be overspecified, as suggested by the variational formulations in the next section, and numerical noise could be generated near the boundaries in a numerical solution as seen in some of our computations (not shown). The fact that (2.4a)–(2.4c) require knowledge of the boundary-normal ageostrophic wind is also consistent with the following boundary condition obtained from the C-vector formulation (Xu 1992b):

$$\mathbf{n}\cdot\mathbf{v} \text{ given at the domain boundary } \partial\Omega, \quad (2.5\text{a})$$

where $\mathbf{n}$ is the unit vector (outward) normal to the domain boundary $\partial\Omega$. Obviously, the boundary flux $\mathbf{n}\cdot\mathbf{v}$ in (2.5a) should satisfy the following integral constraint obtained from the mass continuity equation (2.1d):

$$\iint \mathbf{n}\cdot\mathbf{v}\, dS = 0, \quad (2.5\text{b})$$

where the integral is over the entire boundary $\partial\Omega$. Note that an arbitrary nondivergent vector function of (x, y) can be added to $\mathbf{\Psi}$ without altering specified boundary conditions for ageostrophic velocity. Therefore, to uniquely determine boundary values of $\mathbf{\Psi}$, a constraint on $\partial_y\psi_1 - \partial_x\psi_2$ should be imposed at the bottom (or top) boundary, that is,

$$\partial_x\psi_2 - \partial_y\psi_1 = 0 \quad \text{at} \quad z = 0, \quad (2.6\text{a})$$

and the following integration constants should be also specified:

$$\psi_1 = 0 \text{ along the line-boundaries (edges) } |x| = L_1 \text{ on the lower surface } z = 0, \quad (2.6\text{b})$$

$$\psi_2 = 0 \text{ along the line-boundaries (edges) } |y| = L_2 \text{ on the lower surface } z = 0. \quad (2.6\text{c})$$

As we will see later, these additional constraint and integration constants are necessary for defining the norm in (3.1b) (which must be positive definite) and for uniquely determining $\mathbf{\Psi}$ from given ageostrophic winds at the boundaries.

3. Variational formulation and natural boundary conditions

The admissible boundary conditions for (2.3a)–(2.3c) are those that in combination with (2.3a)–(2.3c) give well-posed problems. A well-posed linear problem should have a uniquely determined solution. In this sense, the admissible boundary conditions are related to the existence and uniqueness of the solution. The existence and uniqueness of the solution can be ensured if the boundary value problem can be formulated into a variational principle and the associated functional is positive definite and, thus, has only one minimum in the function space. In this case, the minimum point gives the generalized "weak" solution for the boundary value problem (Reddy and Rasmussen 1982; section 3.6.1–2, 398–404) and the admissible boundary conditions can be derived from the related variational formulation [Reddy and Rasmussen (1982) section 3.3.6, 317–327; Zienkiewicz and Taylor (1989) section 9.3, 212–214]. In particular, the variational formulation and admissible boundary conditions for the psi equations (2.3a)–(2.3c) can be derived as follows.

In association with (2.3a)–(2.3c) and under the constraints (2.6a)–(2.6c), we can define the following functional and norm:

$$\Phi(\mathbf{\Psi}) \equiv \frac{\|\mathbf{\Psi}\|^2}{2} + 2\int \mathbf{Q}\cdot\mathbf{\Psi}\, d\mathbf{x}, \quad (3.1\text{a})$$

$$\|\mathbf{\Psi}\|^2 \equiv \int \left[N^2\left(\frac{\partial\psi_1}{\partial x} + \frac{\partial\psi_2}{\partial y}\right)^2 + f^2\left(\frac{\partial\psi_1}{\partial z}\right)^2 + f^2\left(\frac{\partial\psi_2}{\partial z}\right)^2 \right] d\mathbf{x}$$

