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2 **against *in-situ* measurements**

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8 **Authors:** Mick Y. Cai<sup>1</sup>, Lixin Wang<sup>2\*</sup>, Stephen D. Parkes<sup>3</sup>, Josiah Strauss<sup>4</sup>, Matthew F.  
9 McCabe<sup>3</sup>, Jason P. Evans<sup>5</sup>, Alan D. Griffiths<sup>6</sup>

10

11 1. Water Research Center, School of Civil and Environmental Engineering, University of  
12 New South Wales, Sydney, NSW, 2052, Australia

13

14 2. Department of Earth Sciences, Indiana University-Purdue University Indianapolis (IUPUI),  
15 Indianapolis, IN, 46202, USA

16

17 3. Water Desalination and Reuse Center, King Abdullah University of Science and  
18 Technology, Thuwal, Saudi Arabia

19

20 4. Dolan Integration Group, Boulder, CO, 80301

21

22 5. Climate Change Research Centre, University of New South Wales, Sydney, NSW, 2052,  
23 Australia

24

25 6. Institute for Environmental Research, Australian Nuclear Science and Technology  
26 Organisation, Lucas Heights, NSW, 2234, Australia

27

28

29 \* Correspondence to: Lixin Wang (wang.iupui@gmail.com)

30 Lixin Wang

31 Department of Earth Sciences

32 Indiana University-Purdue University Indianapolis (IUPUI)

33 Indianapolis, Indiana 46202, USA

34 Office phone number: 317-274-7764

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35 **ABSTRACT**

36 The stable isotopes of water are useful tracers of water sources and hydrological processes.  
37 Stable water isotope-enabled land surface modeling is a relatively new approach for  
38 characterising the hydrological cycle, providing spatial and temporal variability for a number  
39 of hydrological processes. At the land surface, the integration of stable water isotopes with  
40 other meteorological measurements can assist in constraining surface heat flux estimates and  
41 discriminate between evaporation (E) and transpiration (T). However, research in this area  
42 has traditionally been limited by a lack of continuous *in-situ* isotopic observations. Here, the  
43 National Centre for Atmospheric Research stable isotope-enabled Land Surface Model  
44 (ISOLSM) is used to simulate the water and energy fluxes and stable water isotope  
45 variations. The model was run for a period of one month with meteorological data collected  
46 from a coastal sub-tropical site near Sydney, Australia. The modeled energy fluxes (latent  
47 heat and sensible heat) agreed reasonably well with eddy covariance observations, indicating  
48 that ISOLSM has the capacity to reproduce observed flux behaviour. Comparison of modeled  
49 isotopic compositions of evapotranspiration (ET) against *in-situ* Fourier Transform Infrared  
50 spectroscopy (FTIR) measured bulk water vapor isotopic data (10 m above the ground),  
51 however, showed differences in magnitude and temporal patterns. The disparity is due to a  
52 small contribution from local ET fluxes to atmospheric boundary layer water vapor (~ 1%  
53 based on calculations using ideal gas law) relative to that advected from the ocean for this  
54 particular site. Using ISOLSM simulation, the ET was partitioned into E and T with 70%  
55 being T. We also identified that soil water from different soil layers affected T and E  
56 differently based on the simulated soil isotopic patterns, which reflects the internal working  
57 of ISOLSM. These results highlighted the capacity of using the isotope-enabled models to  
58 discriminate between different hydrological components and add insight into expected  
59 hydrological behavior.

60

61 **Keywords:** FITR, hydrogen, ISOLSM, isotope, oxygen, spectroscopy

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63

## 64 1. INTRODUCTION

65 Land surface models (LSMs) provide an established computational approach to describe  
66 energy and water exchanges between the land surface and overlying atmosphere. LSMs  
67 have led to improvements in agriculture and forest water management (Ingwersen et al.,  
68 2011; Patil et al., 2011), weather forecasting (Devonec and Barros, 2002; Kang et al., 2007)  
69 and the description of hydrological exchange processes from local to global scales (Rodell et  
70 al., 2004). However, as with any modeling application, there are necessary caveats associated  
71 with their use. Amongst a number of related studies, the Project for Intercomparison of Land-  
72 surface Parameterization Schemes (PILPS) demonstrated that despite the level of model  
73 sophistication, results for latent heat (LE) and sensible heat (H) fluxes from a range of LSMs  
74 can vary considerably due to uncertainties in surface observations (Henderson-Sellers et al.,  
75 2003) and underutilization of meteorological inputs (Abramowitz et al., 2008). Furthermore,  
76 Abramowitz et al. (2008) demonstrated a lack of confidence in flux calculations by  
77 comparing the performance of three independent models: the Common Land Model (CLM)  
78 (Dai et al., 2003), the Organizing Carbon and Hydrology in Dynamic Ecosystems  
79 (ORCHIDEE) (Krinner et al., 2005) and the Community Atmosphere Biosphere Land  
80 Exchange (CABLE) (Kowalczyk et al., 2006). One outcome of such examinations is the  
81 recognition of the need for additional observational constraints to increase the robustness of  
82 model simulations (McCabe et al., 2005).

