

An inconvenient “truth” about using sensible heat flux as a surface boundary condition in models under stably stratified regimes

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Abstract

In single column and large-eddy simulation studies of the atmospheric boundary layer, surface sensible heat flux is often used as a boundary condition. In this paper, we delineate the fundamental shortcomings of such a boundary condition in the context of stable boundary layer modelling and simulation. Using an analytical approach, we are able to show that for reliable model results of the stable boundary layer accurate surface temperature prescription or prediction is needed. As such, the use of surface heat flux as a boundary condition should be avoided in stable conditions.

Key words: boundary condition, land-atmosphere interaction, large-eddy simulation, PBL modelling, stable boundary layer

GLOSSARY OF SYMBOLS

g	gravitational acceleration
L	the Obukhov length $(= -\Theta_0 u_*^3 / \kappa g \langle w\theta \rangle)$
U	wind speed at height z
u, v, w	velocity fluctuations (around the average) in x, y and z directions
u_*	friction velocity $(= \sqrt[4]{\langle uw \rangle^2 + \langle vw \rangle^2})$

$\langle uw \rangle, \langle vw \rangle$	vertical turbulent surface momentum fluxes
$\langle w\theta \rangle$	vertical surface sensible heat flux
z	height above the surface
z_0	surface roughness length for momentum
z_{0H}	surface roughness length for heat
$\Delta\Theta$	potential temperature difference between first model grid-level and surface ($= \Theta - \Theta_s$)
κ	von Karman's constant ($= 0.40$)
Ψ_M, Ψ_H	velocity and potential temperature profile functions
θ	temperature fluctuations (around the average)
Θ	mean potential temperature at height z
Θ_0	reference potential temperature
Θ_s	surface potential temperature
θ_*	potential temperature scale ($= -\langle w\theta \rangle / u_*$)
ζ	stability parameter ($= z/L$)

1. INTRODUCTION

Modelling of the stable boundary layer (SBL) over land is still a great challenge because of the occurrences of many complex physical processes, such as turbulence burstings, Kelvin–Helmholtz instabilities, gravity waves, low-level jets, meandering motions, et cetera (e.g., Hunt *et al.* 1996, Mahrt 1998, Derbyshire 1999, Holtslag 2006, Steeneveld *et al.* 2006). To enhance our understanding and to improve the representation of the boundary layer in atmospheric models for weather forecasting, climate modelling, air quality, and wind energy research, frequently model evaluation and intercomparison studies are organized (e.g., Lenderink *et al.* 2004, Cuxart *et al.* 2006, Beare *et al.* 2006, Svensson and Holtslag 2006, Steeneveld *et al.* 2007). Overall the aim of such studies is to identify the strengths and weaknesses of boundary layer turbulence parameterization schemes.

Usually evaluation studies are done with atmospheric column (1D) or large-eddy simulation (LES) models with simplified boundary conditions and forcing conditions, such as prescribing a constant geostrophic wind and a prescribed surface temperature (tendency). So far this has also been the approach within the GEWEX Atmospheric Boundary Layer Study (GABLS); see Cuxart *et al.* (2006) and Beare *et al.* (2006) for overviews of the 1D and LES model results for the first GABLS model intercomparison, respectively, and Svensson and Holtslag (2006) for the initial results of the second GABLS 1D model intercomparison.

Instead of prescribing surface temperature, one may also consider to prescribe surface sensible heat flux. This has been a useful approach for case studies over day-

time conditions over land (e.g., Wyngaard and Coté 1974, Sun and Chang 1986, Nieuwstadt *et al.* 1993, Lenderink *et al.* 2004, Kumar *et al.* 2006). Due to the existence of ‘dual’ nature of sensible heat flux in stable conditions (see Malhi 1995, Mahrt 1998, Basu *et al.* 2006, Sorbjan 2006), application of sensible heat flux as a surface boundary condition is intuitively troublesome (elaborated later on). Notwithstanding, several SBL modelling studies opted for this type of boundary condition (e.g., Brown *et al.* 1994, Beljaars and Viterbo 1998, Saiki *et al.* 2000, Jiménez and Cuxart 2005, Kumar *et al.* 2006, Esau and Zilitinkevich 2006).

