



Effect of Surface Temperature Heterogeneity on Turbulent Mixing in the SBL

Dmitrii Mironov

German Weather Service Offenbach am Main, Germany (dmitrii.mironov@dwd.de) Peter Sullivan National Center for Atmospheric Research Boulder, CO, USA (pps@ucar.edu)

Ekaterina Machulskaya

German Weather Service Offenbach am Main, Germany (ekaterina.machulskaya@dwd.de)









Outline

Motivation

- → LES of stably stratified PBL over temperaturehomogeneous vs. temperature-heterogeneous surfaces
- Analysis of mean fields and second-order moment budgets
- Enhanced mixing in horizontally-heterogeneous PBL an explanation
- → Prospects for improving turbulence parameterisations
- Conclusions and outlook



Motivation

Models of stably stratified PBL, incl. surface layer, do not account for many important features (e.g. gravity waves, meanders of cold air, radiation flux divergence, and <u>horizontal heterogeneity of the underlying surface</u>)

- Mixing is typically underestimated
- Models tend to quench turbulence in strongly stable stratification
- Ad hoc tuning devices like "minimum diffusion coefficients" do not help much (they are often detrimental for the NWP/climate model performance)

Motivation (cont'd)

- Although most turbulence models are based on truncated second-moment budget equations, no comprehensive account of second-moment budgets in stably stratified PBL (SBL), neither in horizontallyhomogeneous nor in horizontally-heterogeneous case (cf. Mason and Derbyshire 1990, Coleman et al. 1992, Andrén 1995, Kosović and Curry 2000, Saiki et al. 2000, Jiménez and Cuxart 2005, Taylor and Sarkar 2008)
- Poor understanding of the role of horizontal heterogeneity in maintaining turbulent fluxes (hence no physically sound parameterisation)

Large-Eddy Simulations

Boundary-layer flows over temperature-homogeneous vs. temperature-heterogeneous surface

- LES code: Moeng (1984), Moeng and Wyngaard (1998), Sullivan et al. (1994, 1996), Sullivan and Patton (2008).
- Domain: $400 \times 400 \times 400$ m, $200 \times 200 \times 192$ mesh points, 2 m mesh size.
- Geostrophic wind: (8,0) m·s⁻¹, Coriolis parameter: 1.39·10⁻⁴ s⁻¹, temperature gradient above the PBL: 10⁻² K·m⁻¹.
- Boundary conditions: doubly periodic in *x* and *y* horizontal directions, the Monin-Obukhov surface-layer similarity relations are applied point-by-point.
- Initial temperature profile: mixed layer of depth 100 m and temperature 265 K, temperature increases linearly aloft at a rate 10⁻² K⋅m⁻¹.
- In homogeneous case, a constant surface cooling rate of -0.375 K·hr⁻¹ over 8 hrs. In heterogeneous case, the surface cooling rate varies sinusoidally in the streamwise direction leading to a surface temperature difference of 6 K between the warm and the cold stripes (cf. Stoll and Porté-Agel 2009). Following this initial 8 hr period, a constant surface cooling rate of -0.375 K·hr⁻¹ in both cases.

Surface Temperature in Homogeneous and Heterogeneous Cases



8h sampling 9.75h



Analysis of LES Data

- In order to obtain approximations to ensemble-mean quantities, the LES data are averaged over horizontal planes and the resulting profiles are then averaged over more than 8000 time steps (the number of samples varies between cases). The sampling time covers the last 1.75 hours of simulations.
- Mean fields, second-order and third-order moments
- Budgets of TKE, of the temperature variance and of the temperature flux with due regard for SGS contributions (important in SBL even at high resolution)
- Implications for SBL turbulence parameterisations

Scalar Variance Budget Derived from LES Data

Resolved-scale scalar variance



Scalar Variance Budget Derived from LES Data (cont'd)

Adding the two budgets, we get the budget of total (resolved + SGS) scalar variance

