Online Supplement

A Large-eddy Simulation Study of Water Vapour and Carbon Dioxide Isotopes in the Atmospheric Boundary Layer

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Figure S1: Modelled leaf - $H_2^{18}O$ composition (δ_L^w) in relation to relative humidity (RH), the kinetic fractionation factor (ϵ_k^w) and surface roughness (z_o). Left panels show the dependence on RH, with the line representing the best fit linear regression. Right panels show the deviation of δ_L^w from the regression line as a function of ϵ_k^w . The xylem water $H_2^{18}O$ composition is set at -5.0 per mil in these simulations.

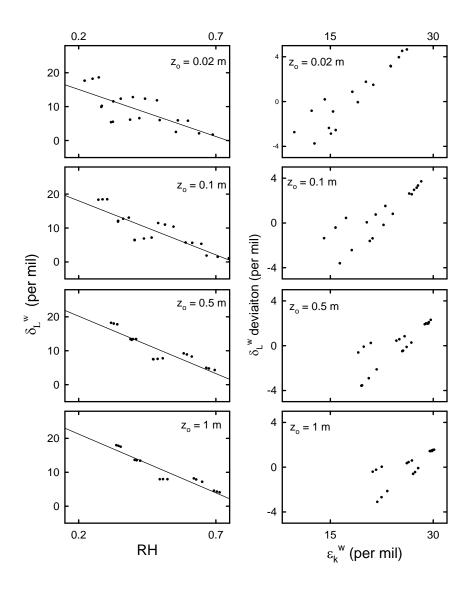


Figure S2: Flux profiles of buoyancy (a), specific humidity (b) and CO₂ mixing ratio (c), and the isoforcing profiles of C¹⁸OO (d), H₂¹⁸O (e) and ¹³CO₂ (f). The simulation is carried out with a time varying solar radiation forcing, surface roughness $z_0 = 0.5$ m, geostrophic wind speed $u_g = 5$ m s⁻¹, and the initial surface specific humidity q = 8 g kg⁻¹. Local solar time is given in panel a.

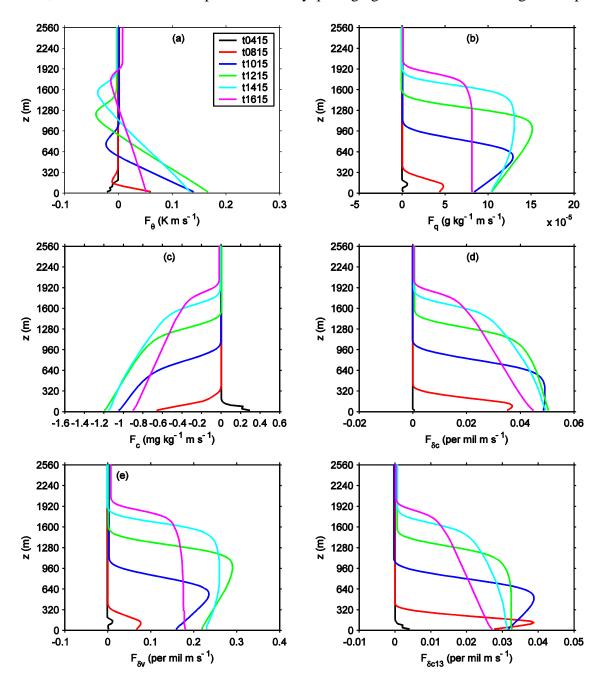


Figure S3: As in Figure S2 but for profiles of potential temperature (a), specific humidity (b), CO_2 mixing ratio (c), and isotopic compositions of $C^{18}OO$ (d), $H_2^{18}O$ (e) and $^{13}CO_2$ (f).