83 Stable isotopes of oxygen ( $^{16}\text{O}$  and  $^{18}\text{O}$ ) and hydrogen ( $^1\text{H}$  and  $^2\text{H}$ ) represent  
84 conservative tracers of the water cycle. They can be used to inform upon various components  
85 of the water cycle, providing new insights into hydrological and meteorological processes.  
86 For example, stable water isotopes are useful tracers of meteoric waters in the hydrologic  
87 cycle (Dansgaard, 1964; Gat, 1996; Soderberg et al., 2013), can quantify the strength of

88 orographic precipitation (Smith and Evans, 2007), can identify vegetation water sources  
89 (Ehleringer and Dawson, 1992) and have been used for discriminating hydrological  
90 components (Wang et al., 2010; Yepez et al., 2003). Stable water isotopes may be  
91 particularly useful in partitioning evapotranspiration (ET), since soil evaporation (E) isotopic  
92 fractionation produces water vapor with a different isotopic composition relative to plant  
93 transpiration (T) and source water (Ehleringer and Dawson, 1992). As a result, the distinct  
94 isotopic compositions of E and T can be determined (Gat, 1996), so that ET can be separated  
95 into its components (Ferretti et al., 2003; Moreira et al., 2003; Sutanto et al., 2012; Wang et  
96 al., 2010; Yepez et al., 2003).

97         Recently, stable isotopes have also been incorporated into land surface models to  
98 better understand energy and water fluxes (Aranibar et al., 2006; Fischer, 2006; Haverd and  
99 Cuntz, 2010; Henderson-Sellers et al., 2006; Riley et al., 2002; Risi et al., 2010). Isotopes in  
100 PILPS (iPILPS) was introduced by Henderson-Sellers (2006) to set up a framework for the  
101 intercomparison of isotope-enabled LSMs. Models participating in iPILPS illustrated the  
102 importance of water isotopes in investigating the transportation and source of fluxes (Fischer,  
103 2006; Henderson-Sellers et al., 2006; Riley et al., 2002; Yoshimura et al., 2006). For  
104 example, by adding a stable water isotope parameterisation to the CHAmeleon Surface  
105 Model (CHASM), Fischer (2006) demonstrated a better reproduction of the behaviour of a  
106 land surface scheme that has additional functionality (such as bare ground evaporation,  
107 canopy interception and aerodynamic, as well as surface and stomatal resistances). However,  
108 disagreement between model outputs suggested that modeled fluxes may not be well  
109 constrained.

110         The National Centre for Atmospheric Research (NCAR) stable isotope-enabled Land  
111 Surface Model (ISOLSM) was developed for the simulation of  $\delta^{18}\text{O}$  of  $\text{H}_2\text{O}$  and  $\text{CO}_2$   
112 exchanges between the atmosphere and the land surface (Riley et al., 2002). It is based on the

113 NCAR Land Surface Model (LSM1.0) (Bonan, 1996; Bonan, 1998) which simulates energy,  
114 water, momentum and carbon dioxide exchanges and interactions between the atmosphere  
115 and terrestrial ecosystem. The isotope modules were integrated into LSM 1.0 for the purpose  
116 of predicting the isotopic compositions of plant water, soil water, water vapor and ecosystem  
117 CO<sub>2</sub> fluxes. Unlike some similar isotope-enabled land surface models (Haverd and Cuntz,  
118 2010; Risi et al., 2010), ISOLSM simultaneously simulates both pools and fluxes in water  
119 isotopes from soil, vegetation and atmosphere reservoirs. In the past, few efforts have been  
120 taken to validate isotope-enabled LSMs using continuous *in-situ* data, due mainly to the  
121 difficulty in undertaking targeted *in-situ* water vapor isotope measurements and the lack of  
122 high resolution field observations. Specifically, to our knowledge no attempt has been made  
123 to test the sensitivity of the response of ISOLSM to uncertainties in input variables. With  
124 recent developments in absorption-spectroscopy based instruments, the collection of  
125 continuous observations of atmospheric water vapor isotopic composition has increased  
126 (Griffis et al., 2011; Lee et al., 2009; Wang et al., 2009; Wen et al., 2008; Zhao et al., 2011),  
127 making model evaluation feasible for different temporal scales. One recent example of  
128 employing high temporal resolution stable water isotopic measurements for LSM validation  
129 was Xiao et al. (2010). Xiao et al. (2010) demonstrated the agreement between modeled and  
130 observed seasonal and diurnal variations in LE and H flux, and they also demonstrated the  
131 agreement between modeled and observed  $\delta^{18}\text{O}$  in bulk leaf water. The observed soil  
132 moisture, however, was not accurately captured by the LSM model in Xiao et al. (2010).

