A coupled equilibrium boundary layer model with stable water isotopes and its application to local water recycling

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ABSTRACT

The contribution of evapotranspiration (ET) to regional precipitation, known as “local water recycling”, is a key process in the water cycle that can affect water management. However, the amount of planetary boundary layer (PBL) moisture that arises from ET is highly uncertain due to complex atmosphere and land surface conditions. In this study, an idealized two-layer equilibrium boundary layer model was coupled with a stable water isotope module including HDO and H\textsubscript{2}^{18}O to constrain PBL growing season water transport processes. The model was validated using turbulent heat fluxes and isotope ratios of water vapor (\$\delta_{P}$) and precipitation (\$\delta_{P}$) measured at a cropland site and a nearby tall tower in the Upper Midwest, United States. The results show that the PBL equilibrium features of \$\delta_{m}$ and \$\delta_{m}$ are well-constrained by thermal and moisture equilibrium in the PBL. For this study region, the summer values of rain evaporation fraction (f) and local water recycling ratio (LRR) are estimated to be 0.09 and 0.29 ± 0.12, respectively. The summer LRR values for the years 2006–2010 were 0.35, 0.36, 0.17, 0.29, and 0.29, respectively. The small value of LRR in 2008 corresponded to a drought condition with the lowest precipitation and second lowest ET among the five years. The summer magnitude of the amount effect is –2.8% (mm day\textsuperscript{-1}) and –0.8% (mm day\textsuperscript{-1}) for HDO and H\textsubscript{2}^{18}O, respectively. The local water recycling is identified as a significant factor influencing the continental isotope effect. Cropland has likely changed the regional LRR by −7.6 to 19.5% under different pre-agriculture land use scenarios. The feedback processes revealed here indicate that local water recycling is expected to be weakened under drought conditions, but it will be enhanced if irrigation is applied more intensely with more frequent drought events as the climate continues to warm.

1. Introduction

Evapotranspiration (ET) is a dominant moisture source in the planetary boundary layer (PBL) affecting the terrestrial water cycle (Oki and Kanae, 2006; Wang and Dickinson, 2012). The contribution of ET to regional precipitation, known as “local water recycling”, is a key mechanism that affects the water cycle and water management (Keys et al., 2019; Treberth, 1999; Van Der Ent and Savenije, 2011). On global average, the ratio of precipitation over land originating from terrestrial ET, the “recycling ratio”, is about 40% (Van Der Ent et al., 2010). However, the contribution of ET to precipitation is highly uncertain at the regional scale.

ET is affected by multiple factors, including meteorological variables (such as air temperature, air moisture, wind speed, and radiation) and land surface characteristics (such as canopy resistance, surface roughness, and albedo) (Haghighi and Kirchner, 2017; McVicar et al., 2012). The water cycle is expected to be intensified in response to global warming (Durack et al., 2012; Huntington, 2006; Santer et al., 2007). Land surface characteristics are changing due to agricultural intensification and other land use changes. For example, the grass-to-corn/soy conversion rate was 1.0–5.4% annually across the western Corn Belt, United States (US) over the period 2006–2012 (Wright and Wimberly, 2013). Such changes in climate and land-use can drive important shifts in ET (Alter et al., 2018), and may significantly alter the magnitude and patterns of local water recycling (de Wierik et al., 2021; Van Der Ent et al., 2014; Zeng et al., 2018).

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Tracing the stable hydrogen and oxygen isotopes in water is a powerful way to study hydrometeorological processes in the soil-plant-atmosphere continuum. The variations of isotope concentrations provide additional information that can reveal the underlying controls on water cycle processes, such as ET partitioning, rain evaporation, local water recycling, and water sources of precipitation (Griffis et al., 2016; Werner et al., 2012; Worden et al., 2007). The isotope ratios of HDO/H2O and H218O/H216O (traditionally presented as δD and δ18O, respectively) in water vapor record the condensation and evaporation history of an air mass (Lee et al., 2005; Worden et al., 2007). For example, Craig and Gordon (1965) proposed a model of evaporation, mixing, and precipitation condensation over the ocean that considered isotope fractionation effects. Worden et al. (2007) compared HDO observations from the Tropospheric Emission Spectrometer (TES) on the Aura spacecraft with process curves of simple isotope models and found that ET is an important source that enriches the water vapor over continents. Isotope observations can also be used to partition ET into evaporation and transpiration, as the transpired vapor is typically more enriched in heavy isotopes than the soil evaporated vapor (Wang et al., 2010; Xiao et al., 2018; Yakir and Wang, 1996).

The isotope ratios, δD and δ18O, found in global precipitation observations are generally linearly correlated, following the Global Meteorological Water Line (GMWL), where δD = 8d[18O] + 10‰ (Craig, 1961). The slope of 8 is determined by the Rayleigh distillation process. Here, ET and rain evaporation can drive the values of δD and δ18O off the GMWL (Dansgaard, 1964). Consequently, the deuterium excess, which is defined as δ = δD − 8δ18O, can also reveal how local hydrometeorological processes influence the water cycle. For example, Lai and Ehleringer (2011) found a diurnal cycle of deuterium excess of water vapor over a coniferous forest with the maximum in the early morning and the minimum around noon, indicating that ET was the primary moisture source in the mid-afternoon PBL. In a global meta-analysis, Welp et al. (2012) found similar diurnal patterns of deuterium excess. Observations of deuterium excess indicate that the isotope composition of water vapor in the PBL is also driven by the solar radiative forcing at the diurnal scale (Lee et al., 2012).

Multiple idealized equilibrium PBL models have revealed that the diurnal averages of the PBL features (such as ET, potential temperature and specific humidity) display a long-term equilibrium with timescales longer than a month in response to the solar radiative forcing (e.g. Betts, 2000; Betts et al., 2004; McColl et al., 2019; Raupach, 2000). For example, Betts (2000) developed an idealized one-layer equilibrium boundary layer model over land, showing a quasi-linear response between the mixed layer (ML) height and the equilibrium specific humidity. Betts et al. (2004) extended the one-layer model into a two-layer PBL model by adding a cloud layer, or the convective boundary layer (CBL) above the ML. The two-layer model showed reasonable equilibrium concentrations of carbon dioxide and radon in the ML. Since the isotope ratios of water vapor in the ML show a well-mixed vertical profile (Bony et al., 2008; Lee et al., 2012) and pronounced diurnal variation (Lai and Ehleringer, 2011; Welp et al., 2012), the equilibrium boundary layer model should reveal the long-term equilibrium of the isotope compositions of water vapor in the PBL. Furthermore, the changes in the hydrometeorological processes, such as ET and local water recycling, are expected to alter the PBL equilibrium values of the water vapor isotope composition.

In this study, we coupled a water isotope module to the idealized equilibrium boundary layer model of Betts (2000) and Betts et al. (2004) (abbreviated as B00 and B04, respectively) to solve for the equilibrium values of oxygen and hydrogen isotope compositions of the water vapor and the water cycle components (e.g., ET, entrainment, and precipitation) within the PBL. We applied this modeling approach in the Upper Midwest US for the growing season to investigate the equilibrium isotope composition of water vapor in the PBL and the local water recycling within the region. The main objectives were to: (1) identify the long-term (seasonal and interannual) equilibrium of surface turbulent fluxes and isotope composition of water vapor in the ML; (2) use this modeling approach with observations to constrain the rain evaporation fraction and local water recycling ratio; and (3) explore the changes of isotope composition equilibrium and local water recycling affected by different vegetation types (broadleaf forest, needleleaf forest, grassland, and cropland).

This paper is organized as follows: First, the model equations are introduced; second, the model is validated using the in-situ observations at a cropland site; third, the sensitivity analyses for five parameters are shown to verify that the model parameters are well-constrained, to quantify the rain evaporation fraction and local water recycling ratio, and to model the isotope amount effect and continental effect; fourth, model results derived for different land surface scenarios are used to examine the influence of croplands on the local water recycling in the Upper Midwest US; and finally, the potential model applications for regional climate and isotope studies are discussed.

2. Model description

The model consists of a base model and a coupled water isotope module. The base model is mainly established using the two-layer framework of B04, defining the climate background with components including surface energy balance, thermal equilibrium in the ML, moisture equilibrium in the ML and the CBL. The water isotope module uses the equilibrium solutions of the base model to solve for the mass mixing ratio equilibrium of HDO and H218O in the ML and the CBL. While the original B04 framework only considers the non-recirculation condition, the base model includes the precipitation-related processes such as condensation, rain evaporation and local water recycling (Fig. 1). The major modifications include: (1) using the observed precipitation and rain evaporation fraction to quantify the parameter of rain evaporation cooling rate originally from B00 and applying the cooling rate to the thermal equilibrium of B04; (2) adding rain evaporation and condensation to the moisture equilibrium of B04; and (3) partitioning the moisture source of precipitation into local ET and advection above the PBL to determine the local water recycling ratio, with the idealized assumption that advection occurs above the PBL and is omitted within the PBL.

