

# Supporting Information for "The climatological impacts of continental surface evaporation, rainout, and sub-cloud processes on $\delta D$ of water vapor and precipitation in Europe."

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## Introduction

This supplementary material summarizes the stable water isotope implementation in the multilayer soil land surface scheme TERRA [Schrodin and Heise, 2001] of the limited-area numerical weather prediction and climate model COSMO [Steppeler et al., 2001]. A validation paper on this implementation is in preparation. The model has also been used by Dütsch [2017] in CCLMiso simulations over Europe. A more detailed description of the processes represented in TERRA can be found in Doms et al. [2011] and for the water isotope part in Dütsch [2017].

## Text S1.

The soil model TERRA provides the lower boundary conditions of temperature and specific humidity for the COSMO model over land by calculating the energy and water budget in the soil. The isotope version TERRA<sub>iso</sub> additionally calculates the land surface water budget of the heavy isotopes HD<sup>16</sup>O and H<sub>2</sub><sup>18</sup>O. The relevant water reservoirs and fluxes for the water budget and the isotope implementation are shown schematically in Fig. S2.

External parameters are used to describe the orography, the land-sea-mask, dominant land use, and dominant soil type. There are eight predefined soil types that are associated with specific hydraulic characteristics. The plant characteristics such as the fractional area covered by plants, the leaf area index, and the root depth are obtained from the dominant land use.

When following a "raindrop's pathway" through TERRA, water can enter the land surface model in the form of precipitation ( $P_r$  and  $P_{\text{snow}}$ ) as given by the atmospheric part

of COSMO. If precipitation falls as snow, it enters the **snow reservoir** (grey reservoir in Fig. S2), if precipitation falls as rain, it enters the intercept reservoir. The snow reservoir is used in the single-layer mode in the setup for this study and contains snow, frozen water and rime. The isotope ratios associated with snow and rain are given by COSMO<sub>iso</sub>. The change in the liquid water content of the snow reservoir is determined by the snowfall rate, the evaporation from the snow reservoir (sublimation), the infiltration contribution from melting snow and the runoff from the snow reservoir. Phase changes of precipitation when it arrives at the surface (freezing rain and snow-rain) are taken into account for the budgets based on surface temperature, but no fractionation is applied for these phase changes.

If the precipitation phase is liquid, a part of it (fraction  $\beta$  in Fig. S2) enters the **intercept reservoir** containing all surface liquid water including dew on plants and on the soil (blue reservoir in Fig. S2). The temporal change in liquid water content of the intercept reservoir is determined from the intercepted fraction of rainfall, the rainfall intensity, the evaporation, percolation and runoff from the intercept reservoir.

The part of the rainfall that is not intercepted as well as the percolation from the intercept reservoir and the melted snow enter the **multilayer soil reservoir** containing all water below the Earth's surface (brown reservoir in Fig. S2). Six active soil layers can be defined in TERRA. Soil layer 7 is hydrologically inactive and uses a prescribed climatological soil water content. Soil layer 8 is also thermally inactive and uses a constant temperature set to the annual mean near surface air temperature. In the first soil layer, the temporal change in liquid water content is determined by the rainfall rate, the snowmelt, the percolation from the intercept reservoir, bare soil evaporation from the first soil layer, transpiration from the first soil layer, surface runoff from infiltration excess, subsurface runoff from the first soil layer and capillary rise from or gravitational loss to layer 2 (depending on the sign of the vertical soil water flux  $F$ ). For the subsequent soil layers (2-6) the temporal change in the liquid water content of the soil is simpler. It only depends on the vertical soil water fluxes (capillary rise or gravitational loss from the adjacent layers), the transpiration rate and the subsurface runoff from the soil layer. The soil mass budget is solved by first computing the evapotranspiration (atmospheric demand) and infiltration fluxes (atmospheric forcing) and then solving Richards' equation [Richards, 1931] for vertical transport of water in the soil due to gravity and capillary forces. Finally the runoff from the soil layers is computed if the total water content of the layer exceeds field capacity (maximum water holding capacity of the soil) and if the divergence of the gravitational and capillary fluxes in this layer is negative.