 $\frac{1}{2}\frac{d}{dt}\left(\left\langle \bar{f}^{\,\prime\prime 2}\right\rangle + \left\langle \bar{f}^{\,\prime 2}\right\rangle\right) = -\left(\left\langle \bar{u}_{i}^{\,\prime\prime}\bar{f}^{\,\prime\prime}\right\rangle + \left\langle \bar{u}_{i}^{\,\prime}f^{\,\prime\prime}\right\rangle\right)\frac{\partial\langle f\rangle}{\partial x_{i}} - \varepsilon_{f^{\,2}}$ $-\frac{1}{2}\frac{\partial}{\partial x_{i}}\left(\left\langle \overline{u}_{i}''\overline{f}''^{2}\right\rangle + \left\langle \overline{u}_{i}''\overline{f''}''\right\rangle + 2\left\langle \overline{f}''\overline{u_{i}'f'}''\right\rangle + \left\langle \overline{u_{i}'f'}^{2}\right\rangle\right)$ **Cannot be estimated Resolved-scale** unless high-order SGS **Important contributions** contribution closure model is used that should be included (presumably small) but are neglected in most LES studies

Components of Mean Wind



Blue – horizontally-homogeneous SBL, red – horizontally-heterogeneous SBL.

Mean Potential Temperature



TKE and Temperature Variance



Blue – homogeneous SBL, red – heterogeneous SBL.

TKE Budget



Left panel – homogeneous SBL, right panel – heterogeneous SBL.

Red – shear production, **blue** – dissipation, **black** – buoyancy destruction, **green** – third-order transport, thin dotted black – tendency . $\partial \overline{u} = \partial \overline{u} = \partial \overline{u}$

$$\frac{\partial e}{\partial t} = -\left(\overline{w'u'}\frac{\partial \overline{u}}{\partial z} + \overline{w'v'}\frac{\partial \overline{v}}{\partial z}\right) + \underline{g\alpha}\overline{w'\theta'} - \frac{\partial}{\partial z}\left(\frac{1}{2}\overline{w'u'^{2}}_{i} + \overline{w'p'}\right) - \underline{\varepsilon}$$

Vertical Temperature Flux Budget



Left panel – homogeneous SBL, right panel – heterogeneous SBL.

 \mathbf{Red} – mean-gradient, **black** – buoyancy, **blue** – pressure gradient-temperature covariance, green – third-order transport, thin dotted black – tendency .

$$\frac{\partial \overline{w'\theta'}}{\partial t} = -\overline{w'^2} \frac{\partial \overline{\theta}}{\partial z} + \underline{g\alpha}\overline{\theta'^2} - \frac{\partial}{\partial z}\overline{w'^2\theta'} - \overline{\theta'}\frac{\partial p'}{\partial z}$$

Temperature Variance Budget



Left panel – homogeneous SBL, right panel – heterogeneous SBL.

Red – mean-gradient production/destruction, blue – dissipation, green – third-order transport, black (thin dotted) – tendency .

$$\frac{1}{2}\frac{\partial {\theta'}^2}{\partial t} = -\overline{w'\theta'}\frac{\partial \overline{\theta}}{\partial z} - \frac{1}{2}\frac{\partial}{\partial z}\overline{w'\theta'}^2 - \varepsilon_{\theta}$$

Key Point: Third-Order Transport of Temperature Variance

LES estimate of $\langle w'\theta'^2 \rangle$ (resolved plus SGS)

$$\left\langle \overline{w}'' \overline{\theta}''^2 \right\rangle + \left\langle \overline{w}'' \overline{\theta'}^2'' \right\rangle + 2 \left\langle \overline{\theta}'' \overline{w' \theta'}'' \right\rangle + \left\langle \overline{w' \theta'}^2 \right\rangle$$

Surface temperature variations modulate local static stability and hence the surface heat flux \rightarrow net production/destruction of $\langle \theta'^2 \rangle$ due to divergence of third-order transport term! In heterogeneous SBL, the third-order transport of temperature variance is non-zero at the surface

