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### Numerical modeling the isotopic composition of evapotranspiration in an arid artificial oasis cropland ecosystem with high-frequency water vapor isotope measurement

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#### ABSTRACT

Stable isotopes of evapotranspiration ( $\delta_{ET}$ ) provide us with useful information for tracing ecosystem processes in the study of biosphere-atmosphere interactions and hydrologic cycling. In this study, a numerical Iso-SPAC model with high frequency isotopic water vapor isotopic measurements was applied in an arid artificial oasis cropland ecosystem. The steady state assumption (SSA) and non-steady state (NSS) sub-models were tested for the isotopic composition of leaf water and transpiration flux. The modeled water/energy fluxes agreed well with eddy covariance observations, indicating that our model has the capacity to reproduce the observed water/energy flux behavior. Comparisons of modeled and estimated  $\delta_{ET}$  by the flux-gradient method using a cavity ring-down spectroscopy water vapor isotope analyzer as well as measured  $\delta_{Lb}$  indicate that  $\delta_T$  with SSA can reproduce better seasonal isotopic variations in ET flux and leaf water during the growing season. Uncertainties/errors for model output ( $\delta_{ET}$ ,  $\delta_E$ ,  $\delta_T$  and  $\delta_{L,b}$ ) under both SSA and NSS were discussed quantitatively. With corn growth, the isoflux of transpiration acted to increase  $\delta_{ET}$  and decrease enrichment in  $\delta_{L,b}$ , inversely, the  $\delta_{ET}$  decreased and isotope enrichment in  $\delta_{L,b}$  increased because of reduction of transpiration caused by frost occurred during 13th and 14th September. The results indicate that the Iso-SPAC model is a useful framework for simulating the dynamics of isotopic composition in the isotopic composition of plant transpiration and soil evaporation separately as well as for simultaneously integrating them for isotopic composition in the ET flux.

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### 1. Introduction

The use of stable water isotopologues (principally  $H_2^{18}O$  and  $H^1DO$ ) as tracers is a new and important technique enabling flux tracing within the soil-plant-atmosphere continuum (SPAC) system (Kendall and McDonnell, 1998; Mook and De Vries, 2000; Sutanto et al., 2014). The stable oxygen isotope ratio of evapotranspiration ( $\delta_{ET}$ ) is the most sensitive isotopic end member of *ET* partitioning and it has been widely applied by many studies on diverse regions worldwide (Moreira et al., 1997; Yakir and Sternberg, 2000; Williams et al., 2004; Yepez et al., 2003, 2005;

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http://dx.doi.org/10.1016/j.agrformet.2015.12.063 0168-1923/© 2015 Elsevier B.V. All rights reserved. Wang et al., 2010; Good et al., 2014; Dubbert et al., 2013, 2014; Wei et al., 2015). That research is one of the most significant ecohydrological challenges and has important implications not only for water budget but also for understanding feedback between vegetation dynamics and water as well as biogeochemical cycles (Jasechko et al., 2013; Newman et al., 2006; Wang et al., 2014).

The isotopic composition of evapotranspiration ( $\delta_{ET}$ ) as a key environmental tracer currently is estimated by a variety of methods, including: Keeling mixing models, the flux-gradient technique, and eddy covariance Good et al. (2012). Traditional methods such as the Keeling plot method (Keeling, 1958; Yakir and Sternberg, 2000; Pataki et al., 2003; Zobitz et al., 2006; Wang et al., 2010; Good et al., 2014), the flux-gradient technique (Yakir and Wang, 1996; Wang and Yakir, 2000; Griffis et al., 2004, 2005; Welp et al., 2008; Huang and Wen, 2014), and the eddy correlation method (*EC*) (Saleska et al., 2006; Griffis et al., 2008, 2010; Sturm et al., 2012)

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are used to measure the value of  $\delta_{ET}$ . However, those approaches focus on the direct measurement of the isotopic composition of the ET flux, which sometimes makes it difficult to be widely applied because of its high cost, complex equipment placement and validation process. Numerical simulation is a good supplement because of its applicability over a wide range of time scales and because modeling can be applied to a spatial scale across an ecosystem (Sturm et al., 2000). Numerous land surface models with isotopic tracers have been developed (e.g. Braud et al., 2005; Riley et al., 2002; Yoshimura et al., 2006; Xiao et al., 2010; Sutanto et al., 2012). Henderson-Sellers et al. (2006) introduced IPILPS (Intercomparison of Land-surface Parameterization Schemes) to promote isotope-enabled LSMs (Land Surface Models) through intercomparsion. Models participating in iPILPS illustrated the importance of water isotopes in ET and its components fluxes (Henderson-Sellers et al., 2006; Riley et al., 2002; Yoshimura et al., 2006). However, as Griffis (2013) noted that simulating and integrating the dynamic variations in the isotopic composition of plant transpiration and soil evaporation remains a challenge. Aside from the aforementioned challenges, whether steady-state assumption (SSA) (the isotopic composition of transpiration flux  $(\delta_T)$  is assumed to be equal to that of xylem water  $(\delta_X)$  is reasonable or not for simulating the isotopic composition of leaf water/transpiration remains unclear under field conditions (Dongmann et al., 1974; Farquhar and Cernusak, 2005; Yepez et al., 2005; Lai et al., 2006; Welp et al., 2008; Dubbert et al., 2014). Furthermore, research in this area has traditionally been limited by a lack of continuous in-situ isotopic observations. The SPAC model is relatively simple but is still capable of considering separate controls on vegetation and soil on water/energy and the isotopic fractionation processes with H<sub>2</sub>O exchange in terrestrial ecosystems (Wang et al., 2015).

