DIRECT NUMERICAL SIMULATIONS OF NEAR-SURFACE TURBULENCE AN EVALUATION OF METHODS FOR ESTIMATING AIR-WATER GAS EXCHANGE

UNIVERSITY OF GOTHENBURG

Sam T. Fredriksson[1], Lars Arneborg[1], Håkan Nilsson[2] , Qi Zhang[3], Robert A. Handler[3]

[1] Department of Earth Sciences, University of Gothenburg, Gothenburg, Sweden

[2] Department of Applied Mechanics, Chalmers University of Technology, Gothenburg, Sweden

[3] Department of Mechanical Engineering, Texas A&M University, College Station, United States

CHALMERS UNIVERSITY OF TECHNOLOGY

Introduction

In this study, direct numerical simulations of free surface flows are used to evaluate three different methods of estimating air-water gas exchange, $F_{gas} = k(C_w - C_0)$ where k is the transfer velocity (or piston velocity) and C_w and C_0 are the gas concentration in the bulk of the water and at the surface respectively. The evaluated methods estimate the piston velocity as a function of; horizontal flow divergence at the surface, dissipation rate of turbulent kinetic energy underneath the surface, and heat flux through the surface and compare these to parameterizations using the wind speed at 10 m above the surface.

The flow is driven by natural convection, applied as a fixed surface heat flux. The heat flux cools the surface resulting in cold plumes going downwards, see **Figure 1**. The influence of a clean and a surfactant-laden surface is studied by applying a slip and a no-slip surface momentum boundary condition at the surface, for the momentum equations, respectively. The results of the present study are compared to previous results with a surfactant boundary condition[1].