Third-Order Transport of Temperature Variance



Vertical Temperature Flux: Algebraic Closure



(*) Using Rotta-type return-to-isotropy model + linear model of the so-called fast terms

$$\overline{\frac{\partial p'}{\partial z}} = \frac{\overline{w'\theta'}}{\tau} + C_b g \alpha \overline{\theta'}^2$$

(*) Neglecting anisotropy

$$\overline{u_i'u_k'} \equiv \left(\overline{u_i'u_k'} - \frac{1}{3}\delta_{ik}\overline{u_j'u_j'}\right) + \frac{1}{3}\delta_{ik}\overline{u_j'u_j'} \to \frac{2}{3}\delta_{ik}e$$



Enhanced Mixing in Horizontally-Heterogeneous SBL An Explanation

increased $\langle \theta'^2 \rangle$ near the surface \rightarrow reduced magnitude of downward heat flux \rightarrow less work against the gravity \rightarrow increased TKE \rightarrow stronger mixing 300 300 200 200 200 Increased **Decreased** (in magnitude) (m) z z (m) **Increased** 100 100 100 0.1 0.02 -0.015 -0.005 0 0 0.2 0.3 0.4 0 0.01 -0.01 $<\theta'^{2}>(K^{2})$ <w'θ'> (K m/s) TKE (m^2/s^2)

(m) z (m)

Implications

Good News

 Analysis of LES results suggests plausible explanation of enhanced mixing in horizontallyheterogeneous SBL – <u>we understand more</u> (increased <θ'²> near the surface is a key point)

Bad News

• Major increase of $\langle \theta'^2 \rangle$ in heterogeneous SBL occurs near the surface – <u>difficult to parameterise</u>

In order to describe enhanced mixing in heterogeneous SBL, an increased $\langle \theta'^2 \rangle$ at the surface should be accounted for.

- **Elegant way**: modify the surface-layer flux-profile relationships. Difficult not for nothing are the Monin-Obukhov surface-layer similarity relations used for more than 50 years without any noticeable modification!
- Less elegant way: use a tile approach, where several parts with different surface temperatures are considered within an atmospheric model grid box.

Tiled TKE-Scalar (Temperature) Variance Closure Scheme

- <u>Transport (prognostic) equations</u> for TKE and for the temperature variances <u>including third-order transport</u>
- <u>Algebraic (diagnostic) formulations</u> for temperature flux, for the Reynolds-stress components, and for turbulence length scale
- <u>Tile approach</u> where different tiles have different surface temperature
- <u>Surface fluxes are computed as weighted means</u> of fluxes over individual tiles
- $\leq w' \theta'^2 >$ is non-zero at the surface in heterogeneous SBL
- Input parameters of numerical experiments are similar to LES (except for piece-wise vs. sinusoidally varying surface temperature)

Coupling of the TKE-Scalar Variance Scheme with the Tiled Surface Scheme



 \rightarrow net gain/loss of $\langle \theta'^2 \rangle$ due to non-zero third-order transport term

Tiled TKE-Scalar Variance Scheme: Results



 \checkmark

SBL in DWD Models: Work in Progress

- Implementation of tile approach (Ekaterina Machulskaya, Jürgen Helmert)
- (i) only a few tiles are considered but the tiles with the maximum difference in terms of their thermal inertia must be included,
- (ii) individual profiles of soil/inland water temperature (and soil water content) are considered for each tile,
- (iii) SGS inland water is crucial (treated with FLake, http://lakemodel.net)
- Further development of parameterization of "circulation terms" (Matthias Raschendorfer)
- Development of the TKE-Scalar Variance scheme, incl. prognostic treatment and third-order transport of scalar variances, and coupling with tiled surface scheme (COSMO, ICON)
- Development of an extended statistical SGS cloud scheme to account for the skewness of scalars (DWD, MPI-M, University of Hannover)

Conclusions and Outlook

- LES results suggests plausible explanation of enhanced mixing in horizontally-heterogeneous SBL
- Turbulent transport of temperature variances (third-order term $\langle w'\theta'^2 \rangle$ in the $\langle \theta'^2 \rangle$ budget) is an important point
- Ways to improve SBL parameterisations are outlined

- Simulations of strongly stable PBL (PS & DM)
- Comprehensive analysis of pressure-scalar and pressure-velocity covariances in the second-moment budgets (DM & PS)
- Development of improved SBL parameterisations, e.g. tile approach, treatment of scalar variances (DWD, NCAR, etc.)