In this paper, we examine in depth the (negative) impact of using heat flux as a surface boundary condition in stable conditions. As such we use an analytical approach. It appears that Taylor (1971), DeBruin (1994), Malhi (1995) and Van de Wiel *et al.* (2007) provide useful corner steps on this issue as will be explained and summarized below. Section 2 gives background information on the subject as well as the implications for modelling when surface sensible heat flux is used as a boundary condition. In contrast, Section 3 gives the results when surface temperature is used as a boundary condition. Finally, Section 4 summarizes and concludes this paper.

2. SENSIBLE HEAT FLUX-BASED SURFACE BOUNDARY CONDITION

To illustrate the issue of this paper, it is useful to start with the wind velocity profile in the atmospheric surface layer. The wind velocity profile is typically written as (Stull 1988):

$$U = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) - \Psi_M \left(\frac{z}{L} \right) \right]. \quad (1a)$$

Using $\Psi_M(z/L) = -\alpha(z/L)$ for $z/L \geq 0$ (Businger *et al.* 1971, Dyer 1974) and utilizing the definition of the Obukhov length, we can re-write eq. (1a) as (Taylor 1971):

$$U = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) + \frac{\beta z}{u_*^3} \right], \quad (1b)$$

where $\beta = -\frac{\alpha \kappa g \langle w\theta \rangle}{\Theta_0} = \frac{\alpha u_*^3}{L}$. Rearranging eq. (1b), we arrive at a third-order polynomial in the friction velocity (Taylor 1971):

$$u_*^3 \left[\frac{1}{\kappa} \ln \left(\frac{z}{z_0} \right) \right] - u_*^2 U + \frac{\beta z}{\kappa} = 0. \quad (2a)$$

Following van de Wiel *et al.* (2007), we divide eq. (2a) by $1/\kappa \ln(z/z_0)$ and arrive at

$$u_*^3 - u_*^2 \frac{U\kappa}{\ln \left(\frac{z}{z_0} \right)} + \frac{\beta z}{\ln \left(\frac{z}{z_0} \right)} = 0. \quad (2b)$$

Now, we define u_{*N} to be the friction velocity which would appear if no stability corrections were applied such as under neutral conditions (i.e., $z/L = 0$). So by definition, $u_{*N} = U\kappa/\ln(z/z_0)$, which can also be inferred from eq. (2b) for $\beta = 0$. Such a definition has been found useful earlier in an analysis of the stable boundary layer (e.g., Holtslag and DeBruin 1988). Using u_{*N} in eq. (2b) and dividing eq. (2b) by u_{*N}^3 , we arrive at the following non-dimensional third-order polynomial:

$$\left(\frac{u_*}{u_{*N}}\right)^3 - \left(\frac{u_*}{u_{*N}}\right)^2 + \frac{\beta z}{u_{*N}^3 \ln\left(\frac{z}{z_0}\right)} = 0, \quad (2c)$$

or

$$\hat{u}_*^3 - \hat{u}_*^2 + \hat{H} = 0, \quad (2d)$$

where

$$\hat{u}_* = \frac{u_*}{u_{*N}} \quad \text{and} \quad \hat{H} = \frac{\beta z}{u_{*N}^3 \ln\left(\frac{z}{z_0}\right)}.$$

The equation as given by eq. (2d) has three roots (Taylor 1971). Let us first explore the results which appear when the surface heat flux has a maximum. As such, we need to impose $d\hat{H}/d\hat{u}_* = 0$ and $d^2\hat{H}/d\hat{u}_*^2 < 0$. Differentiating eq. (2d), we get:

$$\frac{d\hat{H}}{d\hat{u}_*} = 2\hat{u}_* - 3\hat{u}_*^2, \quad (3a)$$

and

$$\frac{d^2\hat{H}}{d\hat{u}_*^2} = 2 - 6\hat{u}_*. \quad (3b)$$

Both the maximum criteria are satisfied for $\hat{u}_* = 2/3$. Resubstitution of $\hat{u}_* = 2/3$ in eq. (2d) leads to $\hat{H}_{\max} = 4/27$. Using the definitions of \hat{H} and β , we arrive at

$$\langle w\theta \rangle_{\min} = -\frac{4}{27} \frac{\Theta_0}{\alpha\kappa g z} u_{*N}^3 \ln\left(\frac{z}{z_0}\right), \quad (4a)$$

or

$$\langle w\theta \rangle_{\min} = -\frac{4}{27} \frac{\Theta_0 \kappa^2}{\alpha g z} \frac{U^3}{\left[\ln\left(\frac{z}{z_0}\right)\right]^2}. \quad (4b)$$

This intriguing result for the minimum surface sensible heat flux, $\langle w\theta \rangle_{\min}$, was first derived by Malhi (1995), albeit following a slightly different derivation route. For the

sake of brevity, in the rest of this paper, the condition $\langle w\theta \rangle = \langle w\theta \rangle_{\min}$ will be denoted as *HMIN*.