2.1. Base model

2.1.1. Surface energy balance

At the land surface, the net available energy (Q) is the difference between the net radiation (Rn) at the canopy top and the ground heat flux (G), which is equal to the sum of the turbulent heat fluxes, i.e. the sum of sensible heat flux (H0) and latent heat flux (LE0):

\[ Q = R_n - G = H_0 + L E_0, \]

where \( L = 2.5 \times 10^6 \) J kg\(^{-1}\) is the specific latent heat of water vaporization, and \( E_0 \) is the surface evapotranspiration.

2.1.2. Thermal equilibrium in the ML

Following B00 and B04, we consider the thermal equilibrium in the ML and ignore the thermal status above the ML top. The three thermal terms include the surface sensible heat flux (\( H_0 \)), thermal entrainment between the ML and the CBL (\( H_b \)), and the cooling term, consisting of radiative cooling (\( F_{\text{rad}} \)) and rain evaporation cooling (\( F_{\text{evap}} \)); these are balanced in the ML:

\[ C_p \frac{P_{\text{LCL}}}{g} \frac{\partial \theta}{\partial z} = \left( \frac{\theta_0}{T_0} \right) H_0 - \left( \frac{\theta_0}{T_r} \right) H_b + (F_{\text{rad}} + F_{\text{evap}}) = 0. \]

Here, \( P_{\text{LCL}} \) is the height of the ML top in pressure coordinates (values increase from zero at the ground surface), which is assumed to be identical to the pressure height of the lifting condensation level (LCL) and the cloud base suggested by B00 and B04. The variables \( T \) and \( \theta \) are
temperature and potential temperature, respectively. The subscripts 0, m, and b represent the surface, ML, and cloud base, respectively. The value of specific heat capacity of air \((C_p)\) is 1005 J kg\(^{-1}\) K\(^{-1}\), and the gravitational acceleration \((g)\) is 9.8 m s\(^{-2}\).

The surface sensible heat flux is determined by the bulk aerodynamic approach in B00 and B04:

\[
H_0 = \rho_0 C_p f_s^{-1} (T_0 - T_m),
\]  
(3)

where \(\rho_0\) is the surface air density, and \(f_s\) is the aerodynamic resistance of air. Here, \(f_s = C_p U^{-1}\), where \(C_p = 100\) is set as a constant aerodynamic transfer coefficient ignoring atmospheric stability; and \(U\) is the 2-m horizontal wind speed above the canopy. \(T_0\) is the surface temperature and \(T_m\) is the 2-m air temperature above the canopy.

The thermal mixing between the ML and the CBL \((H_b)\) is the product of entrainment mass flux \((\rho b W_b)\) and the potential temperature difference \((\theta_{b,\text{ml}} - \theta_{m})\) of the two layers (B04):

\[
\theta_b \left(\frac{\rho b W_b}{T_b}\right) = -\rho_0 C_p (\theta_{b,\text{ml}} - \theta_m),
\]  
(4)

where \(W_b\) is the entrainment velocity at the cloud base; \(\theta_{b,\text{ml}}\) is the potential temperature at the bottom of the cloud layer; \(\theta_m\) is the potential temperature in the ML; and \(T_b\) and \(T_m\) are the potential temperature and air temperature at the cloud base, respectively.

The radiative cooling \((F_{rad})\) is determined by the radiative cooling rate \((\partial \theta_{rad}/\partial t < 0)\), which is set as a prescribed parameter in the model:

\[
F_{rad} = C_r \left( \frac{P_{LCL}}{g} \right) \frac{\partial \theta_{rad}}{\partial t}.
\]  
(5)

The rain evaporation cooling \((F_{evap})\) is equivalent to the latent heat absorbed by the rain evaporation \((E_p)\):

\[
F_{evap} = C_r \left( \frac{P_{LCL}}{g} \right) \frac{\partial \theta_{evap}}{\partial t} = -L E_p.
\]  
(6)

Therefore, the rain evaporation cooling rate \((\partial \theta_{evap}/\partial t < 0)\) is determined by the mass flux of rain evaporation \((E_p)\) and the height of the ML \((P_{LCL})\):

\[
\frac{\partial \theta_{evap}}{\partial t} = -\frac{L g}{C_r P_{LCL}} E_p.
\]  
(7)

The radiative cooling \((F_{rad})\) is approximated by:

\[
F_{rad} = C_r \left( \frac{P_{LCL}}{g} \right) \frac{\partial \theta_{rad}}{\partial t} = \frac{L g}{C_r P_{LCL}} E_p.
\]

2.1.3. Moisture equilibrium in the ML

In the ML, the change rate of specific humidity \((d q_m/\partial t)\) is determined by the moisture fluxes of surface ET \((E_0)\), entrainment at the ML top \((E_b)\) and rain evaporation \((E_p)\). In the equilibrium state, the change rate of \(q_m\) is zero and the three flux terms are in balance:

\[
\left( \frac{P_{LCL}}{g} \right) \frac{dq_m}{dt} = E_0 - E_b + E_p = 0.
\]  
(8)

Using the aerodynamic approach from B00 and B04, the surface ET is given as:

\[
E_0 = \rho_0 (r_c + r_c)^{-1} (\theta_s(T_0) - q_m),
\]  
(9)

where \(\theta_s(T_0)\) is the saturation specific humidity near the soil surface, \(q_m\) is the equilibrium specific humidity in the ML and \(r_c\) is the canopy resistance. The model uses \(r_c\) as the independent variable.

Entrainment at the ML and the CBL is the product of entrainment mass exchange \((\rho b W_b)\) and moisture difference \((q_{cld} - q_m)\) of the two layers (B04); and \(\rho_0\) and \(W_b\) are the cloud-base air density and subsidence velocity, respectively:

\[
E_b = -\rho_0 W_b (q_{cld} - q_m).
\]  
(10)

We assume that rain evaporation only occurs in the ML:

\[
E_p = f \frac{P}{1 - f}.
\]  
(11)

where \(f\) is the fraction of rain evaporation, \(P\) is the precipitation rate measured at the ground level, and \(P/(1 - f)\) is the total condensed rainwater.
2.1.4. Moisture equilibrium in the CBL

B04 suggested that the growth and subsidence of the CBL are balanced by entrainment, and therefore a long-term equilibrium in the CBL is maintained. For the CBL moisture equilibrium, the change rate of specific humidity in the CBL \( \frac{dq_{c,b}}{dt} \) is zero with the balance among entrainment at the ML top \( (E_{b}) \), entrainment at the CBL top \( (E_{c}) \), and rainwater condensation \( (E_{c}) \):

\[
\frac{P_{c,b}}{g} \frac{dq_{c,b}}{dt} = E_{b} - E_{c} = 0, \tag{12}
\]

where \( P_{c,b} \) is the pressure depth of the cloud layer, or the CBL, defined as the pressure height difference between the CBL top and the ML top \( (P_{c,b} - P_{b}) \). Here, we follow the B04 assumption that the pressure height of the CBL top \( (P_{c}) \) or the PBL top as well, is 350 hPa (i.e. the pressure level of the CBL top is 350 hPa lower than the surface pressure, or typically 3500 m altitude above sea level).

B04 assumes a constant subsidence rate \( (\rho_{W}W_{s}) \) in the CBL. Our model follows this assumption and partitions the water vapor entrained from the ML to the CBL \( (E_{b}) \) into the condensation in the CBL \( (E_{c}) \) and the entrainment to the upper free atmosphere above the PBL \( (E_{c}) \):

\[
E_{b} = E_{c} = -\rho_{W}W_{s}(q_{i} - q_{s}), \tag{13}
\]

where \( \rho_{W}W_{s} \) is the entrainment mass exchange in the CBL, and \( q_{i} \) is the boundary condition prescribed by the specific humidity in the free atmosphere.

2.1.5. Local water recycling ratio

The total precipitated water to the ground \( (P) \) is ideally divided into two parts: the precipitation contributed by local ET \( (P_{L}) \) and the precipitation from free-atmosphere advection \( (P_{A}) \):

\[
P = P_{L} + P_{A}, \tag{14}
\]

where the subscripts \( L \) and \( A \) represents the local and advected components, respectively.

The condensation in the CBL \( (E_{c}) \) resulting from local ET \( (E_{c,L}) \) is described as:

\[
E_{c} = E_{c,L} = \frac{P_{L}}{1 - f}, \tag{15}
\]

The condensation from the free-atmosphere advected water is described as:

\[
E_{c,A} = \frac{P_{A}}{1 - f}. \tag{16}
\]

The local water recycling ratio \( (LRR) \) is defined as the ratio of local precipitation to the total precipitation \( (Van Der Ent et al., 2014) \):

\[
LRR = \frac{P_{L}}{P}. \tag{17}
\]

In the model, LRR is set as an input parameter. However, it will be shown later in the sensitivity analyses that LRR can be constrained with observations of ET and isotope ratios by the model-generated sensitivity diagrams. \( P_{L} \) can be determined from the observed total precipitation as \( P_{L} = LRR \cdot P \).