In TERRA<sub>iso</sub> the corresponding **water budget of the heavy isotopes HD<sup>16</sup>O and H<sub>2</sub><sup>18</sup>O** is computed diagnostically from the water budget of the light isotope H<sub>2</sub><sup>16</sup>O.

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Similar to COSMO<sub>iso</sub>, the isotope ratios used in TERRA<sub>iso</sub> are always defined as  $r_i = \frac{R_i}{R_{VSMOW}}$ . To obtain the corresponding  $\delta$ -values in ‰:  $\delta_i = (r_i - 1) \cdot 1000$ .

The **isotope forcing** for TERRA<sub>iso</sub> includes the near surface water vapour and precipitation isotopes:

$$r_v = \frac{R_v}{R_{VSMOW}}$$

$$r_r = \frac{R_r}{R_{VSMOW}}$$

The water fluxes in TERRA<sub>iso</sub> are mostly **non-fractionating** and act as passive tracers and the isotope ratio in the flux is equal to the isotope ratio in the reservoir where the flux originates. Note that the fluxes are defined positive toward the Earth's surface (downward in the atmosphere, upward in the soil). Hence, in Fig. S2,  $P$ ,  $E$ ,  $I$  and  $T$  are positive downward and negative upward, while  $F$  is positive upward (capillary rise) and negative downward (gravitational flow).  $N$  is always positive, and the ice melting flux  $M$  (not shown in Fig. S2) is defined positive from ice to liquid.

We thus use the following isotope ratios for the different fluxes in TERRA<sub>iso</sub>:

- **Infiltration:**

$$r_{I_{perc}} = r_{int}$$

$$r_{I_{melt}} = r_{snow}$$

- **Vertical transport:** (with the layer index  $k$  increasing towards lower soil layers)

$$r_{F_{k,k+1}} = r_k, \text{ if } F_{k,k+1} < 0$$

$$r_{F_{k,k+1}} = r_{k+1}, \text{ if } F_{k,k+1} > 0$$

- **Runoff:**

$$r_{NS,int} = r_{int}$$

$$r_{NS,snow} = r_{snow}$$

$$r_{N_{infil}} = \frac{(1 - \beta) \cdot r_{Pr} \cdot P_r + r_{I_{perc}} \cdot I_{perc}}{(1 - \beta) \cdot P_r + I_{perc}}$$

- **Melting of soil ice:**

$$r_{M_k} = r_{ice,k}, \text{ if } M_k > 0$$

$$r_{M_k} = r_k, \text{ if } M_k < 0$$

- **Snow sublimation:**

$$r_{E_{snow}} = r_{snow}, \text{ if } E_{snow} < 0$$

- **Plant transpiration:** Plant transpiration is often assumed to occur without fractionation [e.g., Washburn and Smith, 1934; Barnes and Allison, 1983], since in steady state the isotopic composition of water leaving the plants through transpiration is equal to the isotopic composition of water entering the plants from the soil. The steady state assumption is valid on long time scales ( $\geq$  days), however, on subdaily time scales variations in leaf water enrichment can occur and the isotopic composition of the transpiration flux is often different from the isotopic composition of the soil [Dongmann et al., 1974; Harwood et al., 1999; Wang et al., 2012]. Plant transpiration in TERRA<sub>iso</sub> can occur with or without fractionation. In the nonfractionating case (steady state), the isotope ratio in the plant transpiration flux is equal to the weighted mean of the isotope ratios of the soil layers from which the plants take up:

$$r_T = \frac{\sum_{k=1}^6 r_k \cdot T_k}{\sum_{k=1}^6 T_k}$$

where  $T_k$  is the contribution to the total transpiration rate from layer  $k$ .