133 To advance a more comprehensive assessment of isotope-enabled LSMs, this paper  
134 seeks to evaluate ISOLSM for surface heat and water isotope flux estimates by integrating  
135 continuous *in-situ* water vapor isotopic measurements. This paper also investigates the  
136 constraints water vapor isotopes provide on land surface modeling. Specifically, the  
137 objectives of this study are: (1) to evaluate ISOLSM accuracy for energy and water fluxes in

138 a coastal sub-tropical site; (2) to perform model sensitivity analyses to identify potential  
139 sources of error for ISOLSM parameterisations and variables that exert large control on the  
140 isotopic fluxes; 3) to examine the local and regional water vapor contributions using modeled  
141 energy and isotopic fluxes, and observed humidity and water vapor isotopes. This is  
142 important because of the coastal setting of the *in-situ* water vapor isotopic measurement and  
143 possible contribution from the ocean; and (4) to partition landscape scale ET into E and T  
144 using process-based modeling. It is noted that due to the coastal location of the site and the  
145 inherent large moisture source from the ocean, the local ET contribution to the atmospheric  
146 vapor was very small and ISOLSM only simulates the local ET flux isotopic composition. In  
147 addition, the final temporal resolution of the isotope measurements in this study is relatively  
148 low (10 min), therefore the comparison of ISOLSM simulated isotopic composition of ET  
149 flux and *in-situ* isotope data is not rigorous.

## 150 **2. DATA AND METHODOLOGY**

### 151 **2.1. Study site description**

152 Meteorological and stable isotope observations were made at a coastal sub-tropical  
153 site at the Australian Nuclear Science and Technology Organization (ANSTO) at Lucas  
154 Heights in NSW, Australia. ANSTO (34.05°S, 150.98°E, 152 m above sea level) is located  
155 40 km southwest of Sydney and approximately 20 km inland. The sensors were located on a  
156 tower over a mown lawn of ~40 m in radius, surrounded by a mixed natural eucalyptus forest  
157 (average canopy height of 10 m) and a sclerophyllous shrub understorey. The tower is 10 m  
158 high and the instruments were at the top of the tower. The site has a temperate climate with  
159 warm to hot summers and mild winters. Based on the site meteorological observations from  
160 2009 to 2011, hourly relative humidity ranged from 30% to 90% throughout the year.  
161 According to the available Bureau of Meteorology data (1958-1982) at the site, rainfall  
162 averages 1000 mm annually and there is no distinct wet or dry season. Average monthly

163 maximum temperature is 21.4°C and average minimum temperature is 12.3°C.

164

## 165 **2.2. Meteorological and evaluation Data**

166 Approximately one month (Dec 22, 2010 to Jan 26, 2011) of meteorological data and  
167 surface heat flux data was used to force and validate ISOLSM, respectively. Meteorological  
168 data consisting of rainfall, relative humidity, air temperature, wind speed, vapor pressure,  
169 incoming solar radiation and net radiation were measured 10 m above ground level.