Taylor (1971) showed that eq. (2a) has two positive real roots if and only if

$$(\kappa U)^3 > \frac{27}{4} \beta z \left[\ln \left(\frac{z}{z_0} \right) \right]^2. \quad (5a)$$

This inequality leads with simple rearrangements to:

$$\kappa^2 U^3 > \frac{27}{4} z \left(-\frac{\alpha g \langle w\theta \rangle}{\Theta_0} \right) \left[\ln \left(\frac{z}{z_0} \right) \right]^2, \quad (5b)$$

or

$$\langle w\theta \rangle > -\frac{4}{27} \frac{\Theta_0 \kappa^2}{g z \alpha} \frac{U^3}{\left[\ln \left(\frac{z}{z_0} \right) \right]^2}, \quad (5c)$$

or

$$\langle w\theta \rangle > \langle w\theta \rangle_{\min} \quad (5d)$$

(recall that $\langle w\theta \rangle$ and $\langle w\theta \rangle_{\min}$ are both negative).

In other words, positive real roots of u_* are guaranteed if and only if eq. (5d) is satisfied. Earlier, we showed that \hat{u}_{*HMIN} is equal to $2/3$. Thus,

$$u_{*HMIN} = \frac{2}{3} u_{*N} = \frac{2}{3} \frac{U \kappa}{\ln \left(\frac{z}{z_0} \right)}. \quad (6)$$

This equation basically signifies that both the positive real roots of u_* become equal to $2/3 u_{*N}$ at *HMIN*. This finding has recently been reported by van de Wiel *et al.* (2007).

Now, the value of the stability parameter, ζ , at *HMIN* can be immediately found using the definitions of Obukhov length (L , see Glossary of Symbols), $\langle w\theta \rangle_{\min}$ (i.e., eq. 4b), and u_{*HMIN} (i.e., eq. 6) as (see also Malhi 1995):

$$\zeta_{HMIN} = \left(\frac{z}{L} \right)_{HMIN} = \frac{\ln(z/z_0)}{2\alpha}. \quad (7)$$

In Fig. 1, we provide an example of the complex $u_* - \langle w\theta \rangle$ relationship. We assume: $U = 5 \text{ m s}^{-1}$, $z = 10 \text{ m}$, $z_0 = 0.1 \text{ m}$, $\Theta_0 = 300 \text{ K}$, $\alpha = 5$, and $g = 9.81 \text{ m s}^{-2}$. We vary $\langle w\theta \rangle$ from 0 to $\langle w\theta \rangle_{\min} \text{ K m s}^{-1}$. From eq. (4b), for this example we get: $\langle w\theta \rangle_{\min} = -0.0855 \text{ K m s}^{-1}$ (see the dashed vertical lines in Fig. 1). In the left subplot, the positive real roots of eq. (2a) are shown. Following Taylor's convention (Taylor

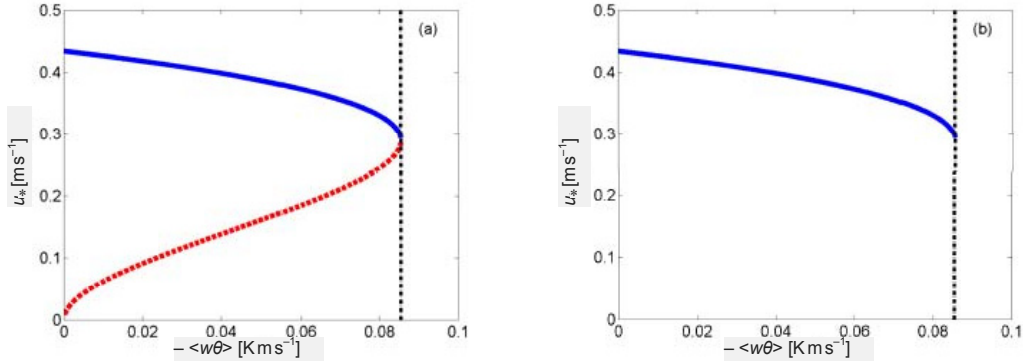


Fig. 1. Friction velocity as a function of prescribed heat flux. The dashed vertical lines denote the maximum achievable heat flux (refer to eq. 4b). The solid and dashed curves in the left subplot show the stable (u_*^+) and unstable (u_*^-) roots of the eq. (2a), respectively. The right subplot portrays the iterative solution for u_* – see Algorithm 1 for details.