<u>Acknowledgements</u>. Thanks are due to Vittorio Canuto, Sergey Danilov, Evgeni Fedorovich, Vladimir Gryanik, Jürgen Helmert, Donald Lenschow, Chin-Hoh Moeng, Ned Patton, Matthias Raschendorfer, and Jeffrey Weil for discussions. The work was partially supported by the NCAR Geophysical Turbulence Program and by the European Commission through the COST Action ES0905.





Appendix

$w'\theta'$ at 12.5 m above the surface



Coupling of the TKE-Scalar Variance Scheme with the Tiled Surface Scheme



 \rightarrow net gain/loss of $\langle \theta'^2 \rangle$ due to non-zero third-order transport term



Surface Temperature (cont'd)



The number of stripes does not affect the results, what matters is the temperature difference between warm and cold stripes (Stoll and Porté-Agel 2009)



Estimation of Total Variances

We apply a <u>triple decomposition</u>, using (i) a low-pass filter whose characteristic horizontal scale, Δ , is much less than the domain size, *L*, and (ii) a horizontal averaging operator over *L*. A fluctuating quantity *f* may then be represented as a sum of the horizontal mean filtered part, a deviation of the filtered quantity from the horizontal mean, and a sub-filter fluctuation,

$$f = \left\langle \bar{f} \right\rangle + \bar{f}'' + f',$$

where an overbar denotes a low-pass filtered quantity, and a prime denotes a deviation therefrom. Angle brackets denote averaging over the horizontal, and a double prime denotes a fluctuation about a horizontal mean.

There is nothing really new in it, cf.

• Mean flow-wave-turbulence decomposition (Hussein and Reynolds 1970, 1972, Reynolds and Hussein 1972)

• A procedure used in LES studies to compute (approximations to) ensemble-mean statistical moments as a sum of resolved scale and sub-grid scale contributions (e.g. Brown 1995, Mironov et al. 2000, Mironov 2001)

• Energy budget scale-by-scale (Frisch 1995, section 2.4)

Estimation of Total Variances

A <u>triple decomposition</u> is applied, using (i) a low-pass filter (overbar) whose characteristic horizontal scale Δ is much less than the domain size *L*, and (ii) a horizontal averaging operator over *L* (angle brackets).

A fluctuating quantity f may then be represented as a sum of the horizontal mean filtered part, a deviation of the filtered quantity from the horizontal mean (double prime), and a sub-filter fluctuation (prime):



$$f = \left\langle \bar{f} \right\rangle + \underline{\bar{f}''} + \underline{f'}$$

Then

total variance =
$$\left\langle \bar{f}''^2 \right\rangle + \left\langle \overline{f'^2} \right\rangle$$

Estimation of Total Variances (cont'd)

Low-pass filtered and high-pass filtered quantity



total variance =
$$\langle \bar{f}''^2 \rangle + \langle \bar{f'}^2 \rangle$$

Velocity Variances



Blue – homogeneous SBL, red – heterogeneous SBL. Short-dashed – $\langle w'^2 \rangle$, long-dashed – $\langle v'^2 \rangle$, solid – $\langle u'^2 \rangle$.

Components of Momentum Flux



Blue – horizontally-homogeneous SBL, red – horizontally-heterogeneous SBL.

Streamwise and Spanwise Temperature Flux



Blue – homogeneous SBL, red – heterogeneous SBL.

Streamwise Temperature Flux Budget



Left panel – homogeneous SBL, right panel – heterogeneous SBL.