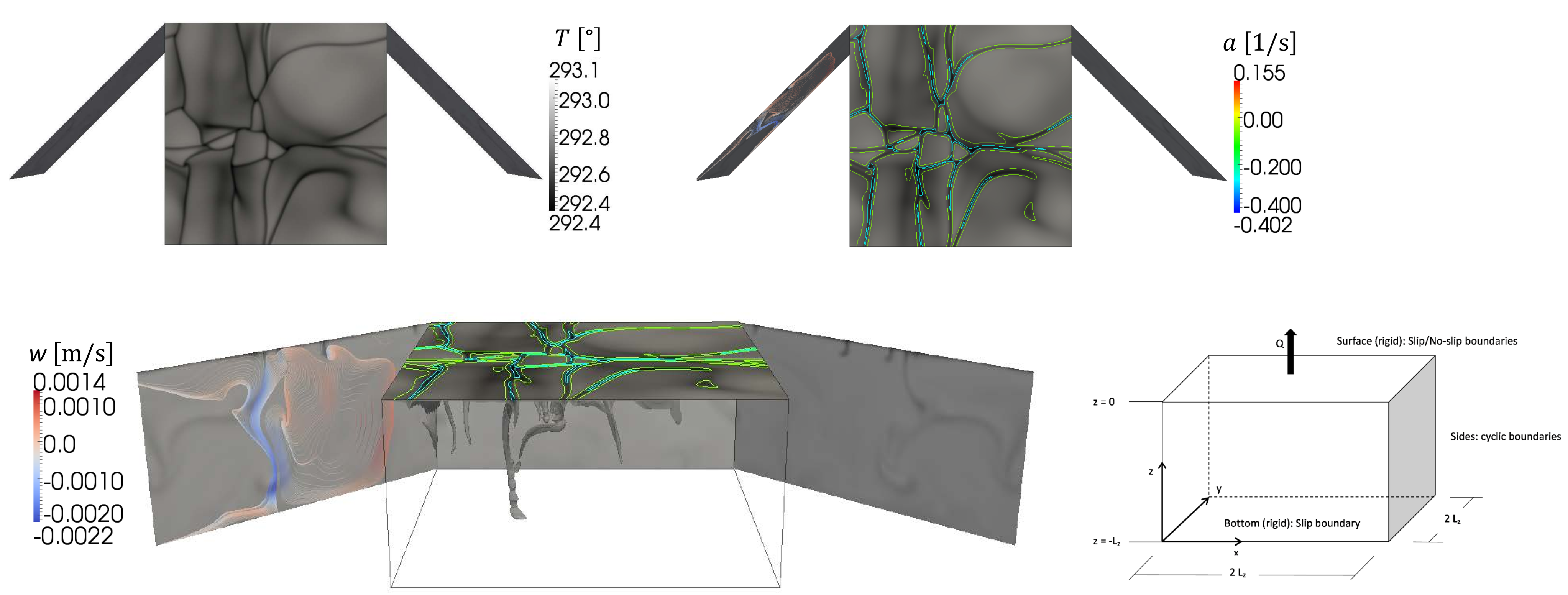

Figure 1. Instantaneous snapshots of the temperature (T), horizontal flow divergence (a) and the vertical velocity (w) corresponding to a surface heat flux Q = 100 W/m². In order to facilitate the understanding only the temperature is given in the plot at the upper left corner and then the divergence is added in the upper right corner and then finally the computational domain is "opened" in order to see the cold plumes of downward moving cold water in the center picture and the streamlines colored with the vertical velocity at the left hand wall. It can be noted that the temperature field of the two "opened" walls are the same since there are cyclic boundary condition in the horizontal directions.

Methods

The flow configuration comprises a fully developed turbulent flow bounded horizontally (x- and y-directions) by cyclic boundary conditions and vertically (z-direction) by parallel walls, with a slip wall boundary condition at the bottom boundary wall and two different kinds of wall boundary conditions at the surface boundary wall (i.e., slip and no-slip) , see **Figure 1**.

The heat flux (Q = 100 W/m²) out of the surface boundary is fixed and the bottom boundary is modeled adiabatic (no heat flux). A volumetric heat source is added equally distributed over the domain to balance the heat loss caused by the heat flux through the surface boundary. A passive scalar is solved in order to study the influence of the different surface boundary conditions appropriate to the surface exchange of heat and a sparsely soluble gas (fixed surface concentration condition).

The simulations are carried out using the OpenFOAM, an open source computational fluid dynamics tool with a collocated finite volume approach. Time and space are discretized using the second-order Crank-Nicholson and the second-order central differencing scheme respectively. The time step δt was dynamically adjusted to keep the courant flow number Co < 0.5 in all cells.

Results and discussion

Figure 2a shows a good agreement between present study and the simulations run with a pseudo-spectral code[1]. It can also be seen that the horizontal velocity rms decreases with increasing amount of surfactants, i.e. increasing Marangoni number (Ma), although the no-slip case and the saturated surfactant case never become equal.

Figure 2b shows that the temperature gradient for the clean and the slip conditions and the saturated surfactant case and the no-slip cases coincide with the intermediate surfactant cases in-between. This implies that a no-slip boundary condition can be used for studying the heat flux for a saturated surfactant case. It can also be seen that a passive tracer shows similar results for the no-slip case but differs somewhat for the slip case.

Figure 2c shows that the turbulent kinetic energy dissipation is almost the same up to a surface boundary layer close to the surface where the no-slip boundary condition gives up to four times increased dissipation. This is interesting when it comes to the use of the dissipation as a measure of the surface exchange velocity of heat and gases. The dissipation used to calculate the piston velocity below is taken at the boundary layer thickness, δ_{bl}, defined as the depth at which molecular diffusion accounts for only 5 % of the total heat flux.

Figure 2d shows that the mean horizontal flow divergence shows a similar pattern as the dissipation with similar values but close to the surface. The divergence is however as expected decreasing as the surface is approached with a no-slip relative to a slip boundary condition.

Figure 3a and 3b show that the piston velocity estimated using the divergence and the dissipation is similar and close to the parameterization of Cole and Caraco[2] whereas the estimation via the heat flux is close to the parameterization of Wanninkhof[3]. It can also be seen that the piston velocity estimated with the dissipation matches the scalar flux within 5% for both slip and no-slip conditions.