1971), the larger root is indicated as u_*^+ , whereas, the smaller root by u_*^- . Taylor (1971) conjectured that u_*^+ and u_*^- are (hydrodynamically) stable and unstable, respectively. A formal proof (based on linear stability analysis) has recently been given by van de Wiel *et al.* (2007).

In planetary boundary layer (PBL) models (single column or LES), u_* is traditionally estimated iteratively by utilizing eq. (1a), rather than by solving the third-order polynomial (eq. 2a). A typical pseudocode is provided in Algorithm 1. Figure 1-right portrays the iterative solution for u_* . Based on Fig. 1, we can conclude that:

- if the magnitude of the prescribed negative heat flux is less than or equal to $\langle w\theta \rangle_{\min}$, the iterative solution always leads to the stable root (i.e., u_*^+);

ALGORITHM 1: SURFFLUX1 ($U, \langle w\theta \rangle, z, z_0$)

Comment: Given $U, \langle w\theta \rangle, z$, and z_0 , compute u_* .

Comment: g, α, κ , and Θ_0 are constants.

Initial value $\psi_M \leftarrow 0$

for iteration $\leftarrow 1$ **to** iteration_{max}

$$\text{do } \begin{cases} u_* \leftarrow \frac{U\kappa}{\ln(z/z_0) - \psi_M} \\ L \leftarrow -\frac{\Theta_0 u_*^3}{\kappa g \langle w\theta \rangle} \\ \psi_M \leftarrow -\frac{\alpha z}{L} \end{cases}$$

- if the magnitude of the prescribed negative heat flux is larger than $\langle w\theta \rangle_{\min}$, there is no real solution for u_* ;
- u_* always resides in the range $[u_{*N}, 2/3u_{*N}]$ for the corresponding prescribed heat flux range of $[0, \langle w\theta \rangle_{\min}]$. For the present example, $u_{*N} = (u_*)_{\langle w\theta \rangle=0} = 0.434 \text{ m s}^{-1}$. We numerically find that u_{*HMIN} is $\sim 0.290 \text{ m s}^{-1}$ – in close agreement with $2/3u_{*N}$.

3. SURFACE TEMPERATURE-BASED SURFACE BOUNDARY CONDITION

To explore the role of a surface temperature condition, it is useful to start with the profile equation for potential temperature. The latter can be written similar to eq. (1a), as in Stull (1988):

$$-\Delta\Theta = \frac{\langle w\theta \rangle}{u_*\kappa} \left[\ln\left(\frac{z}{z_{0H}}\right) - \Psi_H\left(\frac{z}{L}\right) \right]. \quad (8a)$$

Using $\Psi_H(z/L) = -\alpha(z/L)$ for $z/L \geq 0$ (Arya 2001):

$$-\Delta\Theta = \frac{\langle w\theta \rangle}{u_*\kappa} \left[\ln\left(\frac{z}{z_{0H}}\right) + \alpha\left(\frac{z}{L}\right) \right]. \quad (8b)$$

If surface potential temperature, Θ_s , or the potential temperature difference between the first model grid-level and surface ($\Delta\Theta = \Theta - \Theta_s$) is provided as a boundary condition, friction velocity and sensible heat flux can be estimated by solving the coupled eqs. (1b) and (8b). Analytical solutions of these coupled equations can be readily found if we further assume $z_0 = z_{0H}$. Bulk Richardson number, Ri_B , for the atmospheric surface layer is typically written as

$$Ri_B = \frac{gz}{\Theta_0} \frac{\Delta\Theta}{U^2}. \quad (9a)$$

Using eqs. (1b) and (8b), we can re-write Ri_B as follows:

$$Ri_B = \frac{\frac{z}{L}}{\ln\left(\frac{z}{z_0}\right) + \alpha\frac{z}{L}}. \quad (9b)$$

Substituting Ri_B into eq. (1b), we get

$$u_* = \frac{U\kappa}{\ln\left(\frac{z}{z_0}\right)} (1 - \alpha Ri_B). \quad (10a)$$