Red – mean temperature gradient, **brown** – mean velocity shear, **blue** – pressure gradient-temperature covariance, **green** – third-order transport, thin dotted black – tendency.

$$\frac{\partial \overline{u'\theta'}}{\partial t} = -\overline{u'w'}\frac{\partial \overline{\theta}}{\partial z} - \overline{w'\theta'}\frac{\partial \overline{u}}{\partial z} - \frac{\partial}{\partial z}\overline{w'u'\theta'} - \overline{\theta'\frac{\partial p'}{\partial x}}$$

Spanwise Temperature Flux Budget



Left panel – homogeneous SBL, right panel – heterogeneous SBL.

Red – mean temperature gradient, **brown** – mean velocity shear, **blue** – pressure gradient-temperature covariance, **green** – third-order transport, thin dotted black – tendency.

$$\frac{\partial \overline{v'\theta'}}{\partial t} = -\overline{v'w'}\frac{\partial \overline{\theta}}{\partial z} - \overline{w'\theta'}\frac{\partial \overline{v}}{\partial z} - \frac{\partial}{\partial z}\overline{w'v'\theta'} - \overline{\theta'\frac{\partial p'}{\partial y}}$$

Vertical Temperature Flux Budget



Increased $\langle \theta'^2 \rangle$ near the surface in horizontally-heterogeneous SBL \Rightarrow reduced magnitude of downward temperature flux

Tiled TKE-Scalar Variance Scheme (cont'd)



• Low boundary condition for $<\theta'^2>$

Tiled TKE-Temperature Variance Closure Model (cont'd)

TKE

$$\frac{\partial e}{\partial t} = -\left(\overline{w'u'}\frac{\partial \overline{u}}{\partial z} + \overline{w'v'}\frac{\partial \overline{v}}{\partial z}\right) + g\alpha\overline{w'\theta'} - \frac{\partial}{\partial z}\left(\frac{1}{2}\overline{w'u'}^2 + \overline{w'p'}\right) - \varepsilon$$

Temperature variance

$$\frac{1}{2}\frac{\partial \theta'^2}{\partial t} = -\overline{w'\theta'}\frac{\partial \overline{\theta}}{\partial z} - \frac{1}{2}\frac{\partial}{\partial z}\overline{w'\theta'}^2 - \varepsilon_{\theta}$$

Temperature (heat) flux, momentum flux, turbulence time (length) scale

$$\overline{w'\theta'} = -C_h \tau e \frac{\partial \theta}{\partial z} + (1 - C_b) \tau g \alpha \overline{\theta'}^2, \quad \overline{u'w'} = -C_m \tau e \frac{\partial \overline{u}}{\partial z}, \quad \overline{v'w'} = -C_m \tau e \frac{\partial \overline{v}}{\partial z},$$
$$\tau = l e^{-1/2}, \quad l = l(z, h, e, N, ...)$$





Kasimir Malevich, Black Square, 1915 (as a conceptual model of nocturnal SBL)

• Ad hoc tuning devices like "minimum diffusion coefficients" do not help much (they are often detrimental for the NWP/climate model performance)

Ensemble-Mean Second-Moment Budget Equations

TKE

$$\frac{\partial e}{\partial t} = -\left(\overline{w'u'}\frac{\partial \overline{u}}{\partial z} + \overline{w'v'}\frac{\partial \overline{v}}{\partial z}\right) + g\alpha\overline{w'\theta'} - \frac{\partial}{\partial z}\left(\frac{1}{2}\overline{w'u'^2} + \overline{w'p'}\right) - \varepsilon$$

Temperature variance

$$\frac{1}{2}\frac{\partial \theta'^2}{\partial t} = -\overline{w'\theta'}\frac{\partial \overline{\theta}}{\partial z} - \frac{1}{2}\frac{\partial}{\partial z}\overline{w'\theta'}^2 - \varepsilon_{\theta}$$

Temperature (heat) flux

$$\frac{\partial \overline{w'\theta'}}{\partial t} = -\overline{w'^2} \frac{\partial \overline{\theta}}{\partial z} + g \alpha \overline{\theta'^2} - \frac{\partial}{\partial z} \overline{w'^2\theta'} - \overline{\theta' \frac{\partial p'}{\partial z}}$$