$$= \int [N^2 w^2 + f^2 u^2 + f^2 v^2] d\mathbf{x}; \quad (3.1\text{b})$$

where $\int(\ )d\mathbf{x} \equiv \int\int\int(\ )dxdydz$ and the integration is over the domain Ω specified in (2.4a)–(2.4c). We denote by $\mathbf{W}(\Omega)$ the function space with the norm defined in (3.1b). This norm requires that derivatives of $\mathbf{\Psi}$ are square integrable but not necessarily continuous. Note also that $\mathbf{v}$ belongs to the Hilbert space if derivatives of $\mathbf{\Psi}$ are square integrable. In other words, the use of variational form or the "weak" form (3.1a) relaxes the continuity requirement on $\mathbf{\Psi}$ [Reddy and Rasmussen (1982) section 3.6.3, p. 429]. By using integration by parts, one can verify that for $\mathbf{\Psi} \in \mathbf{W}(\Omega)$

$$\delta\Phi(\mathbf{\Psi}) = \int \{2\mathbf{Q} - \mathbf{D}\mathbf{\Psi}\} \cdot \delta\mathbf{\Psi} d\mathbf{x} + \delta\mathrm{BT}_1 + \delta\mathrm{BT}_2 + \delta\mathrm{BT}_3, \quad (3.2)$$

where $\mathbf{D}$ is the (matrix) differential operator defined in (2.3b), and

$$\delta\mathrm{BT}_1 \equiv \int\int \delta\psi_1 N^2(\partial_x\psi_1 + \partial_y\psi_2)|_{-L_1}^{L_1} dydz, \quad (3.3\text{a})$$

$$\delta\mathrm{BT}_2 \equiv \int\int \delta\psi_2 N^2(\partial_x\psi_1 + \partial_y\psi_2)|_{-L_2}^{L_2} dzdx, \quad (3.3\text{b})$$

$$\delta\mathrm{BT}_3 \equiv \int\int f^2(\delta\psi_1\partial_z\psi_1 + \delta\psi_2\partial_z\psi_2)|_0^H dxdy, \quad (3.3\text{c})$$

are the boundary variation terms. In the derivation of (3.2)–(3.3), the boundary conditions have not yet been considered.

The variational formulation (3.1a) and (3.1b) can be interpreted physically as follows. In the space obtained by stretching the psuedoheight by the factor N/f (Eliassen 1984; Davies-Jones 1991), $\|\mathbf{\Psi}\|^2/(2f^2)$ is the kinetic energy of the ageostrophic winds and $(2/f^2)\int \mathbf{Q}\cdot\mathbf{\Psi}d\mathbf{x} = (2/f^2)\int(\mathbf{k}\times\mathbf{C}_H)\cdot\mathbf{\Psi}d\mathbf{x} = (2/f^2) \times \int(\mathbf{\Psi}\times\mathbf{k})\cdot\mathbf{C}_H d\mathbf{x}$ may be interpreted as a generalized potential energy associated with the $\mathbf{C}_H$-vector forcing. Here, $\mathbf{k}$ is the unit vertical vector, $\mathbf{C}_H \equiv \mathbf{Q}\times\mathbf{k}$ is the horizontal component of the $\mathbf{C}$ vector (Xu 1992b), and $\mathbf{\Psi}\times\mathbf{k} = \psi_2\mathbf{i} - \psi_1\mathbf{j}$ is a rotated (by 90° to the right) vector psi streamfunction. The vector direction of $\mathbf{\Psi}\times\mathbf{k}$ is along the horizontal axis of the vertical circulation composed of two vertical circulations: ψ_2 in (y, z) plane and $-\psi_1$ in (x, z) plane. As explained in Xu (1992b), $\mathbf{C}_H$ is the rate of change of horizontal curl of body force (Coriolis force and buoyancy) due to the geostrophic motion alone. Therefore, $\int(\mathbf{\Psi}\times\mathbf{k})\cdot\mathbf{C}_H d\mathbf{x}$, the volume-integrated dot product of the body force curl $\mathbf{C}_H$ and the rotated vector psi streamfunction $\mathbf{\Psi}\times\mathbf{k}$ (which represents the effect of a virtual ageostrophic circulation) may be interpreted as a generalized potential energy associated with the $\mathbf{C}_H$-vector forcing. Thus, apart from the lack of time integration, the minimization of the functional in (3.1a) is analogous to Hamilton's principle in classical mechanics with $\Phi(\mathbf{\Psi})$ playing the role of the Lagrangian function. The lack of time integral may be associated with the *instantaneous* restoration of thermal-wind balance in QG theory.