170 Surface heat fluxes of latent heat (LE) and sensible heat (H) (all in  $W/m^2$ ) were  
171 measured at half hourly intervals from an eddy covariance system positioned on the tower.  
172 Ground heat flux (G) was measured at the ground level using a soil heat flux plate (Model  
173 HFT3, Campbell Scientific, Utah, USA). Fluxes were computed from the 20 Hz output of a  
174 sonic anemometer (Gill Windmaster Pro) and open path infra-red gas analyser (Licor 7500)  
175 following standard methods (Aubinet et al., 2012; Lee et al., 2004). Data were screened for  
176 spikes and grouped into 30-minute blocks, the data streams were time-shifted to maximize  
177 the correlation between temperature and moisture fluctuations (Kristensen et al., 1997), each  
178 30-minute block was rotated into the mean flow direction by applying a three-angle rotation  
179 (Kaimal and Finnigan, 1994), sonic temperature was corrected for the effect of water vapor at  
180 the full data rate (Schotanus et al., 1983), and the Webb-Pearman-Leuning (Webb et al., 1980)  
181 correction was applied to moisture flux. The lag time between the sonic anemometer and  
182 water vapor sensor was due to the physical separation between the instruments, ~0.2 m, and  
183 differences in the instruments' internal signal processing times. As a result, the lag was small,  
184 with typical values between 0 and 6 samples at 20Hz. The measured ground heat flux  
185 (Campbell Scientific HTF3) was corrected for the finite size of the heat flux sensor  
186 (Overgaard Mogensen, 1970) and the harmonic correction (Heusinkveld et al., 2004) used to  
187 correct for the attenuation of the ground heat flux with depth. Modeled results were averaged  
188 to 30-min resolution to match meteorological and surface heat flux observations. The lack of

189 energy balance closure in eddy covariance measurement is a common problem and has been  
190 discussed in many studies (Aranibar et al., 2006; Ingwersen et al., 2011; Xiao et al., 2010).  
191 For the data set compiled for this study, the measured energy fluxes of LE and H accounted  
192 for about 75% of the available energy. This imbalance is within the acceptable range  
193 according to Aranibar et al. (2006) and Xiao et al. (2010). Both Aranibar et al. (2006) and  
194 Xiao et al. (2010) have previously demonstrated the need to force energy balance closure to  
195 improve LSM model performance. Haverd et al. (2007) also showed that canopy energy  
196 storage can prevent energy budget closure in eddy covariance data. For simplification, the  
197 observed energy fluxes were adjusted to achieve energy balance closure by assuming the  
198 energy imbalance was due to measurement bias of LE and H and ignoring the canopy energy  
199 storage. Thus for this research, LE and H were both multiplied by an adjustment factor  
200 derived from the Bowen ratio (H/LE) correction method to force energy balance closure  
201 (Aranibar et al., 2006). ISOLSM requires solar radiation measurements of visible direct,  
202 visible diffuse, near-infrared direct and near-infrared diffuse to drive the model (Bonan,  
203 1996). To derive the radiation components from shortwave radiation, we have assumed that  
204 the ratio of visible to near-infrared radiation is 1:1, and the ratio of direct to diffuse radiation  
205 is 7:3 (Henderson-Sellers et al., 2006).

206

### 207 **2.3 *In-situ* monitoring of water vapor isotopic composition**

208 We present stable water isotopic compositions using the standard delta notation (e.g.,  
209  $\delta^{18}\text{O}$  or  $\delta^2\text{H}$ ), defined in terms of the ratio of a sample relative to the Vienna Standard Mean  
210 Ocean Water (VSMOW):

$$211 \delta = R_{\text{sample}}/R_{\text{VSMOW}} - 1 \quad (1)$$

212 where R is the ratio of  $^{18}\text{O}/^{16}\text{O}$  or  $^2\text{H}/\text{H}$ . The isotope ratios are typically multiplied by 1000 to  
213 express in per mil (‰). The  $\delta$  value represents the isotopic enrichment ( $\delta > 0$ ) or depletion ( $\delta$   
214  $< 0$ ) with respect to VSMOW.

215 Real time stable water vapor isotopic compositions of oxygen and hydrogen  
216 synchronous with the meteorological data were measured using a Fourier Transform Infrared  
217 (FTIR) spectrometer deployed at Lucas Heights, which sampled air through heated sampling  
218 lines from a height of 10 m (Parkes et al., 2011). FTIR measurements were averaged to  
219 present 10 minute values with a precision of better than 1‰ and 0.4‰ for  $\delta^2\text{H}$  and  $\delta^{18}\text{O}$   
220 respectively, at water vapor mixing ratios between 5,000 and 30,000 ppm on a dry air basis.  
221 Measurements of the isotopic compositions of precipitation were not available during the  
222 study period. The  $\delta^{18}\text{O}$  and  $\delta^2\text{H}$  of precipitation were assumed to be 0. Based on the Online  
223 Precipitation Isotope Calculator  
224 ([http://wateriso.utah.edu/waterisotopes/pages/data\\_access/form.html](http://wateriso.utah.edu/waterisotopes/pages/data_access/form.html)), the January rainfall  
225  $\delta^{18}\text{O}$  is -4.2‰. Based on the sensitivity results (Section 2.6), it would induce some biases in  
226 estimating the isotopic compositions of other components. For example, the bias is 2.52‰ in  
227 soil water  $\delta^{18}\text{O}$ .