2.1.6. Closure scheme

Following B00 and B04, three upper boundary conditions at the ML top are necessary closures that are applied to solve the base model. These include the potential temperature at the cloud base, the relative humidity at the cloud base, and the virtual heat flux at the ML top. These three closures are described in Section S2.1 in the supplemental material.

2.2. Water isotope module

After solving the base model, the equilibrium solutions of temperature and mass mixing ratio of water vapor for each layer were used to drive the water isotope module. To be consistent with the units in the base model, we express the heavy isotope fluxes and concentrations in terms of mass fluxes and mass mixing ratios, respectively. The equation forms of the hydrogen and oxygen isotopes are identical, except for the values of their fractionation factors. Here, we present the isotope terms with a subscript \( i \) to represent either HDO or H\textsuperscript{18}O.

2.2.1. ML equilibrium

In the ML, the change rate of water isotope mass mixing ratio \( (dq_{i,ml}/dt) \) is determined by the mass fluxes of surface ET \( (E_{i,s}) \), entrainment at the ML top \( (E_{i,b}) \) and rain evaporation \( (E_{i,p}) \). In equilibrium, the three terms are balanced:

\[
\frac{P_{i,ml}}{g} \frac{dq_{i,ml}}{dt} = E_{i,s} - E_{i,b} + E_{i,p} = 0. \tag{18}
\]

The isotope mass flux of ET over a canopy is presented in a dynamic form with a kinetic fractionation factor \( (Worden et al., 2007) \):

\[
E_{i,s} = \rho_{W}W_{s}(q_{i,s} - q_{s}). \tag{19}
\]

where \( \rho_{W}W_{s} \) is the kinetic fractionation factor related to the differences in isotopic molecular diffusivity ratios \( (Merlivat & Jouzel, 1979; Cappa et al., 2003) \). \( R_{0} \) is the isotope molar ratio of soil water at the surface, which is a specified boundary condition; \( \alpha \) is the liquid-vapor equilibrium fractionation factor \( (\alpha > 1) \) depending on temperature \( (Horita and Wesolowski, 1994) \), and \( R_{0}/\alpha(T_{0}) \) is the isotope molar ratio of vapor just above the surface. \( M_{i}/M_{W} \) is a factor converting molar ratio to mass mixing ratio, where \( M_{i} \) is the molecular weight of HDO or H\textsuperscript{18}O and \( M_{W} \) is the molecular weight of H\textsubscript{2}O.

Entrainment is assumed to mix air completely without a fractionation effect. Therefore, we can use a similar parameterization in the PBL model to represent the water isotope mixing at the ML top:

\[
E_{i,b} = \rho_{W}W_{s}(q_{i,b} - q_{s}). \tag{20}
\]

2.2.2. CBL equilibrium

Similar to the water vapor mixing ratio in the CBL, the isotope fluxes are balanced by entrainment at the ML top \( (E_{i,b}) \), entrainment at the CBL top \( (E_{i,c}) \), and condensation \( (E_{i,c}) \):

\[
\frac{P_{i,c}}{g} \frac{dq_{i,c}}{dt} = E_{i,b} - E_{i,c} = 0. \tag{21}
\]

The entrainment at the cloud base \( (E_{i,b}) \) is divided into the condensation \( (E_{i,c}) \) in the CBL and the entrainment to the free atmosphere above the PBL \( (E_{i,p}) \) as:

\[
E_{i,b} = E_{i,c} = \rho_{W}W_{s}(q_{i,b} - q_{s}). \tag{22}
\]

where the isotope mixing ratio above the PBL \( (q_{i}) \) is the boundary condition determined by the prescribed isotope ratio above the PBL \( (\delta_{0}) \).

\( \alpha R C \) suggested the isotope condensation term as \( \alpha RC \), where \( \alpha \) is the temperature-dependent equilibrium fractionation factor \( (\alpha > 1) \), \( R \) is the isotope molar ratio, and \( C \) is the condensation rate. Therefore, the isotope mass flux of the CBL condensation is given by:

\[
E_{i,c} = E_{i,c,L} = \alpha(T_{c})E_{c,B} - \frac{E_{i,b}}{E_{b}}. \tag{23}
\]

where \( T_{c} \) is the average temperature of the CBL, which is equivalent to the temperature at the middle of the CBL while assuming a constant temperature lapse rate \( \Gamma \) (See Eq. S1).
Table 1

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</tr>
<tr>
<td>$q_i$</td>
</tr>
<tr>
<td>$\delta^{18O}$</td>
</tr>
</tbody>
</table>

2.2.3. Isotope composition of precipitation and rain evaporation

According to Worden et al. (2007), the isotope mass flux of the rain evaporation can be calculated by:

$$E_{i,F} = E_{i,P} + E_{i,PA} = \frac{f}{\alpha_i(T_{ML})} (E_{i,CL} + E_{i,CA}),$$

(25)

where $f$ is the evaporated rain fraction, $T_{ML}$ is the average temperature of the ML, and $\alpha_i$ is the kinetic fractionation factor accounting for molecular diffusive transport in the rain drops (Stewart, 1975).

Finally, the isotope mass mixing ratio in accumulated precipitation water is what remains in the condensed water after rain evaporation and is calculated as:

$$P_i = P_{i,L} + P_{i,A} = (E_{i,CL} - E_{i,P}) + (E_{i,CA} - E_{i,PA})$$

$$= (E_{i,CL} + E_{i,CA}) \left(1 - \frac{f}{\alpha_i(T_{ML})}\right).$$

(26)

2.3. Iterative process

The input parameters and variables to drive the model are listed in Table 1 and described in Section 3.1. The base model and the water isotope module were solved by iteration in two steps. First, in the base model, a range of $r_c$ values were given as the independent variable, other variables such as $P_i$, $\theta_{i}$, $q_i$, $q_{18O}$, and $\delta^{18O}$ were solved at each value of $r_c$ iteratively. Second, these solved meteorological equilibrium states were passed to the water isotope module to solve the equilibrium states of the isotope mass mixing ratios, such as $q_{i,0}$, $q_{i,cl}$, $q_{18O,0}$, and $\delta^{18O,cl}$. Finally, we have expressed the isotope compositions in the familiar delta $\delta$ notation as:

$$\delta^{(\%)} = \left( \frac{R}{R_{ref}} - 1 \right) \times 1000,$$

(27)

where $R$ is the molar ratio of the less abundant over the more abundant isotopic species and $R_{ref}$ is a standard molar ratio corresponding to the Vienna Standard Mean Ocean Water (VSMOW) scale, which is 1013.5 ppm for D/H2O and 1005.2 ppm for $H_2^{18}$O/$H_2^{16}$O.

2.4. Model limitations

First, consistent with the models of B00 and B04, the equilibrium model applied here is an idealized model that represents a climate average of the daily mean boundary layer over a long-term period (monthly or longer timescales). The atmospheric may not be strictly in equilibrium on the 24-hour timescale. However, the average of the day-to-day variation should approach a climate equilibrium provided that the long-term atmospheric thermal and moisture conditions are in balance. We note that the model is not expected to explain variations at the daily or sub-daily timescales.

Second, for some parameter settings, the model will not converge to a solution during iteration. This implies a non-equilibrium condition. For example, at very low $r_c$ values, the model will not converge to a solution. Here, the sensible heat flux is too strong to maintain the equilibrium at the low PBL height.

Finally, there are limitations with the simplified assumptions in the model. For example, advection below the PBL top is ignored, which could influence the background isotope composition (Worden et al., 2007). The microphysical processes in cloud and precipitation are largely simplified, which might potentially affect the isotope equilibrium. For instance, the rainwater formation only considers the vapor-liquid phase changes in condensation and ignores the ice phase. However, we note that ice-phase processes can be important in summertime precipitation associated with deep convection (Fu and Qin, 2014; Mülmenstädt et al., 2015). Furthermore, the model does not separate the convective precipitation and large-scale stratiform precipitation, while rainwater in convective precipitation tends to be more enriched (Aggarwal et al., 2016). Despite these simplifications, the model can capture some essential isotope features of ET, precipitation, and local water recycling during summer and can provide valuable insights regarding the interpretation of the isotope composition of atmospheric water vapor and precipitation.

3. Materials and methods

3.1. Model parameters

The study site for model setup and validation is the AmeriFlux core site US-Ro1 (44° 42′52″N, 93° 5′23″W, 260 m above sea level), which is a corn-soybean rotation cropland located in Rosemount, MN (Baker & Griffis, 2005). The model was run and validated for summer seasons (June to August), because the model only considers the vapor-liquid phase changes in condensation and precipitation.