If $\mathbf{\Psi} \in \mathbf{W}(\Omega)$ is a generalized solution of (2.3a)–(2.3c) with either the essential or natural homogeneous boundary conditions, then $\mathbf{\Psi}$ has to ensure the variational principle: $\delta\Phi(\mathbf{\Psi}) = 0$, that is, not only the volume integral in (3.2) but also the surface integrals [i.e., the boundary variation terms in (3.3a)–(3.3c)] vanish for any $\delta\mathbf{\Psi} \in \mathbf{W}(\Omega)$. The vanishing of the boundary variation terms suggests that the admissible homogeneous boundary conditions should be specified as follows:

$$\psi_1 = 0 \quad \text{or} \quad \partial_x\psi_1 + \partial_y\psi_2 = 0 \quad \text{at} \quad |x| = L_1, \quad (3.4\text{a}),(3.4\text{b})$$

$$\psi_2 = 0 \quad \text{or} \quad \partial_x\psi_1 + \partial_y\psi_2 = 0 \quad \text{at} \quad |y| = L_2, \quad (3.5\text{a}),(3.5\text{b})$$

$$(\psi_1, \psi_2) = 0 \quad \text{or} \quad (\partial_z\psi_1, \partial_z\psi_2) = 0 \quad \text{at} \quad z = 0, H. \quad (3.6\text{a}),(3.6\text{b})$$

Alternatively, linear combinations of the (a) and (b) conditions in (3.4)–(3.6) may be chosen. All the (a) in (3.4)–(3.6) are called the essential homogeneous boundary conditions (similar to the Dirichlet boundary condition for the Poisson equation). These boundary conditions can be specified explicitly as constraints on $\mathbf{\Psi} \in \mathbf{W}(\Omega)$. All the (b) in (3.4)–(3.6) are the natural homogeneous boundary conditions [similar to the Neumann boundary condition for the Poisson equation in sense that the boundary values are given for the derivatives and, thus, the solution allows arbitrary integration constants unless the integration constants are specified as in (2.6b) and (2.6c)]. Note that (3.6a) corresponds to a rigid boundary condition $w = 0$ at $z = 0, H$, so the combination of (3.4b), (3.5b), and (3.6a) is the same as the conventional homogeneous boundary conditions for the ω equation.

Like the essential homogeneous boundary conditions [i.e., all the (a) in (3.4)–(3.6)], the essential nonhomogeneous boundary conditions (2.4a)–(2.4c) can be explicitly imposed on $\mathbf{\Psi} \in \mathbf{W}(\Omega)$. In this case, the variational formulation (3.2) and functional $\Phi(\mathbf{\Psi})$ defined in (3.1a) will not change, because $\delta\psi_1$ and $\delta\psi_2$ vanish at the boundaries in (3.3a)–(3.3c). As explained in the text after (3.1b), the derivatives of $\mathbf{\Psi}$ are integrable, but not necessarily continuous in $\mathbf{W}(\Omega)$, so the natural boundary conditions cannot be explicitly imposed on the "weak" solution in $\mathbf{W}(\Omega)$ [Reddy and Rasmussen (1982) section 3.6.3, p. 429]. Note that the natural homogeneous boundary conditions [all the (b) in (3.4)–(3.6)] correspond to the vanishing of the boundary variation terms in (3.3a)–(3.3c), so the natural nonhomogeneous conditions can be implicitly imposed on the solution by adding the following boundary forcing terms to the functional (3.1a), that is,

$$\Phi(\boldsymbol{\Psi}) \equiv \frac{\|\boldsymbol{\Psi}\|^2}{2} + 2\int \mathbf{Q}\cdot\boldsymbol{\Psi}d\mathbf{x} + \mathrm{BF}_1 + \mathrm{BF}_2 + \mathrm{BF}_3, \tag{3.7}$$