#### 228 **2.4. Physical model description**

229 ISOLSM is a one-dimensional multiple process LSM that simulates atmospheric (e.g.,  
230 net radiation and outgoing longwave radiation), ecological (e.g., plant photosynthesis and  
231 stomatal conductance) and hydrological (e.g., surface runoff and infiltration) processes. The  
232 model is capable of land surface simulation at multiple spatial scales (point, regional or  
233 global) and supports 28 surface types (e.g., grassland, forest and shrubland) and multiple  
234 different soil types. Evergreen forest vegetation cover was used for the current simulation  
235 based on leaf area index and phenology. The surface heat fluxes of LE and H are calculated  
236 as a function of surface types and the forcing meteorological conditions using standard water  
237 and energy balance assumptions, described by Still et al. (2009). With respect to soil layers,  
238 soil water movement, soil textures, boundary conditions, and plant rooting depth, ISOLSM  
239 follows LSM1.0 with detailed description in Bonan et al. (1996). Specifically, six soil layers

240 were used (0.10 m, 0.20 m, 0.40 m, 0.80 m, 1.60 m, 3.20 m). The dynamics of infiltration and  
 241 surface runoff is determined by the relative relationship of throughfall, snow melt, dew, soil  
 242 water content and infiltration capacity.

243 For the calculation of stable water vapor isotopic flux from vegetation, leaf water is  
 244 considered as liquid phase and surface water vapor isotopic composition is calculated based  
 245 on the Craig and Gordon model (1965). The total water vapor isotopic ratio at canopy surface  
 246 is then summarised as:

$$247 \quad R_s = \frac{c_s R_{atm} e_{atm} + c_l \alpha_{V/L}(T_v) R_l e_l + c_g \alpha_{V/L}(T_g) R_g e_g}{e_s (c_s + c_l + c_g)}, \quad (2)$$

248 where  $C_s$  (m/s) is the land surface aerodynamic conductance,  $C_l$  (m/s) is the aerodynamic  
 249 conductance between the leaf interior and land surface,  $C_g$  (m/s) is the aerodynamic  
 250 conductance between the ground and land surface,  $R_{atm}$ ,  $R_l$  and  $R_g$  are isotopic ratios of the  
 251 atmospheric water, leaf water and the surface soil water respectively,  $e_{atm}$  (Pa) is the water  
 252 vapor pressure at atmospheric reference height and  $e_s$  (Pa),  $e_l$  (Pa) and  $e_g$  (Pa) are water vapor  
 253 pressure at the land surface, within the leaf and within the surface soil layer respectively, and  
 254  $\alpha_{V/L}(T_v)$  and  $\alpha_{V/L}(T_g)$  are the equilibrium isotope fractionation factors at the vegetation  
 255 evaporating surface temperature ( $T_v$ ) and ground temperature ( $T_g$ ) (Riley et al., 2002).

256 The model computes fluxes of each isotopologue (e.g.,  $H_2^{16}O$ ,  $H_2^{18}O$  and HDO)  
 257 individually (in units of mm/s), from which we derived the isotopic compositions of T, E and  
 258 canopy evaporation (CE, which refers to evaporation at canopy level) fluxes (e.g.,  $\delta^{18}O$  and  
 259  $\delta^2H$ ). For example, the isotopic compositions of T ( $\delta^{18}O$ ) is calculated as:

$$260 \quad R_{sample} = \frac{T(H_2^{18}O)}{T(H_2^{16}O)} \quad (3)$$

261 where  $T(H_2^{18}O)$  and  $T(H_2^{16}O)$  represent the transpiration rates of each isotopologue (mm/s).  
 262 Further details on ISOLSM isotopic processes have been documented by Riley et al. (2002),  
 263 Aranibar et al. (2006) and Still et al. (2009).

264

## 265 2.5. Model evaluation

266 For model evaluation, the performance of ISOLSM in predicting energy and water  
267 fluxes was examined during two different weather regimes: a wet period and a dry period.  
268 The modeled fluxes during the wet period (Jan 5-15, 2011 and with a total of 45 mm rainfall)  
269 and the dry period (Jan 16-25, 2011, <1 mm rainfall) were selected from the approximately  
270 36 days of total simulation (Dec 22, 2010 to Jan 26, 2011) to compare with observations. The  
271 simulation includes a short initialization period (Dec 22, 2010 to Jan 5, 2011) for priming the  
272 model (e.g., initialize soil moisture content).