5
A group of reference parameters and variables were prescribed to define a climate normal for the base model and the water isotope module (Table 1). The conceptual parameters in the base model such as radiative cooling rate, entrainment parameter, stability, reference potential temperature and pressure height of the CBL top were determined following B00 and B04 (see supplemental material Section S2.1). The input meteorological variables, such as net available energy, surface pressure, aerodynamic resistance (calculated from wind speed) and precipitation, were the ensemble averages of the summer observations at US-Ro1 from June to August 2004–2012 (Table S1). Both the rain evaporation fraction and the local recycling ratio are tunable parameters in the model. The reference value of rain evaporation fraction was arbitrarily prescribed as 0.1. The reference value of local recycling ratio was set as 0.3 according to previous studies in the same region (Griffis et al., 2016). We will assess if these two parameters are well constrained by comparing them with the results from the model sensitivity tests. The kinetic fractionation factors of evaporation (θ0 and η2θ0) in Eq. (19) were tuned and determined by model validation.

For the boundary conditions, the base model only needs the specific humidity above the PBL (q), while the isotope module requires isotope ratios of HDO and H218O both above the PBL (δD and δ18O) and at the surface (δD0 and δ18O0) (Table 1). The values of q, δD0 and δ18O0 were both retrieved from the Tropospheric Emission Spectrometer (TES) Level 3 daily products on the Aqua satellite (Beier et al., 2001; Worden et al., 2006). The reference values were the average summer measurements of the grid point nearest to US-Ro1 at the pressure level of 680 hPa in the TES product from 2005 to 2011. Since TES did not measure the profile of H218O and δ18O, both above the PBL (δD and δ18O) and at the surface (δD0 and δ18O0), we used the isotope ratios of δ18O in soil water at US-Ro1 was about −5% (Griffis et al., 2011; Welp et al., 2008), and δD0 was set as −50‰ with the soil water line δD = 5.3δ18O − 21.6 at US-Ro1 (Griffis et al., 2016).

### 3.2. Data for model validation

Applying the same rationale as B00 and B04 in the model validation, the model outputs were compared with the climate equilibrium presented by the daily averaged observations. The base model was validated by the surface fluxes and the ML variables observed in June to August 2004–2012. The surface fluxes for validation were measured at US-Ro1 by the eddy covariance method following AmeriFlux standard procedures. Data were obtained from the MPX weather station (44°57′N, 93°42′W; 290 m above sea level) in Rosemount, MN, which is 3 km away from US-Ro1 (Griffis et al., 2016). The water vapor was sampled at the height of 185 m and the isotope compositions were analyzed using a tunable diode laser (TGA200, Campbell Scientific Inc., Logan, UT, USA) (Griffis et al., 2016, 2010). The rainwater samples were collected in summer from 2006 to 2010 at a weather station on the Saint Paul Campus, University of Minnesota, which is 31.5 km north to US-Ro1 (Griffis et al., 2016) (Table S2). The isotope compositions of the samples were analyzed using a the Liquid Water Isotope Analyzer DLT-100 (Los Gatos Research Inc., Mountain View, CA, USA) following Schultz et al. (2011).

### 4. Results and discussion

#### 4.1. Model validation

##### 4.1.1. ML equilibrium of base model

The equilibrium solutions of the ML variables and the surface fluxes of the base model are compared with the linear regression of observations against PCL (Eq. 2). The modeled 𝜃₀, q₀, H, and LE are all quasi-linearly correlated to PCL. Here, the linear regression is treated as a first guess of the “observed” climate equilibrium and used as a benchmark for model validation. The modeled equilibrium is considered closer to the observed equilibrium when the model line deviates less from the regression line within the range of model output (i.e. PCL is between 70 and 280 hPa).

Both observed and modeled 𝜃₀ increase with PCL, with slopes of 0.0099 K hPa⁻¹ (p < 0.01) and 0.054 K hPa⁻¹, respectively (Fig. 2a). The observed and modeled q₀ are both negatively correlated to PCL with slopes of −0.043 (g kg⁻¹) hPa⁻¹ (p < 0.01) and −0.020 (g kg⁻¹) hPa⁻¹, respectively (Fig. 2b). The slope of modeled q₀ is 5.4 times the observed trend, while the slope of modeled q₀ is only half of the observation. Here we infer that the slope inconsistencies between model and observation reveal the disequilibrium condition in the soundings that were measured twice a day (i.e. weather soundings at 0600 and 1800 hr) and did not include hourly information of PBL development and diel dynamics. The measured soundings in early morning and late afternoon were less in equilibrium than noon and early afternoon. With PBL growth, the surface forcing warms and moistens the atmosphere less efficiently due to larger entrainment at the ML top, which causes flattened slopes in observed 𝜃₀ and steeper slopes in observed q₀ compared with the modeled equilibrium condition.

The observed and modeled H are both positively correlated to PCL, with similar slopes of 0.20 (W m⁻²) hPa⁻¹ (p < 0.01) and 0.21 (W m⁻²) hPa⁻¹, respectively (Fig. 2c), which indicates that the cooling terms are well-constrained (see Eq. S6). In the reference case, the radiative cooling rate is specified as −2 K day⁻¹, and the modeled rain evaporation cooling rate varies from −1.3 to −0.3 K day⁻¹ as the PBL grows (Fig. S2). The magnitude of the rain evaporation cooling rate is about 15 to 65% of the radiative cooling rate, indicating that the radiative cooling is dominant on clear days with large PBL height and that the rain evaporation cooling will be more important on cloudy/rainy days with relatively small PBL height. This supports that rain evaporation is a key cooling process in the ML equilibrium as proposed by B00.

When PCL increases, the observed LE shows an increased trend with a slope of 0.11 (W m⁻²) hPa⁻¹ (p < 0.01), but the modeled LE declines with a slope of −0.21 (W m⁻²) hPa⁻¹ (Fig. 2d). The negative correlation between the modeled H and LE is consistent with the “surface flux equilibrium” (SFE) theory, which is a one-layer model for daily or monthly equilibrium H and LE over water-limited inland continental regions (McCoy et al., 2019; McCoy and Ridgway, 2020). In SFE, when Q is fixed, a high H increases air temperature, induces a warmer atmosphere near the surface, and leads to declines in LE and surface moisture and vice versa for a low H situation. Therefore, LE determines the near-surface RH in the equilibrium condition, and the near-surface RH in
turn controls LE in the non-steady state (McColl and Rigden, 2020). The observations at US-Ro1 imply that the surface fluxes are consistent with SFE when the ML is well-developed. Although the entire set of observed LE is positively correlated to \( P_{LCL} \) (Fig. 2d), the observed LE is negatively correlated to \( P_{LCL} \) from 110 to 280 hPa (LE = –0.25\( P_{LCL} \) + 142.9, \( r = -0.19, p < 0.01 \)), whose linear regression is closer to the model output. The large values of \( P_{LCL} \) are related to large values of \( r_c \) that correspond to a water-limited condition, which drives the surface fluxes toward the SFE condition.

The base model also shows good performance in surface energy partitioning with the constraint on observed \( Q \) and the assumption of complete energy balance closure. While the surface energy balance ratio (\( EBR = (H + LE)/Q \)) of Eq. (1) is assumed to be 100% in the model, the average EBR of the eddy covariance data at US-Ro1 for summer seasons (2004 to 2012) is 86% (Table S1), which is within the typical range of eddy covariance measurements across FLUXNET sites (Stoy et al., 2013; Wilson et al., 2002). The sensitivity analysis on \( Q \) indicates that the evaporative fraction \( LE/(H + LE) \) is well constrained by using the observed \( Q \) as the reference value in the base model (Fig. S3).

### 4.1.2. ML equilibrium of water isotope compositions

Fig. 3 shows that the model generates reasonable isotope ratios and deuterium excess values in the ML compared with the observations at US-Ro1 in summer 2010 to 2012. The observed \( \delta D \) and \( \delta^{18}O \) both weakly decrease with \( P_{LCL} \) with slopes of –0.097 % hPa\(^{-1} \) (\( p = 0.03 \)) and –0.005 % hPa\(^{-1} \) (\( p = 0.49 \)), respectively (Fig. 3a). The model solutions of \( \delta D \) and \( \delta^{18}O \) display the same negative trends with slopes of –0.033 % hPa\(^{-1} \) and –0.018 % hPa\(^{-1} \), respectively (Fig. 3b). The modeled and observed \( \delta D \) both increase with \( P_{LCL} \) with slopes of 0.038 % hPa\(^{-1} \) (\( p = 0.17 \)) and 0.11 % hPa\(^{-1} \), respectively (Fig. 3c). The modeled curves of \( \delta D \), \( \delta^{18}O \), and \( \delta^{2} \) all pass between, or approach, the 95% confidence bounds of the corresponding linear regressions of the observations. Therefore, although the isotope module calculated the mass mixing ratio of \( H_2O \), HDO and \( H^2^{18}O \) independently, the modeled values and trends of isotope ratios and deuterium excess are realistic when compared with the observations, demonstrating that the ML isotope equilibrium of each isotopologue is well-constrained by the model.