where

$$\mathrm{BF}_1 \equiv -\iint (\psi_1 N^2 w)|_{-L_1}^{L_1}\, dydz, \tag{3.8a}$$

$$\mathrm{BF}_2 \equiv -\iint (\psi_2 N^2 w)|_{-L_2}^{L_2} dzdx, \tag{3.8b}$$

$$\mathrm{BF}_3 \equiv \iint f^2(\psi_1 u + \psi_2 v)|_0^H dxdy \tag{3.8c}$$

are the boundary forcing terms with w specified at the lateral boundaries and (u, v) specified at the lower and upper boundaries. The variational formulation for the first two terms in (3.7) is as in (3.2)–(3.3). The variations of the boundary forcing terms ($\delta\mathrm{BF}_1$, $\delta\mathrm{BF}_2$, $\delta\mathrm{BF}_3$) should cancel the boundary variation terms ($\delta\mathrm{BT}_1$, $\delta\mathrm{BT}_2$, $\delta\mathrm{BT}_3$) in (3.3a)–(3.3c), so the natural nonhomogeneous boundary conditions should be specified as

$$\partial_x\psi_1 + \partial_y\psi_2 = w \quad \text{(given)} \quad \text{at} \quad |x| = L_1 \tag{3.9a}$$

$$\partial_x\psi_1 + \partial_y\psi_2 = w \quad \text{(given)} \quad \text{at} \quad |y| = L_2, \tag{3.9b}$$

$$(\partial_z\psi_1, \partial_z\psi_2) = -(u, v) \quad \text{(given)} \quad \text{at} \quad z = 0, H. \tag{3.9c}$$

Clearly, (3.9a) and (3.9b) require knowledge of the vertical velocity at the lateral boundaries and (3.9c) requires knowledge of the horizontal ageostrophic wind at the lower and upper boundaries. Note that adding the "divergence expression," $\nabla\cdot[-\psi_1 N^2 w, -\psi_1 N^2 w, -f^2(\psi_1 u + \psi_2 v)]$, to the integrand in (3.7) is equivalent to adding the boundary forcing terms $\mathrm{BF}_1 + \mathrm{BF}_2 + \mathrm{BF}_3$ by virtue of Gauss's integral theorem. Thus, either technique can be used in calculus of variations to impose the natural boundary conditions without changing the Euler–Lagrange equations.

4. Extraction of the boundary values from observational data

The boundary ageostrophic wind can be extracted from observational data in two ways. Here, by "observational data" we mean the observed horizontal wind field $(u_{\mathrm{ob}}, v_{\mathrm{ob}})$, geopotential height field φ_{ob}, and potential temperature field θ_{ob}. Since the geostrophic components $(u_g, v_g, \theta_g) \equiv (-\partial_y\varphi_g/f, \partial_x\varphi_g/f, \partial_z\varphi_g/\gamma)$ can be extracted from observational data by using the variational method (Sasaki 1970) or normal-mode method (Temperton 1988), the horizontal ageostrophic wind field can be obtained from $(u_{\mathrm{ob}}, v_{\mathrm{ob}}) - (u_g, v_g)$ and the vertical wind can be obtained from the mass continuity equation (2.1d). [Although the ageostrophic wind is extracted over the entire (limited) domain, only the boundary ageostrophic wind is used to obtain the boundary conditions for the psi equations, which are then solved for the ageostrophic winds in the interior.] In this way, the boundary ageostrophic wind satisfies the constraint (2.5b) automatically. This is the first way to extract the boundary ageostrophic wind. The second method extracts the geostrophic components $(\partial_x\varphi_g, \partial_y\varphi_g, \partial_z\varphi_g)$ from observational data on two consecutive time levels. By computing the tendency terms on the right side of (2.1a)–(2.1c), the ageostrophic wind is obtained from the left side of (2.1a)–(2.1c). The boundary ageostrophic wind obtained in this second way needs to be adjusted under the constraint (2.5b) (by using the variational method), because the boundary ageostrophic wind does not automatically satisfy (2.5b) due to data errors and the QG approximation in (2.1a)–(2.1c).