273 To investigate ISOLSM energy simulation, four performance measures including the  
274 root mean square error (*RMSE*, eq. 4), index of agreement (*I*, eq. 5) (Willmott, 1981), bias  
275 (eq. 6) and the correlation coefficient (*R*, eq. 7) were adopted to examine the total number (*N*)  
276 of modeled values (*m*) in comparison with observed values (*o*). These expressions are  
277 detailed below:

278

279

$$280 \quad RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (m_i - o_i)^2} \quad (4)$$

$$281 \quad I = 1 - \frac{\sum_{i=1}^N (m_i - o_i)^2}{\sum_{i=1}^N (|m_i - \bar{o}| + |o_i - \bar{o}|)^2} \quad (5)$$

$$282 \quad bias = \frac{1}{N} \sum_{i=1}^N (m_i - o_i) \quad (6)$$

$$283 \quad R = \frac{\sum_{i=1}^N (m_i - \bar{m})(o_i - \bar{o})}{\sqrt{\sum_{i=1}^N (m_i - \bar{m})^2 \sum_{i=1}^N (o_i - \bar{o})^2}} \quad (7)$$

284 where  $\bar{m}$  and  $\bar{o}$  are the average values of the predictions and observations respectively. An  
285 RMSE and bias equal to 0, and *I* and *R*<sup>2</sup> (*R* x *R*) equal to 1 is indicative of the “best” model  
286 performance. Performance measures were calculated on predictions of LE, H and G for the  
287 wet period and dry period.

288

## 289 **2.6 Model sensitivity to variation in isotope forcing**

290 A sensitivity study of ISOLSM was designed to test the model output response to  
291 changes in the isotopic composition of input waters: in particular to demonstrate the response  
292 of modeled  $\delta^{18}\text{O}$  in soil water, T and E to a range of input  $\delta^{18}\text{O}$  values for initial soil water  
293 and precipitation. This procedure is essential to quantify the potential model output biases  
294 that may arise due to uncertainties or lack of data in model inputs. The analysis focussed on  
295 the wet period as no significant rainfall occurred during the dry period. The wet period  
296 meteorological data was used to force ISOLSM, with initial soil water content obtained from  
297 the initialization run. A set of values ranging from -20 to 0 ‰ in 1 ‰ increments, were  
298 assigned as the precipitation  $\delta^{18}\text{O}$  input, to establish the response of soil water isotopic  
299 compositions. The soil water isotopic composition  $\delta^{18}\text{O}$  was also initialized with isotopic  
300 values of 0 ‰, -5 ‰, -10 ‰ and -15 ‰ for the same set of precipitation  $\delta^{18}\text{O}$  input values to  
301 understand the interactions between isotopic compositions of precipitation, soil water and ET.  
302

## 303 **3. RESULTS AND DISCUSSION**

### 304 **3.1. Simulation and evaluation of energy and water fluxes**

305 To address our first objective of evaluating ISOLSM accuracy for energy and water fluxes in  
306 a coastal sub-tropical site, the observed and modeled surface heat fluxes from the  
307 meteorological site at the ANSTO field location were shown in Figure 1. An expected diurnal  
308 variation was evident in the observed LE, H and G. On average larger LE and H were  
309 observed during the dry period, with LE peaks of  $350 (\pm 109 (1\sigma)) \text{ W/m}^2$ , whilst an average  
310 of  $300 (\pm 105 (1\sigma)) \text{ W/m}^2$  was observed in the wet period. The regression between the  
311 observed net radiation ( $R_n$ ) and the sum of LE, H and G ( $F_t$ ) radiation ( $R_n$ ) was,  $R_n = 0.76 F_t$   
312  $+ 6.04$ , with an  $R^2$  of 0.92, indicating an energy budget closure of 76%.

313 The modeled data show that ISOLSM captured the diurnal cycle for the LE fluxes

314 (Figure 1). For the dry period, the magnitude and diurnal cycle were in general agreement  
315 between modeled and observed energy fluxes (LE, H and G). Modeled wet period H matched  
316 observations until January 9, but then underestimated measured H by up to  $200 \text{ W/m}^2$  (Figure  
317 1) due to the heavy rainfall events that bring the top soil layer to near saturation (Figure 5a).  
318 The better match between modeled and observed results in the dry period is potentially a  
319 response to less variability in weather related variables such as rainfall and relative humidity.  
320 Lower quality measurements due to conditions that deviate from EC assumptions during the  
321 rainy days could also contribute to the poorer match in the wet period. These results may also  
322 indicate that the modeled H is too sensitive to the soil moisture in the top soil layer when it is  
323 very wet.