The sensitivity tests on the kinetic fractionation factors of evaporation (\( \eta_0 \) and \( \eta_{18O} \)) indicate that these factors can significantly influence the relationship between isotope ratios and \( P_{LCL} \). The kinetic fractionation during evaporation is caused by the differences in molecular diffusivities of isotopic species, and it is not a constant, as it is influenced by the near-surface atmospheric condition (Lee et al., 2009; Merlivat and Jouzel, 1979). The laboratory ranges of \( \eta_0 \) and \( \eta_{18O} \) are 0.9796–0.9955 and 0.9724–0.9943, respectively (Horita et al., 2008). The sensitivity tests showed that \( \delta D \) is insensitive to \( \eta_0 \), so \( \eta_0 \) takes the average lab value of 0.9892. The value of \( \eta_{18O} \) is determined as 0.9930 by best fitting the model outputs to the linear regression of observation and is consistent with the results of Lagrangian simulations of the isotope composition of evaporation in Europe (Pfahl and Wemli, 2009) and the estimates found for a soybean field calculated under low-wind condition (Lee et al., 2009).

### 4.1.3. Sensitivity to canopy resistance

Figs. 4 and S4 take two choices of canopy resistance (\( r_c = 263 \) and 460 s m\(^{-1} \)) with reference parameters to show the modeled equilibrium solutions of fluxes and variables. In the base model, when \( r_c \) increases from 263 to 460 s m\(^{-1} \), \( H_2O \) increases and LE decreases, and the ML pressure height \( P_{LCL} \) increases from 150 to 200 hPa corresponding to the enhanced \( H_2O \) (Fig. S4). The radiative cooling term \( F_{rad} \) increases with \( P_{LCL} \) at a given radiative cooling rate \( \partial T_a/\partial t \). The thermal entrainment at the cloud base \( H_2O \) increases to maintain the thermal equilibrium. The surface temperature \( T_a \), potential temperature \( \theta_m \), and \( \theta_{ld} \) also increase to the new equilibrium. As ET decreases, both the entrainment terms \( E_0 \) and \( E_1 \) decrease, and the specific humidities \( q_m \) and \( q_{ld} \) also decrease. Because the precipitation rate \( P \) and the rain evaporation fraction \( f \) are
isotope compositions at the tall tower in Rosemount, MN from June to August prescribed, the condensation–Fig. 3.

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4.2. Sensitivity analyses of the water isotope module

4.2.1. Sensitivity to precipitation rate

Sensitivity tests show that when precipitation rate (P) increases by about 80% (from 3.3 to 6 mm day⁻¹), both hydrogen and oxygen isotope compositions of P and EP get enriched by less than 1.5%, indicating that these isotope compositions are insensitive to P (Tables 2b and 3b). Taking the assumption that the isotope composition of raindrops is in equilibrium with the surrounding air in the CBL (Eqs. (25) and (26), the isotope molar ratios of precipitation (RP) and rain evaporation (RP) are calculated as:

\[
R_P = \frac{P - \frac{M_o}{M_i}}{1 - \frac{1}{\alpha(T_{CL})} \left[ LRR \frac{E_i}{E_0} (1 - LRR) \frac{q_i}{q_i} \frac{M_o}{M_i} \right]}
\]

\[
R_{EP} = \frac{E_P - \frac{M_o}{M_i}}{1 - \frac{1}{\alpha(T_{CL})} \left[ LRR \frac{E_i}{E_0} (1 - LRR) \frac{q_i}{q_i} \frac{M_o}{M_i} \right]}
\]

These two equations show that P does not explicitly affect the isotope composition of either rainwater or rain evaporated vapor. Instead, P indirectly affects RP and REP through the thermal and moisture variables, such as TML and TCL, by changing EP and Fep in the base model.

4.2.2. Sensitivity to rain evaporation fraction

Tables 2c and 3c show that when rain evaporation fraction (f) increases, the isotope composition of all moisture fluxes decreases, except for the surface ET. The isotope mass fluxes of ET are weakened in order to balance the increased mass fluxes of rain evaporation to reach the new ML equilibrium. The precipitation is more enriched in heavy isotopes responding to the stronger EP, but the isotope ratios of EP do not change significantly. Eqs. (29) and (30) show that REP is explicitly determined by f while RPE is not. RP increases as f increases because light isotopes are more preferentially evaporated and leave the remaining water more enriched in heavy isotopes. REP represents the isotope mixing between the moisture of surface ET and the free atmosphere, and it is indirectly affected by f through the changes of thermal and moisture equilibrium in the base model.

Fig. 5a-c show that when f increases, the equilibrium isotope composition of water vapor in the ML decreases and the corresponding deuterium excess values increase. When f varies from 0 to 0.4, the ranges of modeled δD and δ18O are ~140.0 to ~130.1‰ and ~25.1 to ~17.5‰, respectively. This explains 7% and 29% of the ranges of observed daily averaged δD ~193.7 to ~51.2‰ and δ18O ~35.7 to ~9.6‰, respectively. The larger variation of modeled δ18O indicates that the equilibrium δ18O is more sensitive to f than δD. In contrast, when f increases, the rainwater gets more enriched in heavy isotopes and the corresponding deuterium excess values decrease (Fig. 5d-f). The observed deuterium excess of precipitation, dp, is well bounded by curves modeled with f varying between 0 and 0.3. This indicates that the range of f can be constrained by dp, and the upper bound for f in the Upper Midwest US is 0.3, which is smaller than the upper bound of 0.5 determined for tropical ecosystems (Worden et al., 2007). This implies that the lower air temperature and weaker convection in mid-latitude regions cause weaker rain evaporation compared to the tropical region. Here we attempt to quantify f with P and rainwater isotope compositions (δD and δ18O) by relating them to the “amount effect”, which is an empirical finding that the monthly mean isotope ratio of rainwater is anti-correlated to the precipitation amount in tropical regions (Dansgaard, 1964; Tharammal et al., 2017). Although the amount effect is most obvious in the tropics, it is also observed in the Midwestern US in summer seasons (Bedaso and Wu, 2020; Simpkins, 1995). There are multiple mechanisms that cause the amount effect, such as the

or variables with r_c given as 263 s m⁻¹ (i.e. P_c is 150 hPa in the reference case). Case (a) is the reference case, and Cases (b) to (f) are scenarios with varied P, f, LRR, free-atmosphere isotope compositions (δD and δ18O), and surface isotope compositions (δD and δ18O), respectively.

4.2. Sensitivity analyses of the water isotope module

In this section, the analyses focus on the sensitivities of the water isotope composition of ML water vapor (δD) and precipitation (δD) and δ18O) to precipitation parameters and boundary variables in the water isotope module. Tables 2 and 3 show the case studies examining the sensitivities of isotope fluxes and compositions to these parameters.
downdraft mixing of deep convection into the ML (Risi et al., 2008), mesoscale convective systems in stratiform rainfall (Kurita, 2013), and moisture convergence (Moore et al., 2014). Here we consider a classic explanation of the amount effect related to the rain evaporation. As the precipitation gets more intense, the raindrops are less equilibrated with the surrounding vapor because of higher ambient relative humidity, larger drops, and shorter residence time of raindrop formation, which causes a smaller fraction of rain evaporation and isotopic depletion of raindrops (Dansgaard, 1964; Lee and Fung, 2008; Risi et al., 2008). The typical ranges of amount effect in the tropical regions for $\partial \delta D / \partial P$ and $\partial \delta^{18}O / \partial P$ are $1$ to $8$ ‰ (mm day$^{-1}$) and $0.5$ to $3$ ‰ (mm day$^{-1}$), respectively (Eastoe and Dettman, 2016; Kurita, 2013; Risi et al., 2008; Tharammal et al., 2017). When $P$ increases as shown in Tables 2b and 3b, the modeled $\partial \delta D / \partial P$ and $\partial \delta^{18}O / \partial P$ are $0.04$ and $0.07$ ‰ (mm day$^{-1}$)$^{-1}$, respectively. Therefore, the model cannot simulate the amount effect when $f$ is independent of $P$. To produce the amount effect, we made an arbitrary assumption that $f$ is inversely proportional to $P$, i.e. $f = c_f / P$, where $c_f$ is a prescribed parameter. A larger $c_f$ indicates a stronger intensity of rain evaporation.

Fig. 5g–i show the sensitivity diagrams of rain evaporation fraction with $c_f$ varying from $0$ to $0.4$ mm day$^{-1}$, on planes with the axes of isotope compositions of rainwater and summer mean precipitation rate. Using the observed summer mean precipitation rate at US-Ro1 and the amount-weighted isotope compositions of rainwater in 2006–2010, the diagrams with isotope ratios of rainwater ($\delta D$ and $\delta^{18}O$) and deuterium excess value ($dP$) consistently estimate that $0.3$ mm day$^{-1}$ is a reasonable value for $c_f$ at US-Ro1. The corresponding $f$ is estimated to be $0.09$ with $c_f = 0.3$ mm day$^{-1}$. The magnitude of the amount effect can be

![Diagram](image_url)
Sensitivity results of mass fluxes and isotope ratios of the hydrogen isotope composition (HDO) corresponding to the model parameters.