In the fractionating case (nonsteady state), the isotope ratio in the transpiration flux is calculated based on the model by Farquhar and Cernusak [2005] with a constant leaf water content. For both settings the root uptake is considered non-fractionating ( $r_{T_k} = r_k$ ). The different treatments of leaf processes (steady-state and non steady-state leaf water enrichment, Peclet Effect) solely impact the daily cycle of the isotope composition of transpiration and the leaf water isotope composition. The daily cycle of the near surface water vapour isotope composition is slightly affected but over longer timescales the effect of non-steady state fractionation is negligible for the isotope composition of atmospheric waters. Thus, in the setup used in this paper the steady state setting is chosen.

Only few fluxes in TERRA<sub>iso</sub> are **fractionating**. The group of the fractionating fluxes can further be separated into equilibrium and nonequilibrium fluxes. The equilibrium fluxes are dew formation ( $E_{int} > 0$ ) and rime formation ( $E_{snow} > 0$ ). For these two fluxes the isotope ratios are calculated with the equilibrium fractionation factors over liquid ( $\alpha_{eq}^{l/v}$ , Majoube [1971a]) and ice ( $\alpha_{eq}^{i/v}$ , Majoube [1971b]):

- **Dew formation:**  $r_{E_{int}} = \alpha_{eq}^{l/v} \cdot r_v$ , if  $E_{int} > 0$

- **Rime formation:**  $r_{E_{snow}} = \alpha_{eq}^{i/v} \cdot r_v$ , if  $E_{snow} > 0$

The **nonequilibrium fluxes** are bare soil evaporation ( $E_{bs}$ ) and evaporation from the interception reservoir ( $E_{int} < 0$ ). For these two fluxes the isotope ratios are calculated with the Craig-Gordon model [Craig and Gordon, 1965]:

- **Bare soil evaporation:**  $r_{E_{bs}} = \alpha_k \cdot \frac{r_1 / \alpha_{eq}^{l/v} - h \cdot r_v}{1 - h}$

As the only modification compared to the TERRA<sub>iso</sub> used by Dütsch [2017], we adjusted  $r_{E_{bs}}$  at locations with skin temperature below the freezing point. For these conditions, the Craig-Gordon-equation is possibly inappropriate because it ignores processes specific to ice such as non-fractionating sublimation. For this reason, we turned off the effect of bare soil evaporation on atmospheric  $\delta D$  in the case of skin temperature below the freezing point by setting  $r_{E_{bs}} = r_v$ . The  $\delta D$  of the other, typically dominating, surface fluxes such as snow sublimation is not affected by this change.