The piston velocity as a function of heat flux Q, turbulent kinetic energy dissipation ε and horizontal flow divergence a is calculated as

Heat[4]: $$k_{gas} = k_{heat}\left[\frac{Sc}{Pr}\right]^{-n},\ k_{heat} = \frac{Q}{\rho c_p \Delta T}$$

Dissipation[5]: $$k_{gas} \propto (\varepsilon\nu)^{1/4} Sc^{-n} \approx 0.42(\varepsilon\nu)^{1/4} Sc^{-n}$$

Divergence[6]: $$k_{gas} = \frac{1}{2}\sqrt{a\nu} Sc^{-n}$$ (a taken at the surface and boundary layer thickness for the free-slip and no-slip case respectively)

where the exponent n varies with boundary condition $1/2 < n < 2/3$ for slip and no-slip conditions respectively. The study of actual values of n for different boundary conditions has not been part of this study.

Conclusions

The piston velocity estimations by Wanninkhof (2009) and Cole and Caraco (1998) match the piston velocity from heat flux calculation for the free-slip boundary condition reasonably well. The piston velocity is approximately three times less for the no-slip compared to the free-slip condition.

k_{heat} is very well modeled with a no-slip boundary condition compared to a saturated surfactant case (high *Marangoni* number).

Altering the domain depth with a factor of two changes k_{heat} with less then ± 5% whereas a change in heat flux alters $k_{heat} \propto Q^{1/4}$ (which matches well with the dissipation model assuming $\varepsilon\sim$ buoyancy production $B = \beta g Q/\rho c_p$) for the free-slip case respecively[7].

The boundary layer thickness δ_{bl} is approximately five times the length scale, z_{sm}, according to the surface strain model[7].