Table 2

<table>
<thead>
<tr>
<th>Case</th>
<th>$r_c$ (s m$^{-1}$)</th>
<th>$P$ (mm day$^{-1}$)</th>
<th>$f$ (l)</th>
<th>LRR</th>
<th>$\delta D$</th>
<th>$\delta O$</th>
<th>$P_{CL}$ (hPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>263</td>
<td>3.3</td>
<td>0.1</td>
<td>0.3</td>
<td>$-160.0$</td>
<td>$-50.0$</td>
<td>150</td>
</tr>
<tr>
<td>b</td>
<td>263</td>
<td>6.0</td>
<td>0.1</td>
<td>0.3</td>
<td>$-160.0$</td>
<td>$-50.0$</td>
<td>141</td>
</tr>
<tr>
<td>c</td>
<td>263</td>
<td>3.3</td>
<td>0.2</td>
<td>0.3</td>
<td>$-160.0$</td>
<td>$-50.0$</td>
<td>136</td>
</tr>
<tr>
<td>d</td>
<td>263</td>
<td>3.3</td>
<td>0.1</td>
<td>0.5</td>
<td>$-160.0$</td>
<td>$-50.0$</td>
<td>150</td>
</tr>
<tr>
<td>e</td>
<td>263</td>
<td>3.3</td>
<td>0.1</td>
<td>0.3</td>
<td>$-200.0$</td>
<td>$-50.0$</td>
<td>150</td>
</tr>
<tr>
<td>f</td>
<td>263</td>
<td>3.3</td>
<td>0.1</td>
<td>0.3</td>
<td>$-160.0$</td>
<td>$-40.0$</td>
<td>150</td>
</tr>
</tbody>
</table>

The local recycling ratio (LRR) primarily affects the isotope mass fluxes and isotope compositions of $E_P$, $P$, and $R_P$, while the isotope composition of ML water vapor is insensitive to LRR Tables 2 and 3d). Fig. 6 shows that the shapes of the sensitivity curves are bounded by the curves with $LRR = 0$ and $LRR = 1$. Eqs. (29) and (30) indicate that LRR represents the two-source mixing ratio for $R_P$ and $R_{EP}$ between the moisture from surface ET and the advected moisture above the PBL. When LRR = 0, $R_P$ and $R_{EP}$ are purely determined by the moisture condition above the PBL (i.e. $\delta D$ and $\delta ^{18}O$); when LRR = 1, $R_P$ and $R_{EP}$ are solely determined by the surface condition (i.e. $\delta D$ and $\delta ^{18}O$) affecting the ET. Therefore, the change of boundary conditions above the PBL and at the surface may affect the sensitivities of $\delta D$ and $\delta ^{18}O$ to LRR. The sensitivity tests on the boundary isotope compositions indicate that these boundary variables are well constrained (see Sections 4.2.4 and 4.2.5).

Comparing with the observation of summer mean ET at US-Ro1 and the amount-weighted isotope compositions of precipitation from 2006 to 2010, the diagrams of $\delta D$–ET and $\delta ^{18}O$–ET estimate LRR as 0.28 and 0.33, respectively. To assess the uncertainty range of LRR due to the observation uncertainties in rainwater isotope composition, a Monte Carlo method was used to randomly resample 30 of the 85 rainfall events for summer recycling ratio can be up to 0.40.

It is well known that LRR depends on the shape and area of the study region. The LRR value increases as a function of spatial scale (Brubaker et al., 2010). The spatial scale of the equilibrium model is on the order of 150–450 km, assuming a daily average wind speed of 2–5 m/s in the lower atmosphere as suggested by B04. The monthly mean ET estimate LRR as 0.28 and 0.33, respectively. To assess the uncertainty range of LRR due to the observation uncertainties in rainwater isotope composition, a Monte Carlo method was used to randomly resample 30 of the 85 rainfall events for summer recycling ratio can be up to 0.40.
over 0.3 might be associated with the PBL advection and reflect the moisture originated from outside of the study domain.

Since the PBL advection is ignored in the model setup, here we try to explore the source of advected moisture by estimating the deuterium excess values of the PBL advection \( \delta_{dab} \). Deuterium excess values associated with precipitation, ET and advection have been used to quantify LRR in previous studies (e.g. Kong et al., 2013; Peng et al., 2005). The value of \( \delta_{dab} \) was calculated using a transformation of their equation:

\[
\delta_{dab} = \frac{d_p - LRR \cdot d_{ET}}{1 - LRR},
\]

where \( d_p \) and \( d_{ET} \) are the deuterium excess values of precipitation and ET, respectively. Using the observed \( d_p \), the modeled \( d_{ET} \), and the mean LRR estimated by the sensitivity diagrams, the summer \( \delta_{dab} \) values from 2006 to 2010 are estimated to be 16.9‰, 2.4‰, 3.9‰, 0.53‰, and 7.1‰, respectively.

According to Eq. (31), \( \delta_{dab} \) is identical to \( d_p \) when there is no water recycling (LRR = 0). Further, the Rayleigh distillation and rainout history will not affect the water vapor deuterium excess, which suggests that \( \delta_{dab} \) will be a passive tracer carrying the oceanic signal without local water recycling (Wei and Lee, 2019). The typical summer deuterium excess value of water vapor from the ocean varies between 0 and 20‰ due to different environmental relative humidity, sea surface temperature, and wind speed of the evaporation source (Benetti et al., 2014; Bonne et al., 2019; Steen-Larsen et al., 2015, 2014; Uemura et al., 2008).

The average mid-afternoon deuterium excess of transpiration from cropland was close to the xylem water value of −3.5‰ (Welp et al., 2012), and thus the continental source of water vapor tends to decrease the value of \( \delta_{dab} \). Therefore, the small values of \( \delta_{dab} \) in 2007, 2008 and 2009 suggest that the dominant source of the advection was continental, while the source of the advection in 2006 and 2010 was mainly oceanic.

Eq. (31) also shows that the values of \( \delta_{dab} \) and LRR are anti-correlated. A continental advection with a small value of \( \delta_{dab} \) suggests a strong effect of local water recycling. Therefore, without the effect of advection, the model assumes that the deuterium excess of upstream advection is identical to the local situation. The LRR value may be overestimated without the information of oceanic advection. However, further research is required to verify these potential influences caused by advection.

4.4.2. Sensitivity to isotope composition above the PBL

Tables 2e and 3e show that when isotope compositions of water vapor above the PBL (\( \delta^{18}O \) and \( \delta^{13}C_{\text{iso}} \)) decrease, \( E_{ELr} \) and \( E_{EP} \) become relatively depleted in the heavy isotopes. Further, the isotope mass fluxes of \( \delta_p \) and \( \delta_{ET} \) increase and the corresponding isotope composition becomes enriched to compensate for the larger vertical isotope gradient induced by the depletion at the PBL top. When \( \delta^{18}O \) decreases by 25% (from −160 to −200‰), the modeled \( \delta_{dab} \) and \( \delta_{dab} \) decrease by 7.5% and 12%, respectively (Table 2e). When \( \delta^{18}O \) decreases by 30% (from −231 to −30%), the modeled \( \delta^{18}O \) and \( \delta^{18}O \) decrease by 8.6% and 14%, respectively (Table 3e). The larger sensitivity of the CBL isotope composition compared to the ML isotope composition illustrates that the depleted isotope signal is transported downward from the free atmosphere to the surface layer.

Fig. 7a and b show that when \( P_{LCL} \) is fixed, the modeled \( \delta_{dab} \) and \( \delta_{dab} \) decrease as \( \delta_{dab} \) declines. As \( P_{LCL} \) increases, their sensitivities to \( \delta_{dab} \) both increase. When \( P_{LCL} \) increases from 70 to 275 hPa, \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) increases from 0.130 to 0.441, and \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) increases from 0.69 to 0.75. Fig. 7c and d show that when \( P_{LCL} \) increases from 70 to 275 hPa, \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) increases from 0.130 to 0.442, and \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) increases from 0.62 to 0.68. The similar sensitivity of the oxygen and deuterium isotope composition indicates that the isotope depletion signal is transported by entrainment (Lee et al., 2012), which mixes different isotopologues at the same rate. The large sensitivities of \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) and \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) imply that the observed \( \delta_{dab} \) and \( \delta_{dab} \) can effectively constrain \( \delta_{dab} \) and \( \delta_{dab} \), respectively. The linear regressions of the observed \( \delta_{dab} \) and \( \delta_{dab} \) against \( P_{LCL} \) suggest that the reference values of \( \delta_{dab} = -160.0‰ \) and \( \delta^{18}O = -23.1‰ \) are reasonable estimates for the upper boundary condition (Fig. 7b and d).