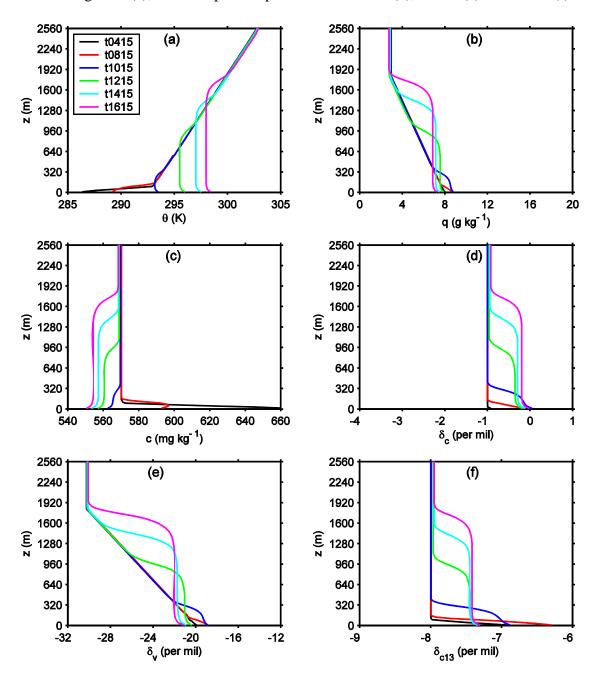


Figure S4: As in Figure S2 but for an initial surface specific humidity $q = 16 \text{ g kg}^{-1}$.

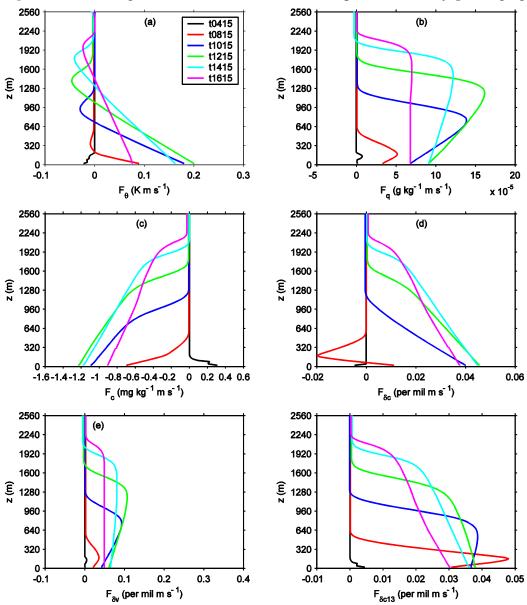


Figure S5: As in Figure S3 but for an initial surface specific humidity $q = 16 \text{ g kg}^{-1}$.

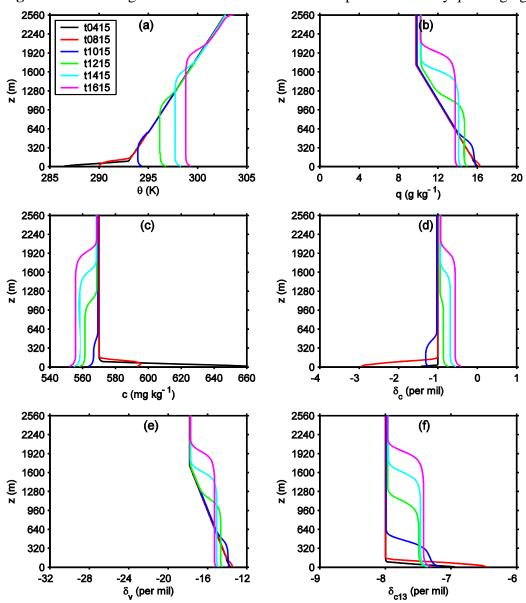


Figure S6: Turbulent fluctuations simulated by the ISOLES model run in the snapshot mode initiated with the profiles shown in Figure 2 with surface roughness $z_0 = 0.5$ m and geostrophic wind speed $u_g = 5$ m s⁻¹. These time series are for the central grid at the height of 100 m above the surface. The mean values have been removed.