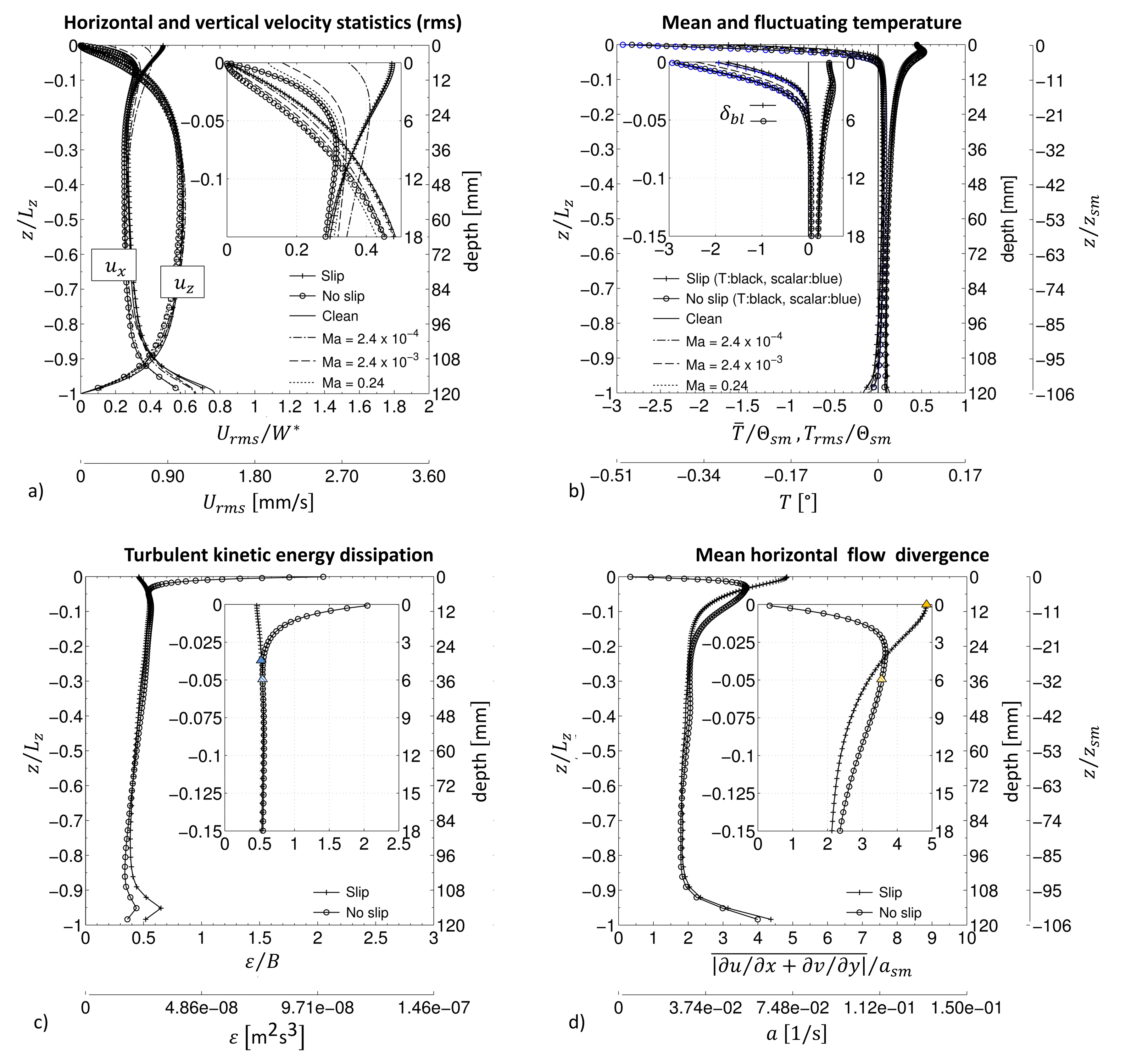

Figure 2. *Vertical and tangential velocity statistics (a) and temperature statistics (b). The velocity and the temperature are normalized with the outer velocity scale $W^* = (BL_z)^{-1/3}$ and the temperature scale $\Theta_{sm} = \sqrt{\pi/2}(g\beta)^{-1}(PrB^3/\alpha)^{1/4}$ of the surface strain model respectively. The cases with a surfactants including the case "Clean" are run with a pseudo-spectral code. Turbulent kinetic energy dissipation (c) and horizontal flow divergence (d). The dissipation and the divergence are normalized with the buoyancy production $B = \beta g Q/\rho c_p$ and the inverse time scale (a_{sm} = 1/t_{sm}) of the surface strain model respectively. The nominal values are also given corresponding to a surface heat flux Q = 100 W/m². Vertical axes are given for scaling with domain depth, depth corresponding to a surface heat flux Q = 100 W/m², and scaling $z_{sm} = \sqrt{2}(B/\upsilon\alpha^2)^{-1/4}$ according to the surface strain model.*