The sensitivity to the isotope composition of water vapor above the PBL may reveal the relative ratio of the continental effect between precipitation and the advected vapor above the PBL. The “continental effect” shows that the isotope ratios of precipitation and ambient vapor are gradually depleted from coastal to inland regions (Dansgaard, 1964; Winnick et al., 2014). The summer average gradient of the continental effect of rainwater \( \delta^{18}O_{\text{iso}} / \delta^{18}O_{\text{iso}} \) in the US is −4.8‰ (1000 km)⁻¹ (Liu et al., 2010; Welker, 2012; Winnick et al., 2014), and \( \delta^{18}O_{\text{iso}} / \delta^{18}O_{\text{iso}} \) is assumed to be −24‰ (1000 km)⁻¹ determined by the slope of the GMWL. The sensitivity test conducted here indicates that \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) is about 0.7, and thus the continental effect of the hydrogen isotope composition of the free atmosphere \( \delta^{18}O_{dab} / \delta^{18}O_{\text{iso}} \) is estimated to be −34‰ (1000 km)⁻¹, which is a relatively good approximation of the gradient of the lower-atmosphere isotope composition from the US East Coast to the Upper Midwest region (Frankenberg et al., 2009; Sutanto et al., 2015). Since the continental effect is a composite phenomenon, caused by condensation from different oceanic sources and local water recycling of vapor from terrestrial ET (Welker, 2000; Winnick et al., 2014), further investigations are needed to partition the specific processes contributing to the relative ratio.

4.4.2.5. Sensitivity to isotope composition at the surface

When the isotope composition of soil water (\( \delta_{dab} \) and \( \delta^{18}O \)) becomes relatively enriched in the heavy isotopes, the isotope mass fluxes and
Fig. 5. Model solutions of sensitivity tests on rain evaporation fraction ($f$) compared with observations. Graphs in the first row are model outputs of water vapor isotope ratios in the ML compared with observations from the tall tower, Rosemount, MN in 2010–2012: (a) $\delta D_m$, (b) $\delta^{18}O_m$, and (c) deuterium excess $d_m = \delta D_m - \delta^{18}O_m$. Graphs in the second row are model outputs of rainwater isotope ratios compared with summer rainwater samples collected on the Saint Paul Campus, University of Minnesota in 2006–2010: (d) $\delta D_P$, (e) $\delta^{18}O_P$, and (f) $d_P = \delta D_P - \delta^{18}O_P$. Diagrams in the third row are the modeled isotope compositions of precipitation against varying seasonal precipitation rate ($P$) with the assumptions of $f$ inversely proportional to $P$: (g) $\delta D_P$, (h) $\delta^{18}O_P$, and (i) $d_P = \delta D_P - \delta^{18}O_P$. The red asterisks in (g), (h) and (i) indicate the summer mean precipitation rate at US-Ro1 and amount-weighted isotope compositions of rainwater in 2006–2010.

Fig. 6. Model solutions of sensitivity tests on local recycling ratio (LRR) compared with observations. Graphs in the first row are model outputs of rainwater isotope ratios compared with summer rainwater samples collected on the Saint Paul Campus, University of Minnesota in 2006–2010: (a) deuterium isotope ratio of precipitation ($\delta D_P$); and (b) oxygen isotope ratio of precipitation ($\delta^{18}O_P$). The second row are the sensitivity diagrams of LRR with modeled isotope compositions of precipitation against varying surface ET: (c) $\delta D_P$ and (d) $\delta^{18}O_P$. In (c) and (d), the red asterisks indicate the summer mean ET at US-Ro1 and amount-weighted isotope compositions of rainwater in 2006–2010; the red triangles indicate the annual average of observations; and the colored circles indicate the resampled data generated in the Monte Carlo tests.
isotope ratios of $E_0$, $E_b$, $E_t$ and $P$ increase (Tables 2f and 3f). When $\delta D_0$ increases by 20% (from $-50$ to $-40\%$), $\delta D_m$ and $\delta D_{lid}$ increase by 5.3% and 3.8%, respectively (Table 2f). When $\delta^{18}O_t$ increases by 50% (from $-5$ to $-2.5\%$), $\delta^{18}O_m$ and $\delta^{18}O_{lid}$ increase by 9.1% and 7.3%, respectively (Table 3f). The larger percentage increase in the isotope composition of the ML compared to the CBL confirms that the enriched surface isotope signal is transported upward.

The isotope composition of the ML and the precipitation both decrease when the surface becomes relatively depleted at a given ML height (Fig. 8). As the ML grows higher, the sensitivities of these isotope signals to the surface isotope composition decrease. When $P_{LCL}$ increases from 70 to 275 hPa, $\partial \delta D_m / \partial \delta D_0$ and $\partial \delta^{18}O_m / \partial \delta^{18}O_0$ decreases from 0.80 to 0.52 and from 0.86 to 0.55, respectively (Fig. 8a and b). $\partial \delta D_m / \partial \delta D_0$ and $\partial \delta^{18}O_m / \partial \delta^{18}O_0$ increases slightly from 0.40 to 0.35 and from 0.39 to 0.33, respectively (Fig. 8c and d). The larger sensitivity of the ML isotope composition indicates that the surface isotope composition plays a major role in constraining the isotope equilibrium in the ML.

### 4.3. ET and local water recycling under different land surface scenarios

In this section, four types of land-cover surfaces, broadleaf forest (BLF), needleleaf forest (NLF), grassland (GRA) and cropland (CRO), were modeled and compared. The typical ranges of canopy resistance ($r_c$), transpiration fraction ($T/ET$), and leaf area index (LAI) of the four different ecosystems are presented in Fig. 9. The ranges of $r_c$ were determined from a global estimate of canopy conductance ($g_c$, the reciprocal of $r_c$) derived from the MODIS remote sensing product (Yebra et al., 2013). The interval between median and 95% percentile of the Q75 value of the annual spatial mean was taken for the summer estimate in our study (Fig. 9a). The value of $T/ET$ was modeled and computed by the isotope method for ET partitioning (Wang et al., 2010), and LAI was estimated from a global regression between $T/ET$ and LAI (Wei et al., 2017) (see supplemental material Section S3.1).

The grassland has the highest range of $r_c$ between 231 and 377 s m$^{-1}$, while the other three types largely overlap in the NLF range of 120–156 s m$^{-1}$, with BLF varying between 82 and 144 s m$^{-1}$, and CRO varying...
from 112 to 204 s m\(^{-1}\) (Fig. 9b). Fig. 9c indicates that the ranking of the upper bound of modeled ET is BLF, CRO, NLF and GRA, which is consistent with the ranking of summer ET across AmeriFlux sites (Xia et al., 2015). Fig. 9d shows that the T/ET of the four land cover types ranges from 0.68 to 0.75, which are within the ranges of \(\delta^{18}O\) measurements in temperate ecosystems (Schlesinger and Jasechko, 2014). The idealized LAIs estimated from the T/ET relation for BLF, NLF, CRO and GRA are 2.3–2.8, 3.5–3.7, 1.5–1.8 and 1.0–1.1, respectively (Fig. 9e), which are smaller than the typical values of the corresponding ecosystems. The exponential regression of LAI is sensitive to T/ET (Eq. (Fig. 9 e)), which are smaller than the typical values of the corresponding ecosystems. The exponential regression of LAI is sensitive to T/ET (Eq. (Fig. 9 e)). The value of \(\delta^{18}O\) of cropland ET (~ \(-15\%\)) is more depleted than \(\delta^{18}O\) of grassland and comparable to forests. The other possible reason for the discrepancy might be the scale difference between the model and the stand-level measurements. Within the tall tower footprint of our study region (with a radius of about 100 km), the land cover percentages of cropland, grassland/pasture, broadleaf forest, and needleleaf forest are 48%, 11%, 12% and <1%, respectively (estimated from Cropland Data Layer, https://nassgeodata.gmu.edu/). The land use is remarkably similar as the radius increases to 400 km away from the tall tower, with land cover percentages of 44%, 11%, 15% and <1%, respectively, for the four land cover types. Therefore, the modeled \(\delta^{18}O\) might correspond to the climate average over a larger region with mixed land covers instead of homogeneous cropland.

The value of \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) quantifies the intensity of local water recycling affecting the oxygen isotope composition of rainwater at a fixed LAI or \(r_c\). Fig. 9f shows that the median value of the cropland \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) is 1.19 times the grassland value and is 0.97 and 0.93 times the needle and broadleaf forest values, respectively. Therefore, the intensity of cropland is larger than grassland and comparable to forests. The change of \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) indicates the sensitivity of \(\delta^{18}O_{\text{P}}\) affected by LAI through the local water recycling. The \(\delta^{18}O_{\text{P}}\)–ET diagram shows that \(\delta^{18}O_{\text{P}}\) increases as ET increases at a given LRR (Fig. 6d). The increase of ET is caused by the increase of LAI (or decrease of \(r_c\)), which induces larger T/ET and more enrichment in oxygen isotope composition of ET (\(\delta^{18}O_{\text{P}}\) (Fig. 10d)). As a result, the rainwater becomes more enriched in \(^{18}O\) by the local water recycling with a larger LAI (and a smaller \(r_c\)). Therefore, when LAI increases (and \(r_c\) decreases), \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) becomes larger, indicating a stronger local water recycling effect on \(\delta^{18}O_{\text{P}}\).