324 The daily Bowen ratios were calculated to assist energy balance closure. For the days  
325 without rain, the Bowen ratio averaged 0.7. For the days with rainfall events (26, 27 Dec  
326 2010 and 7 to 15 Jan 2011), the Bowen ratios were generally higher than 1.2 with maximum  
327 values up to 2 (data not shown). Prueger (2005) also reported that the relationship between  
328 measured LE and H was influenced by the rainfall events. Both Aranibar et al. (2006) and  
329 Xiao et al. (2010) drew the conclusion that forcing energy balance closure using Bowen ratio  
330 approach can improve the LSM model performance. However neither of these studies  
331 investigated eddy covariance measurements on raining days since eddy covariance sensors  
332 typically do not work properly during precipitation. Further study on the utility of the Bowen  
333 ratio correction method for eddy covariance data closure under such conditions is required.

334 To statistically evaluate ISOLSM energy simulation against observed data, the four  
335 performance measures in Section 2.5 were calculated. Overall, the performance measures  
336 show that the model provided more accurate measures of LE and H during the dry period,  
337 whereas the accuracy of G was similar for both wet and dry periods. Specifically, H was the  
338 most improved measure from wet to dry, with the *bias* improving from  $-84.90 \text{ W/m}^2$  to  $-52$

339  $\text{W/m}^2$ , the *RMSE* decreasing from  $107.35 \text{ W/m}^2$  to  $70.16 \text{ W/m}^2$ , the  $R^2$  increasing from 0.43  
340 to 0.71 during the dry period, and  $I$  increasing from 0.65 to 0.82. The modeled LE was  
341 similarly more accurate during the dry period, with *RMSE* and *bias* decreasing from 88.94 to  
342  $58.06 \text{ W/m}^2$  and 66.67 to 28.15 respectively, while  $I$  and  $R^2$  increased from 0.82 to 0.93 and  
343 0.69 to 0.81. Figure 2 illustrates that both LE and H were less scattered during the dry period  
344 compared with the wet period. The rainfall (wet vs. dry period) had only a small influence on  
345 the G prediction relative to LE and H. The  $I$  of G increased marginally from 0.91 during the  
346 wet period to 0.92 during the dry period and its  $R^2$  increased from 0.82 to 0.86 respectively.  
347 There was a negative bias of modeled H during both wet ( $-84.90 \text{ W/m}^2$ ) and dry ( $-52.00$   
348  $\text{W/m}^2$ ) periods that can also be observed in the scatter plots between modeled results and  
349 observations (Figure 2). This indicates that on average ISOLSM underestimates H for the  
350 entire simulation period. Table 2 and Figure 2 also show that the overall model performance  
351 was poorer for H than for the LE and G fluxes.

352

### 353 **3.2. Model sensitivity to variation in isotope forcing**

354 To address our second objective of testing ISOLSM sensitivity to parameterisations,  
355 Figure 3 shows the time series of modeled soil water  $\delta^{18}\text{O}$  for the top two soil layers [(a)  
356 layer1 (0-0.1 m) and (b) layer2 (0.1-0.2 m)] with an initial soil water  $\delta^{18}\text{O}$  of 0 ‰ and  
357 precipitation  $\delta^{18}\text{O}$  ranging from -20 ‰ to 0 ‰. For the top soil layer (Figure 3a) there was no  
358 change in soil water  $\delta^{18}\text{O}$  before 50 hours (the time when precipitation appears) due to the  
359 lack of precipitation. Following 50 hours, rainfall caused modeled soil water  $\delta^{18}\text{O}$  to decrease  
360 sharply after each rainfall event. This decrease was proportional to the rainfall amount and  
361 the  $\delta^{18}\text{O}$  of the rainfall. Due to the removal of light isotopes by ET, the soil water  $\delta^{18}\text{O}$   
362 becomes gradually more enriched between rainfall events. A mean difference ( $MD_{soil}$ ) was  
363 defined as  $\Delta\delta_{soil}/\Delta\delta_{precipitation}$ , which was the averaged difference for  $\delta_{soil}$  between all the

364 adjacent increments (e.g., -20 ‰ to -19 ‰, -1 ‰ to 0 ‰) across the wet period. The standard  
365 error of the difference ( $SE_{soil}$ ) was the standard error of all the  $\Delta\delta_{soil}$  across the wet period. For  
366 every 1‰ increment of  $\delta^{18}O$  of precipitation, soil water  $\delta^{18}O$  within this layer increased by a  
367  $MD_{soil}$  of about 0.6 ‰, with a  $SE_{soil}$  of 0.07 ‰.