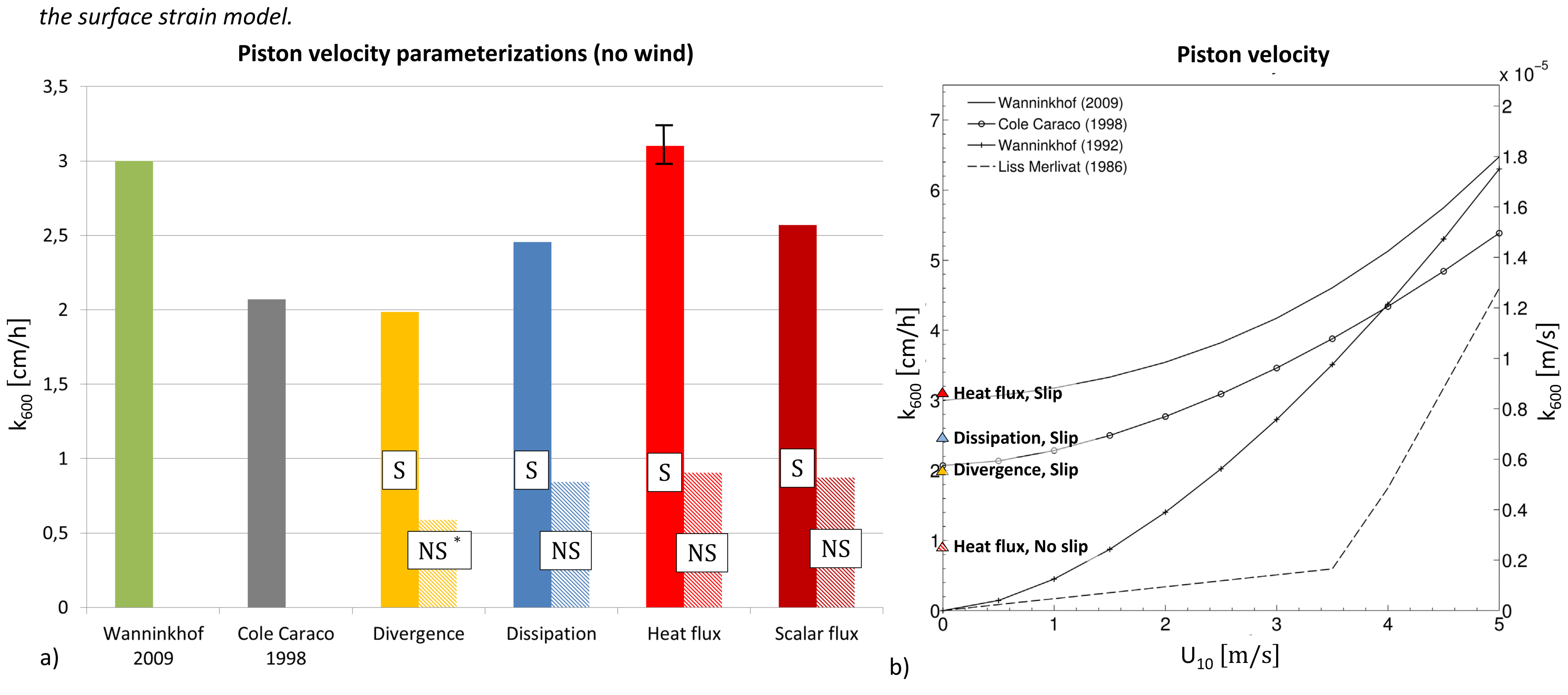

Figure 3. *(a) Piston velocity for no wind conditions for two parameterizations as in Figure 2b compared to present study. NS* implies that the horizontal flow divergence is taken at the boundary layer thickness for the no-slip case. The black bar at the top of the estimation of piston velocity via k_{heat} during slip condition is indicating the approximate change while altering the domain depth $0.5L_z$ - $2.0L_z$ [7]. (b) Piston velocity as a function of wind speed 10 m above the surface. (Animations of temperature flow field from present study and from field measurements with an IR-camera during poster session)*

References

[1] Zhang, Q., R. A. Handler and S. T. Fredriksson (2013). "Direct numerical simulation of turbulent free convection in the presence of a surfactant." International Journal of Heat and Mass Transfer 61: 82-93.

[2] Bade, D. L. (2009). Gas exchange at the Air-Water interface. Encyclopedia of Inland Waters, Elsevier. 1: 70-78.

[3] Wanninkhof, R., W. E. Asher, D. T. Ho, C. Sweeney and W. R. McGillis (2009). "Advances in Quantifying Air-Sea Gas Exchange and Environmental Forcing." Annual Review of Marine Science 1: 213-244.

[4] Frew, N. M., E. J. Bock, U. Schimpf, T. Hara, H. Haussecker, J. B. Edson, W. R. McGillis, R. K. Nelson, S. P. McKenna, B. M. Uz and B. Jahne (2004). "Air-sea gas transfer: Its dependence on wind stress, small-scale roughness, and surface films." Journal of Geophysical Research-Oceans 109.

[5] Zappa, C. J., W. R. McGillis, P. A. Raymond, J. B. Edson, E. J. Hintsa, H. J. Zemmelink, J. W. H. Dacey and D. T. Ho (2007). "Environmental turbulent mixing controls on air-water gas exchange in marine and aquatic systems." Geophysical Research Letters 34.

[6] McKenna, S. P. and W. R. McGillis (2004). "The role of free-surface turbulence and surfactants in air-water gas transfer." International Journal of Heat and Mass Transfer 47(3): 539-553.

[7] Leighton, R. I., G. B. Smith and R. A. Handler (2003). "Direct numerical simulations of free convection beneath an air-water interface at low Rayleigh numbers." Physics of Fluids 15(10): 3181-3193.

Acknowledgement

The computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at C3SE (Chalmers Centre for Computational Science and Engineering) computing resources.