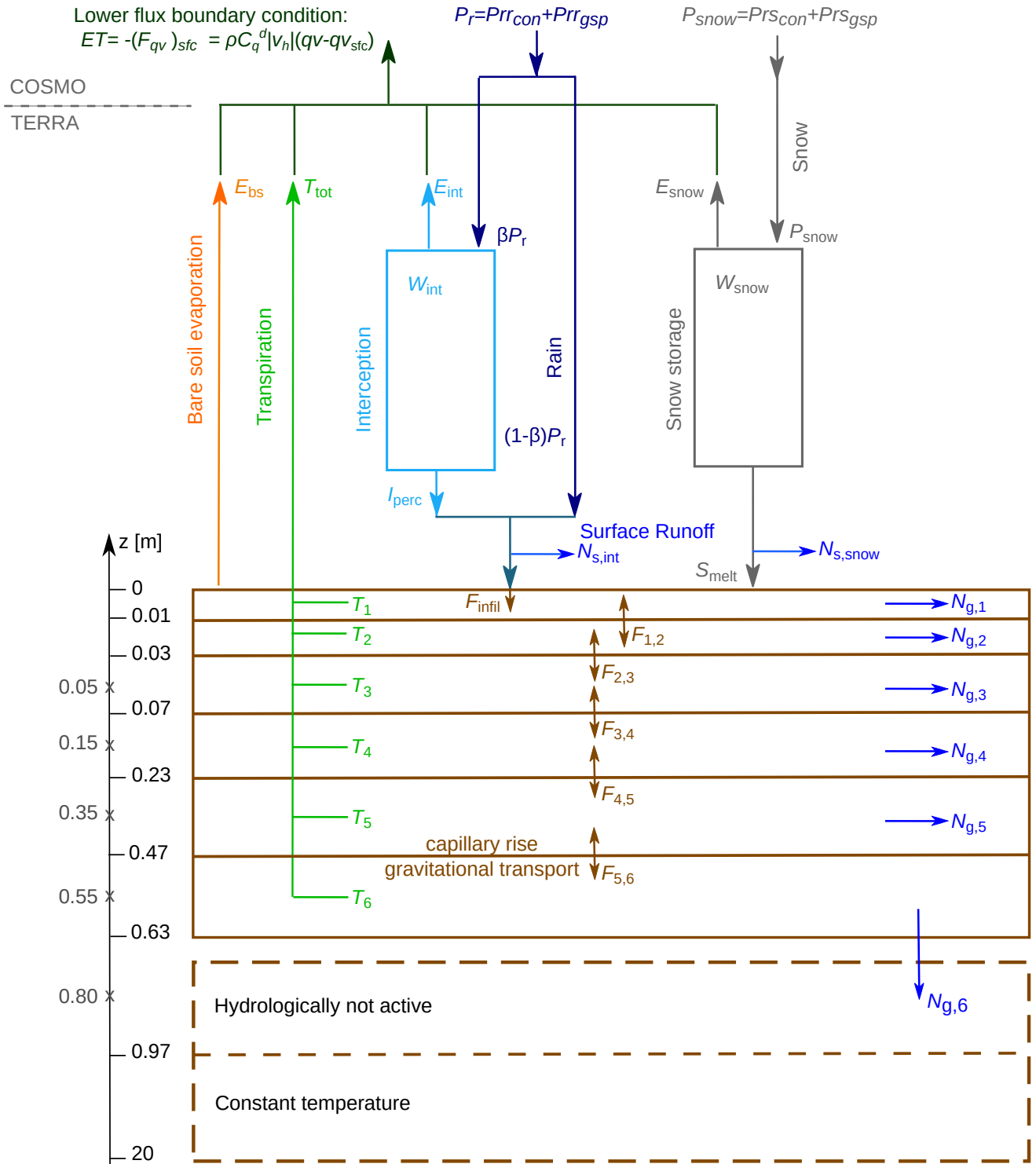
- **Evaporation from the intercept store:**  $r_{E_{int}} = \alpha_k \cdot \frac{r_{int} / \alpha_{eq}^{l/v} - h \cdot r_v}{1 - h}$ , if  $E_{int} < 0$  where  $r_1$  and  $r_{int}$  refer to the isotope ratios in the first soil layer and in the interception reservoir, respectively,  $h$  is the relative humidity with respect to the surface temperature, and  $\alpha_k$  is the nonequilibrium fractionation factor defined as the  $n^{\text{th}}$  power of the molecular diffusivity ratio in air [Mathieu and Bariac, 1996]:

$$\alpha_k = \left( \frac{D^{\text{iso}}}{D} \right)^n \quad (1)$$

with  $n = 0.67$  [Riley et al., 2002]. Thus, with the diffusion coefficients from Merlivat [1978],  $\alpha^{18O_k} = 0.981$  and  $\alpha^{2H_k} = 0.984$ . The equilibrium fractionation factor  $\alpha_{eq}^{l/v}$  is again parameterised following Majoube [1971a].

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**Figure S2.** Schematic of the water fluxes in the soil currently used in TERRA<sub>iso</sub>.

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