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Single-column model and large eddy simulation of the evening transition in the planetary boundary layer

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The transition from the convective boundary layer during the daytime to the stable stratified boundary layer during nighttime after sunset plays an important role in the transport and dispersion of atmospheric pollutants. However, our knowledge regarding this transition and its feedback on the structure of the subsequent nocturnal boundary layer is still restricted. This also prevents forecast models from accurate prediction of the onset and development of the nighttime boundary layer, which determines the redistribution of pollutants within the nocturnal surface layer and the residual layer aloft. In the present study, the well-known case of day 33 of the Wangara experiment is resimulated using the Weather Research and Forecasting (WRF) model in an idealized single-column mode to assess the performance of a frequently used planetary boundary layer (PBL) scheme, the Yonsei University (YSU) PBL scheme. These results are compared with two large eddy simulations (LES) for the same case study imposing different surface fluxes: one using previous surface fluxes calculated for the Wangara experiment and a second one using output from the WRF model. The results show a reasonable agreement of the PBL scheme in WRF with the LES. Overall, all the simulations presented a cold bias of $\sim$3 Kelvin for the potential temperature and underestimation of the wind speed, especially after the transition to nighttime conditions (biases were up to 4 ms-1). Finally, an alternative set of eddy diffusivity equations was tested to represent the transition characteristics of a sunset period, with a stable layer below and a new parameterization for the convective decay regime typically observed in the RL aloft. This set of equations led to a gradual decrease of the eddy diffusivity, which replaces the instantaneous collapse of traditional diagnostics for eddy diffusivities. More appreciable changes were observed in air temperature, wind speed and specific humidity (up to 0.5 K, 0.6 ms-1, and 0.003 gkg-1, respectively). Although the representation of the convective decay in the standard parameterization did not show noticeable improvements in the simulation of state variables for the selected Wangara case study day, small changes in the eddy diffusivity over consecutive hours throughout the night can impact the simulation of distribution of trace gases in air quality models. So, this work points out the relevance of simulating the turbulent decay during sunset, which could help air quality forecast models to better represent the distribution of pollutants storage in the residual layer during the entire night.