The land cover change to cropland could induce changes in local water recycling. Within the study region, grassland and broadleaf forest are two major natural vegetation types. If grassland is converted to cropland, the increase in LAI will cause a decline in the regional canopy resistance. Therefore, the total ET is expected to increase and the PBL height will decrease. The local water recycling will be intensified and cause an increase in \(\delta^{18}O\). In contrast, the local water recycling will be weakened if broadleaf forest is converted to cropland. Assuming all cropland was originally grassland in the pre-agriculture era, the model estimates that the median LRR would have increased 19.5% in the growing season (Xia et al., 2018). The larger estimates in measurements might overestimate the daily average value because the isotope ET partitioning is usually applied with high transpiration in midday hours and soil evaporation is not accounted for when transpiration is weak (Wei et al., 2017). The other possible reason for the discrepancy might be the scale difference between the model and the stand-level measurements. Within the tall tower footprint of our study region (with a radius of about 100 km), the land cover percentages of cropland, grassland/pasture, broadleaf forest, and needleleaf forest are 48%, 11%, 12% and <1%, respectively (estimated from Cropland Data Layer, https://nassgeodata.gmu.edu/). The land use is remarkably similar as the radius increases to 400 km away from the tall tower, with land cover percentages of 44%, 11%, 15% and <1%, respectively, for the four land cover types. Therefore, the modeled \(\delta^{18}O_{\text{P}}\) might correspond to the climate average over a larger region with mixed land covers instead of homogeneous cropland.

The value of \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) quantifies the intensity of local water recycling affecting the oxygen isotope composition of rainwater at a fixed LAI or \(r_c\). Fig. 9f shows that the median value of the cropland \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) is 1.19 times the grassland value and is 0.97 and 0.93 times the needle and broadleaf forest values, respectively. Therefore, the intensity of cropland is larger than grassland and comparable to forests. The change of \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) indicates the sensitivity of \(\delta^{18}O_{\text{P}}\) affected by LAI through the local water recycling. The \(\delta^{18}O_{\text{P}}\)–ET diagram shows that \(\delta^{18}O_{\text{P}}\) increases as ET increases at a given LRR (Fig. 6d). The increase of ET is caused by the increase of LAI (or decrease of \(r_c\)), which induces larger T/ET and more enrichment in oxygen isotope composition of ET (\(\delta^{18}O_{\text{P}}\) (Fig. 10d)). As a result, the rainwater becomes more enriched in \(^{18}O\) by the local water recycling with a larger LAI (and a smaller \(r_c\)). Therefore, when LAI increases (and \(r_c\) decreases), \(\partial\delta^{18}O_{\text{P}}/\partial\text{LRR}\) becomes larger, indicating a stronger local water recycling effect on \(\delta^{18}O_{\text{P}}\).

The land cover change to cropland could induce changes in local water recycling. Within the study region, grassland and broadleaf forest are two major natural vegetation types. If grassland is converted to cropland, the increase in LAI will cause a decline in the regional canopy resistance. Therefore, the total ET is expected to increase and the PBL height will decrease. The local water recycling will be intensified and cause an increase in \(\delta^{18}O\). In contrast, the local water recycling will be weakened if broadleaf forest is converted to cropland. Assuming all cropland was originally grassland in the pre-agriculture era, the model estimates that the median LRR would have increased 19.5% in the modern time; and the median LRR would have decreased 7.6% compared with a pure broadleaf forest scenario.

The water management of croplands could also influence the local water recycling. Under drought conditions, the overall canopy resistance of the vegetative surface is expected to increase due to the increased water stress, and therefore it will decrease both ET and local recycling intensity. Broad-scale irrigation can counter these effects and increase local water recycling. Further, Alter et al. (2018) have
suggested that the increase of moist static energy near the surface and local water recycling are two major mechanisms through which the large-scale irrigation can contribute to enhanced rainfall recently observed in the central US. Here, the feedback process demonstrated by our equilibrium model further confirm that irrigation can enhance the local water recycling. Since the precipitation in the Upper Midwest US is predicted to be more variable under global warming scenarios (Zhang et al., 2021), irrigation use is expected to increase to offset variability in precipitation and to avoid more frequent drought events. Currently, about 3% of croplands are irrigated in the Upper Midwest US, and the annual total irrigation withdrawals about 1.48 billion tons of water in 2015 (Dieter et al., 2018). With the large coverage of cropland area and low percentage of irrigated ratio in the region, irrigation is expected to increase in the future and will likely enhance local water recycling.

4.4. Implications

The regional climate parameters (i.e. the rain evaporation fraction and local water recycling ratio) were quantified from flux and isotope observations using the model-generated sensitivity diagrams. According to the cooling effect and the influence on the isotope composition, the model results suggest that the rain evaporation is a key process in the ML equilibrium during the summer in the humid continental climate. The model results for different vegetation scenarios implies that cropland in the Upper Midwest US has changed the intensity of local water recycling compared with the pre-agriculture era. The feedback processes in the model also reveal that the local water recycling is expected to be enhanced if irrigation is more frequently applied when considering future global warming scenarios. In future studies, the model can be coupled with other analytical land surface models to design more sophisticated water and agricultural management scenarios.

Global observations of stable water isotopes have identified multiple significant isotope effects in the global distribution, including the “amount effect”, “continental effect”, “temperature effect”, and “latitude effect” (Dansgaard, 1964; Sutanto et al., 2015; Worden et al., 2007). Our model shows the potential capacity to simulate these isotope effects over monthly or longer timescales. For instance, by relating the rain evaporation fraction to the precipitation amount, the model can quantify the magnitude of the amount effect with the constraint of observed isotope composition of rainwater. The magnitude of the continental effect can be estimated by the model sensitivity between the isotope composition of rainwater and free-atmosphere water vapor. These results imply that the local water recycling is a key process influencing the continental effect.

Further research is needed to test the model performance across a broader range of ecosystems and environments. For example, the model

![Fig. 10. Model outputs of different variables against leaf area index (LAI) under land cover scenarios of broadleaf forest (BLF), needleleaf forest (NLF), grassland (GRA) and cropland (CRO): (a) canopy resistance; (b) modeled pressure height of ML; (c) modeled transpiration fraction; and (d) the left y-axis and solid lines indicate the oxygen composition of ET represented by the modeled $E_0$, and the right y-axis and dotted lines indicate the oxygen composition of soil evaporation calculated by the Craig–Gordon (CG) model.](image-url)
could be evaluated at other locations by utilizing the global isotope databases for precipitation and water vapor, such as the Global Network of Isotopes in Precipitation (GNIP) dataset and the Stable Water Vapor Isotope Database (SWVID) (Wei et al., 2019). In addition to the variables tested here (i.e. the isotope ratios of rainwater and the ML water vapor), the isotope fluxes of ET, entrainment and condensation are potential quantities to further constrain the equilibrium model. B00 suggested that the equilibrium model is a plausible zero-order fit to the reanalysis data of a climate model. This implies that our model can be used to identify the patterns of isotope effects or the changes of water isotope equilibrium over the longer timescales. Such analytical analyses are simple but provide an important check on the more sophisticated isotope-enabled land-atmosphere models, which require more forcing data, more complex parameterization, and intensive computational resources.

5. Conclusion

(1) We developed an idealized water isotope model with precipitation processes and coupled it to a two-layer equilibrium boundary layer model. The model performed well in describing the summer PBL equilibrium of the hydrogen and oxygen isotope composition (HDO and H$_2$O) of water vapor and precipitation in the Upper Midwest, United States. The equilibrium values of these isotope isotopologues were well-constrained by the thermal and moisture equilibrium in the PBL.

(2) Two graphical methods were developed within the model framework to constrain the summer rain evaporation fraction and the local recycling ratio, respectively. For the Upper Midwest, United States region, we estimated the rain evaporation fraction to be 0.09 and local water recycling ratio to be 0.29 ± 0.12. The local water recycling ratios for the years 2006–2010 were 0.35, 0.36, 0.17, 0.29, and 0.29, respectively. The small recycling ratio in 2008 corresponded to a drought condition with the lowest precipitation and second lowest ET among the five years.

(3) Model sensitivity tests were used to quantify the isotope effects related to the amount effect and the continental effect. The summer magnitude of the amount effect for the study region is estimated as $–2.8\%$ (mm day$^{-1}$)$^{-1}$ and $–0.8\%$ (mm day$^{-1}$)$^{-1}$ for HDO and H$_2$O, respectively. The local water recycling is identified as a significant factor influencing the continental effect.

(4) The analyses of four land cover types (broadleaf forest, needleleaf forest, grassland, and cropland) and the feedback processes revealed by our model indicate that the local water recycling will decrease if broadleaf forest is converted to cropland, and it will increase if grassland is converted to cropland. The anthropogenic land use change in the Upper Midwest, United States has likely changed the local water recycling ratio by $–7.6$ to $19.5\%$ under different land use change scenarios. The local water recycling is expected to be weakened under drought conditions, but it will be enhanced if irrigation is applied more intensely with more frequent drought events under global warming scenarios.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

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Supplementary materials


References