After the boundary ageostrophic wind is extracted from observational data, the natural nonhomogeneous boundary conditions (3.9a)–(3.9c) are known immediately. As mentioned at the end of section 2, however, the boundary values for $\boldsymbol{\Psi}$ required by the essential nonhomogeneous boundary conditions (2.4a)–(2.4c) cannot be uniquely determined from (2.2) and the boundary-normal ageostrophic wind, unless an additional constraint and integration constants are given, such as those in (2.6a)–(2.6c). The constraint (2.6a) allows us to introduce a scalar field χ_0 on $z = 0$ such that $(\partial_x\chi_0, \partial_y\chi_0) \equiv (\psi_1, \psi_2)$. Substituting this into the last formula of (2.2) gives

$$(\partial_x^2 + \partial_y^2)\chi_0 = w\,(=0) \quad \text{on} \quad z = 0. \tag{4.1}$$

The boundary conditions for (4.1) are given by (2.6b) and (2.6c) with $\partial_x\chi_0 = \psi_1 = 0$ along $|x| = L_1$ and $\partial_y\chi_0 = \psi_2 = 0$ along $|y| = L_2$ on the lower boundary surface $z = 0$. The solution of (4.1) is χ_0 = constant on $z = 0$, which gives the following lower boundary values for (2.4c):

$$\psi_1 = \psi_2 = 0 \quad \text{on} \quad z = 0. \tag{4.2}$$

Integrating the first two formulas in (2.2) vertically gives the following lateral boundary values for (2.4a) and (2.4b):

$$\psi_1 = -\int_0^z u dz' \quad \text{at} \quad |x| = L_1, \tag{4.3a}$$

$$\psi_2 = -\int_0^z v dz' \quad \text{at} \quad |y| = L_2, \tag{4.3b}$$

where (4.2) is used.

To find the upper boundary values for (2.4c), we integrate the ageostrophic vorticity equation (or, equivalently, the QG divergence equation) derived from $\partial_x(2.1\mathrm{b}) - \partial_y(2.1\mathrm{a})$ and obtain

$$\partial_y\psi_1 - \partial_x\psi_2 = \int_0^H (\partial_x v - \partial_y u)$$
$$= \frac{2}{f^2}\int_0^H Q_3 dz \quad \text{at} \quad z = H, \qquad (4.4\text{a})$$

where

$$Q_3 \equiv \frac{-f\partial(u_g, v_g)}{\partial(x, y)} \qquad (4.4\text{b})$$

and (2.6a) is used for the lower boundary value of the curl of $\mathbf{\Psi}$. Note that Q_3 is the vertical component of the **C** vector (Xu 1992b), while (4.4a) is just the barotropic ageostrophic vorticity equation (2.9a) of Xu and Keyser (1993) that relates the upper and lower boundary values of the curl of $\mathbf{\Psi}$ to the vertical integration of Q_3 and, thus, gives a constraint in specifying the lower and upper boundary conditions for $\mathbf{\Psi}$. Since the curl of $\mathbf{\Psi}$ is already set to zero at the lower boundary value in (2.6a), the upper boundary value of the curl of $\mathbf{\Psi}$ cannot be freely specified and has to be given by (4.4a). Because $\mathbf{\Psi}$ is not irrotational at the upper boundary, we need to introduce two scalar fields φ_1 and χ_1 such that $(\partial_x\chi_1 - \partial_y\varphi_1, \partial_y\chi_1 + \partial_x\varphi_1) \equiv (\psi_1, \psi_2)$ on $z = H$. Substituting this into (4.4a) and the last formula of (2.2) gives

$$(\partial_x^2 + \partial_y^2)\varphi_1 = -\frac{2}{f^2}\int_0^H Q_3 dz \quad \text{at} \quad z = H, \qquad (4.5\text{a})$$
$$(\partial_x^2 + \partial_y^2)\chi_1 = w \quad \text{at} \quad z = H. \qquad (4.5\text{b})$$