Similarly, substituting Ri_B into eq. (8b) and using eq. (10a), we get

$$\langle w\theta \rangle = -\frac{U\kappa^2\Delta\Theta}{\ln\left(\frac{z}{z_0}\right)^2}(1-\alpha Ri_B)^2. \quad (10b)$$

Thus, in the case of $z_0 = z_{0H}$, given U and $\Delta\Theta$, u_* and $\langle w\theta \rangle$ could be easily estimated from eqs. (10a) and (10b) with the help of eq. (9a). For more general cases (e.g., $z_0 \neq z_{0H}$), the analytical solutions might become untractable. Then, Algorithm 2 or its variants could be effectively used for iterative solutions. Please note that eqs. (10a) and (10b) are valid for $Ri_B \leq 1/\alpha$. From eqs. (9a), (10a), and (10b), we also observe that u_* and $\langle w\theta \rangle$ depend on $\Delta\Theta$ in linear and cubic fashions, respectively.

Now, we revisit the example problem discussed in the previous section. However, in this occasion instead of prescribing surface sensible heat flux, $\langle w\theta \rangle$, we vary the potential temperature difference between the first model grid-level and surface ($\Delta\Theta$). All other variables remain the same. We further assume $z_0 = z_{0H}$ and $\Psi_M = \Psi_H = -\alpha z/L$.

The dual nature of surface sensible heat flux is clearly visible in Fig. 2a. The downward heat flux achieves its maximum possible value for a certain value of potential temperature difference between first model grid-level and surface, denoted as $\Delta\Theta_{HMIN}$ in this work. In the very stable regime ($\Delta\Theta \gg \Delta\Theta_{HMIN}$) due to suppression of turbulence, the heat flux vanishes. Of course, the heat flux should also go to zero in the near-neutral limit ($\Delta\Theta \rightarrow 0$) since the temperature fluctuations become quite

ALGORITHM 2: SURFFLUX2 ($U, \Delta\Theta, z, z_0, z_{0H}$)

Comment: Given $U, \Delta\Theta, z, z_0$, and z_{0H} , compute u_* and $\langle w\theta \rangle$.

Comment: g, α, κ , and Θ_0 are constants.

Initial value $\Psi_M \leftarrow 0$

Initial value $\Psi_H \leftarrow 0$

for $iteration \leftarrow 1$ **to** $iteration_{max}$

$$\text{do } \left\{ \begin{array}{l} u_* \leftarrow \frac{U\kappa}{\ln(z/z_0) - \Psi_M} \\ \langle w\theta \rangle \leftarrow \frac{-\Delta\Theta u_* \kappa}{\ln(z/z_{0H}) - \Psi_H} \\ L \leftarrow -\frac{\Theta_0 u_*^3}{\kappa g \langle w\theta \rangle} \\ \Psi_M \leftarrow -\frac{\alpha z}{L} \\ \Psi_H \leftarrow \Psi_M \end{array} \right.$$

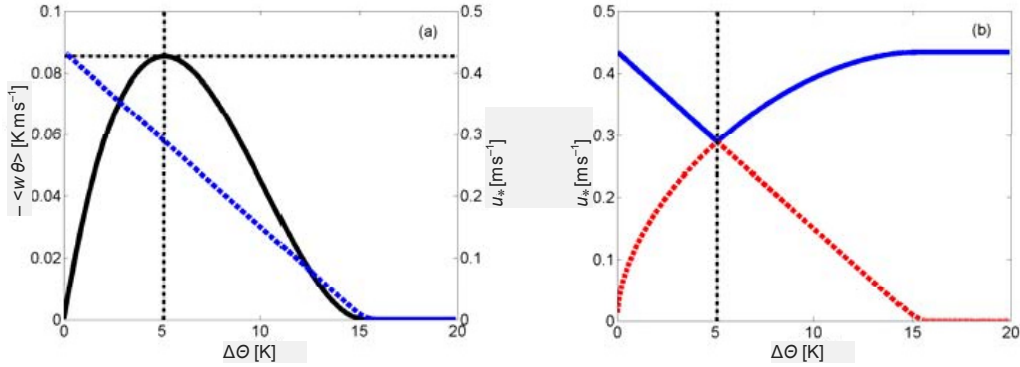


Fig. 2: (a) Sensible heat flux and friction velocity as functions of potential temperature difference between surface and first atmospheric model level. Algorithm 2 has been used to estimate these fluxes. The dashed horizontal line denotes the maximum achievable heat flux, refer to eq. (4b). The dashed vertical line indicates $\Delta\theta_{HMIN}$, see eq. (11a), and related discussions; (b) The solid and dashed curves represent the stable (u_*^+) and unstable (u_*^-) roots of eq. (2a), respectively, given the estimated sensible heat flux of the left subplot as input. Similar to the left subplot, the dashed vertical line indicates $\Delta\theta_{HMIN}$.