◀ ▶

Ensemble-Mean Second-Moment Budget Equations

TKE

$$\frac{1}{2}\left(\frac{\partial}{\partial t} + \overline{u}_k \frac{\partial}{\partial x_k}\right)\overline{u_i'^2} = -\overline{u_i'u_k'}\frac{\partial\overline{u_i}}{\partial x_k} + g_i\alpha\overline{u_i'\theta'} - \frac{\partial}{\partial x_k}\left(\frac{1}{2}\overline{u_k'u_i'^2} + \overline{u_k'p'}\right) - \varepsilon$$

Temperature variance

$$\frac{1}{2} \left(\frac{\partial}{\partial t} + \overline{u}_i \frac{\partial}{\partial x_i} \right) \overline{\theta'}^2 = -\overline{u'_i \theta'} \frac{\partial \overline{\theta}}{\partial x_i} - \frac{1}{2} \frac{\partial}{\partial x_i} \overline{u'_i \theta'}^2 - \varepsilon_{\theta}$$

Temperature (heat) flux

$$\left(\frac{\partial}{\partial t} + \overline{u}_k \frac{\partial}{\partial x_k}\right) \overline{u'_i \theta'} = -\overline{u'_k \theta'} \frac{\partial \overline{u}_i}{\partial x_k} - \overline{u'_i u'_k} \frac{\partial \overline{\theta}}{\partial x_k} + g_i \alpha \overline{\theta'}^2 - 2\varepsilon_{ijk} \Omega_j \overline{u'_k \theta'} - \frac{\partial}{\partial x_k} \overline{u'_k u'_i \theta'} - \overline{\theta' \frac{\partial p'}{\partial x_i}}$$

Ensemble-Mean Second-Moment Budget Equations

Reynolds stress

$$\left(\frac{\partial}{\partial t} + \overline{u}_k \frac{\partial}{\partial x_k} \right) \overline{u'_i u'_j} = - \left(\overline{u'_i u'_k} \frac{\partial \overline{u}_j}{\partial x_k} + \overline{u'_i u'_k} \frac{\partial \overline{u}_j}{\partial x_k} \right) - \left(g_i \alpha \overline{u'_j \theta'} + g_j \alpha \overline{u'_i \theta'} \right) - 2 \left(\varepsilon_{ilk} \Omega_l \overline{u'_k u'_j} + \varepsilon_{ilk} \Omega_l \overline{u'_k u'_j} \right) - \left(\overline{u'_i \frac{\partial p'}{\partial x_j}} + \overline{u'_j \frac{\partial p'}{\partial x_i}} - \frac{2}{3} \delta_{ij} \frac{\partial}{\partial x_k} \overline{u'_k p'} \right) - \frac{\partial}{\partial x_k} \left(\overline{u'_k u'_i u'_j} + \frac{2}{3} \delta_{ij} \overline{u'_k p'} \right) - \varepsilon_{ij}$$

Temperature variance

$$\frac{1}{2} \left(\frac{\partial}{\partial t} + \overline{u}_i \frac{\partial}{\partial x_i} \right) \overline{\theta'}^2 = -\overline{u'_i \theta'} \frac{\partial \overline{\theta}}{\partial x_i} - \frac{1}{2} \frac{\partial}{\partial x_i} \overline{u'_i \theta'}^2 - \varepsilon_{\theta}$$

Temperature (heat) flux

$$\left(\frac{\partial}{\partial t} + \overline{u}_k \frac{\partial}{\partial x_k}\right) \overline{u'_i \theta'} = -\overline{u'_k \theta'} \frac{\partial \overline{u_i}}{\partial x_k} - \overline{u'_i u'_k} \frac{\partial \overline{\theta}}{\partial x_k} + g_i \alpha \overline{\theta'^2} - 2\varepsilon_{ijk} \Omega_j \overline{u'_k \theta'} - \frac{\partial}{\partial x_k} \overline{u'_k u'_i \theta'} - \overline{\theta' \frac{\partial p'}{\partial x_i}}$$