The Heihe River Basin is the second largest inland river basin in the arid region of northwestern China. In middle reaches, agricultural oasis is a typical landscape providing precious fertile soil, living space, food, and ecological services. Owing to shortage of water resources, mulching is a common and effective practice to reduce evaporation artificially. Many studies have attempted to evaluate the effect of gravel mulch on evaporation (e.g. Li et al., 2000, 2001; Yamanaka et al., 2004), however, little attention has been paid to the impacts on isotopic composition in evaporation/evapotranspiration as a result of mulching. In general, few Iso-SPAC models have been developed or sufficiently validated by high-frequency isotopic observation in arid cropland ecosystem. The isotopic variation of ET should be well understood based on field observations and modeled as an isoflux mixture of plant transpiration and soil evaporation. The objectives of the present study were as follows: (1) to test the model performance for a cropland ecosystem in an arid oasis, (2) to examine the validity of the methodology and mulch effects for the isotopic composition of ET flux, (3) to identify potential sources of error for modeling parameterizations and variables that exert a large degree control on the isotopic fluxes of ET.

### 2. Materials and methods

### 2.1. Study site

The study site (38°51′ N, 100°22′ E, 1550m) is located in an arid artificial oasis spring maize in the middle reaches of the Heihe River Watershed in Zhangye, Gansu Province which was part of the Heihe Watershed Allied Telemetry Experimental Research (HiWA-TER) program (Li et al., 2013; Cheng et al., 2014). Around the site, a field about 13 ha is used exclusively for planting maize. It provides a sufficient fetch of uniform land cover for the determination of fluxes and isotope measurement. The mean annual precipitation and air

temperature were approximately 128.7 mm and 7.4 °C, respectively, from 1961 to 2010. Mean annual pan evaporation were about 2002.5 mm, Plastic films were used for water conservation and keeping warm in seeding stage, covering approximately 60% of the soil surface. Irrigation was applied four times (DOY 158, 184, 210, and 238) during the growing season. Spring maize was planted in April 20 and harvested on September 22, 2012. The frost was happened at 13th and 14th, September during growing season which result in sharp decrease of leaf area index from 2.9 to 0.7 m<sup>-2</sup> m<sup>-2</sup>.

### 2.2. Numerical model description

The Iso-SPAC model of was adopted here to simulate the hourly heat and water fluxes and isotope output (canopy folia enrichment and isotopic composition of ET). The model framework is illustrated in Fig. 1 and details were described in Wang et al. (2015). In a short, the Iso-SPAC is composing of two parts. The first part is an energy balanced two source model (soil surface and canopy interface) for soil evaporation and plant transpiration, and second part is an isotopic budget at soil surface and canopy interface, which integrating the isotopic fractionation processes with soil evaporation and plant transpiration process. The model was selected for several reasons. First, this model treats water flux and the isotopic composition in *T* and *E* properly at both the vegetation canopy and at the ground surface with respect to interaction with the atmosphere in the terrestrial ecosystem. Moreover, the sensitivity analysis reveals that the model is relatively insensitive to uncertainties/errors in the assigned models parameters and in measured input variables for our partitioning of water flux (Wang and Yamanaka, 2014). Second, this model treats the radiation/energy balance properly in both vegetative canopy and at the ground surface with respect to interaction between them and it is solved by Newton-Raphson scheme, enabling us to estimate vegetation canopy  $(T_L)$  and ground temperature  $(T_G)$  separately, The scheme can easily integrate the isotopic fractionation processes with H<sub>2</sub>O exchange and it has the advantage of enabling long-term assessment of ET partitioning as well as isotopic enrichment output at the plant-atmosphere interface. Third, this model simulates the isotopic composition of leaf/transpiration considering SSA and NSS and it can be validated not only by physical components (e.g. ET, T, E, leaf temperature, and energy flux) but also by the isotopic component ( $\delta_{ET}$ ,  $\delta_T$ ,  $\delta_E$ ,  $\delta_{Lb}$ ), so it is expected to be more robust and reliable. The SSA (Craig and Gordon, 1965), NSS-D74 (Dongmann et al., 1974), and NSS-F05 (Farguhar and Cernusak, 2005) submodules were adopted here for the isotopic composition in leaf water and transpiration. The Iso-SPAC model was driven by input variables of (1) micrometeorological variables, including air temperature  $(T_a)$ , relative humidity of air  $(h_a)$ , downward short-wave radiation  $(S_d)$ , downward longwave radiation  $(L_d)$ , wind speed (u) and air pressure (P); (2) plant variables, including leaf area index (LAI), canopy height  $(Z_V)$  and leaf water content per unit ground area (W) (if we considering NSS, W is necessary input); (3) soil variables, including surface soil temperature at a depth  $Z_{soil}(m)(T_{soil})$  with hourly mean data set, volumetric soil moisture content; and (4) the isotope composition of atmospheric vapor, the average stem water, as well as soil water at depth of 5 cm. The input parameters in the Iso-SPAC including minimum stomata resistance, ( $r_{st\_min}$ ), maximum stomata resistance ( $r_{st\_max}$ ), albedo of fully vegetated interface ( $\alpha_V$ ), albedo of bare soil ( $\alpha_G$ ), clumping factors for canopy structure (CLAI), and height of placement of equipment  $(Z_h, Z_m)$  and thermal conductivity of surface soil ( $\lambda_{ss}$ ). To measure the model performance, we used root mean square error (RMSD), the I index (Willmott et al., 1985) and  $R^2$  (R is the correlation coefficient) to evaluate the model performance for water and energy fluxes and isotope ratios of ET flux and bulk leaf water. Our model simulation was restricted to a maize growing period (from 26-May to 24-September) in 2012.

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