small. We would like to point out that Malhi (1995) reported qualitatively very similar stability parameter (ζ) *versus* heat flux curves. We would like to stress that the dual nature of sensible heat flux is not a numerical artifact, it has been reported in several recent observational studies. Malhi (1995) reported ζ_{HMIN} to be around 0.20. Based on the Microfont data, Mahrt (1998) found ζ_{HMIN} to occur at 0.05. Basu *et al.* (2006) performed extensive analyses of turbulence data from several field campaigns and wind-tunnel experiments. They also provided convincing evidences of the duality of sensible heat flux. Based on CASES-99 observations and utilizing the ‘gradient-based’ local scaling hypothesis, Sorbjan (2006) found the normalized minimum surface sensible heat flux to be around $Ri \approx 0.25$ (here Ri denotes the so-called gradient Richardson number).

Using eqs. (4b), (6), and (8b), along with the assumption of $z_0 = z_{0H}$, it is quite straightforward to show that

$$\Delta\theta_{HMIN} = \frac{U^2 \theta_0}{3gz\alpha}. \quad (11a)$$

Thus, $\Delta\theta_{HMIN}$ strongly depends on wind speed and height. Recent single column modelling study by Holtslag *et al.* (2007) also arrived at this conclusion numerically. Using the definition of Ri_B , eq. (11a) can be re-arranged in the following dimensionless (quasi-universal) form:

$$(Ri_B)_{HMIN} = \frac{1}{3\alpha}. \quad (11b)$$

For $\alpha = 5$, eq. (11b) basically implies that minimum heat flux occurs at $Ri_B = 1/15$. In our future works, we will attempt to validate this interesting finding via extensive analyses of field observations.

Figure 2a portrays that the friction velocity (estimated using Algorithm 2) decreases monotonically with increasing surface inversion, as would be physically anticipated. Both u_* and $\langle w\theta \rangle$ eventually go to zero (the so-called “collapse” phenomenon) for $\Delta\theta \gg \Delta\theta_{HMIN}$. However, we earlier found that, if surface sensible heat flux is prescribed, the (hydrodynamically) stable root u_*^+ only decreases upto $2/3 u_{*N} \gg 0$ (see eq. (6) and Fig. 1). In order to resolve this anomaly, in Fig. 2-right, we have plotted both u_*^+ and u_*^- using the iteratively estimated sensible heat flux of Fig. 2a and eq. (2a). Interestingly, for $\Delta\theta \leq \Delta\theta_{HMIN}$, the iteratively estimated u_* (Fig. 2a) follows the stable root u_*^+ (Fig. 2b, solid curve). But, for $\Delta\theta > \Delta\theta_{HMIN}$, the trend reverses, as it follows the unstable root u_*^- . We would like to emphasize that the stable root u_*^+ increases with increasing stability for $\Delta\theta > \Delta\theta_{HMIN}$, which is physically unfeasible.

4. SUMMARY AND CONCLUSION

In this paper, we have discussed how the use of a prescribed sensible heat flux as a lower boundary condition will impact on the results of a PBL model. It is argued that any PBL model (single column or LES) will only be able to capture the near-neutral to weakly stable regime ($\Delta\theta \leq \Delta\theta_{HMIN}$) if surface sensible heat flux is prescribed. As a result, the estimated u_* will never become less than 67% of the neutral estimate for the friction velocity (e.g., $2/3 u_{*N}$ in the case of the Businger–Dyer-type profiles). In order to represent the moderate to very stable regime ($\Delta\theta > \Delta\theta_{HMIN}$ and $u_* < 2/3 u_{*N}$) in a boundary layer model for stably stratified conditions, unquestionably one needs to use surface temperature as a boundary condition as shown in this paper. In addition, model results also seem to depend on how the surface temperature condition is applied. Using a prescribed surface temperature or a surface temperature as predicted by a simple energy balance model, indicated strong impacts on the model results. This has been discussed by Holtslag *et al.* (2007).

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