The boundary conditions for (4.5a) and (4.5b) need to be considered together and can be given in many ways. The simplest way is to use the homogeneous essential boundary condition for (4.5a), that is, $\varphi_1 = 0$ along $|x| = L_1$ and $|y| = L_2$ on the upper boundary surface $z = H$. Then the boundary condition for (4.5b) can be obtained from (4.3a) and (4.3b), that is, $\partial_x\chi_1 = \psi_1$ along $|x| = L_1$ and $\partial_y\chi_1 = \psi_2$ along $|y| = L_2$ on $z = H$. By using (2.5b) and (4.3a) and (4.3b), one can verify that the solvability condition for (4.5b) is satisfied, that is, $\oint \mathbf{n}\cdot\nabla\chi_1 dl = \iint_{S_1} w dxdy$, where S_1 is the upper boundary surface of Ω and $\mathbf{n}$ is the horizontal unit vector (outward) normal to the boundary lines of S_1. Once φ_1 and χ_1 are solved, $(\partial_x\chi_1 - \partial_y\varphi_1, \partial_y\chi_1 + \partial_x\varphi_1) \equiv (\psi_1, \psi_2)$ give the upper boundary values for (2.4c).

5. Conclusions

In this paper, the admissible essential (Dirichlet-type) and natural (Neumann-type) boundary conditions are derived from the variational formulations of the QG psi equations. The essential nonhomogeneous boundary conditions (2.4a)–(2.4c) require knowledge of the boundary-normal ageostrophic wind, which is consistent with the boundary conditions for the **C**-vector diagnostic equations of ageostrophic circulation (Xu 1992b). Since the ageostrophic wind is related to the derivatives of the psi functions, the essential boundary values of psi functions cannot be uniquely determined by the boundary-normal ageostrophic wind unless an additional boundary constraint and constants of integration are specified [see (2.6a)–(2.6c)]. The natural nonhomogeneous boundary conditions (3.9a)–(3.9c) require knowledge of the vertical velocity at the lateral boundaries and knowledge of the horizontal ageostrophic wind at the lower and upper boundaries. The conventional (homogeneous) boundary conditions for the QG ω equation correspond to a hybrid-type of boundary conditions for the psi equations—a combination of the natural homogeneous lateral boundary conditions (3.4b) and (3.5b) and essential homogeneous lower and upper boundary conditions (3.6a). Mathematically admissible hybrid-type boundary conditions can be obtained by various combinations of the essential and natural boundary conditions, either homogeneous or nonhomogeneous. But a physically appropriate combination should, at least, exclude the homogeneous lateral boundary conditions (of both types) and the natural homogeneous lower and upper boundary conditions. Furthermore, the essential homogeneous boundary condition applies only to a rigid flat (lower) boundary (as assumed in this paper).

The boundary ageostrophic wind can be extracted from observational data in two ways. In the first way, the geostrophic wind is first extracted from observational data (on a single time level) by using the variational method (Sasaki 1970) or normal-mode method (Temperton 1988). Then, the boundary ageostrophic wind is directly obtained from the difference field between the observed wind and geostrophic wind. The second method extracts the geostrophic wind from observational data on two consecutive time levels, so the boundary ageostrophic wind can be estimated from the geostrophic tendency terms by using the QG momentum equation (2.1a)–(2.1c). This boundary ageostrophic wind needs to be further adjusted to satisfy the mass-flux conservation (2.5b).

Although only the QG psi equations are considered here, the results obtained in this paper can be directly applied, with no additional complexity, to the counterpart semigeostrophic (SG) psi equations in geostrophic-coordinate space (Hoskins and Draghici 1977) and to the more general diagnostic equation—the iterative form of the alternative balance (AB) psi equations [obtainable from (6.3a) and (6.3b) of Davies-Jones (1991) with the time derivative terms set to zero and the generalized **Q** vector evaluated at each iteration from the previous iterate]. The variational formulations can be used to derive the admissible boundary conditions for an irregular domain, such as a domain with a complex terrain at the lower boundary, though only a regular domain is considered in this paper. The technique of using variational formulations to derive the admissible boundary conditions can be applied to other types of linear elliptic equations, such as the SG psi equations in physical space (appendix of Xu 1990; Xu et al. 1991) and the viscous Sawyer–Eliassen equation (appendix of Xu 1992a).

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