368         Precipitation did not have an influence on layer2 soil water  $\delta^{18}O$  until 117 hours. This  
369 delayed response to precipitation input is due to the response time of infiltration. The soil  
370 water  $\delta^{18}O$  in layer2 was less sensitive to the precipitation, with an average ( $MD_{soil}$ ) of about  
371 0.005‰ changes with  $SE_{soil}$  of 0.001 ‰, for every 1‰ increment of  $\delta^{18}O$  of precipitation.  
372 The  $\delta^{18}O$  in soil water below layer2 was not isotopically influenced by the precipitation,  
373 suggesting infiltration stops above soil depth of 0.2 m with the assigned soil properties (Table  
374 1).

375         The mean difference in transpiration ( $MD_T$ , defined similarly to  $MD_{soil}$ ) and  
376 evaporation ( $MD_E$ ) in response to each 1‰ increment of precipitation  $\delta^{18}O$  (varying from -20  
377 ‰ to 0 ‰) and with an initial soil water  $\delta^{18}O$  of 0 ‰, was calculated as 0.26 ‰ and 0.6 ‰,  
378 with a  $SE$  of 0.16 ‰ and 0.34 ‰ respectively. These results indicate that the  $\delta^{18}O$  of soil  
379 evaporation is twice as sensitive as T to the  $\delta^{18}O$  of precipitation. The different  $MD_T$  and  
380  $MD_E$  responses could be due to the different moisture sources (e.g., T uses deeper soil layers  
381 than E). This would explain the lower  $SE$  in T (0.16 ‰ vs. 0.34 ‰) since deeper soil layers  
382 will buffer the variability in isotopic compositions of precipitation. Both  $MD_T$  and  $MD_E$   
383 followed the same pattern as the  $MD_{soil}$  of layer1. These relative sensitivities need to be  
384 considered in the context of precipitation and initial soil moisture isotopic ratios being  
385 prescribed model variables.

386

### 387 **3.3. Modeled ET isotopic compositions against FTIR *in-situ* measurements**

388         To address our third objective, the diurnal composites for the *in-situ* water vapor

389 isotope observations, the modeled  $\delta_{ET}$  as well as the modeled and observed LE fluxes are  
 390 shown in Figure 4. The modeled  $\delta^{18}O$  and  $\delta^2H$  showed similar and clear diurnal patterns with  
 391 more enriched values observed during the daytime (Figure 4a and b). Interestingly, the FTIR  
 392 observations did not show a clear diurnal cycle, suggesting that the isotopic composition of  
 393 atmospheric water vapor at the site was largely unaffected by local ET fluxes. A calculation  
 394 was conducted to estimate the ET contribution to the total water vapour, which involved three  
 395 steps. Firstly, using the ideal gas law, the total absolute humidity ( $q$  ( $g/m^3$ )) was calculated  
 396 following Koh et al., (2010) as:

$$397 \quad q = \frac{217e}{T}, \quad (8)$$

398 where  $T$  (K) is the atmospheric temperature,  $e$  is actual vapour pressure, which is the product  
 399 of observed relative humidity and saturation vapour pressure calculated from temperature.  
 400 The atmospheric water vapor ( $mm/s$ ) was then calculated as  $q$  ( $g/m^3$ ) multiplied by the  
 401 measured wind speed ( $m/s$ ). Lastly, using the measured ET flux ( $mm/s$ ) as local water vapor,  
 402 the mean ratio ( $f_{ET}$ ) of local water vapor over total atmospheric water vapor was calculated.  
 403 The calculated  $f_{ET}$  was 0.75%, suggesting that advective processes dominates water vapor at  
 404 the study site. The small ET contribution is not surprising considering the location of the  
 405 study site, which is approximately 20 km from the coast. This agrees with previous study  
 406 which has estimated that the majority of moisture for the Murray-Darling basin is from the  
 407 Pacific ocean (Stohl and James, 2005). Using the calculated  $f_{ET}$ , an isotopic water mass  
 408 balance equation was used to attain a rough estimate of  $\delta_{ET}$ :

$$409 \quad \delta_{FIS} = \delta_{ET} f_{ET} + \delta_{atm} (1 - f_{ET}) \quad (9)$$

411 where  $\delta_{atm}$  is the background atmospheric isotopic compositions, which were assumed as the  
 412 standard marine air values ( $\delta^{18}O = -11.4 \text{ ‰}$  and  $\delta D = -85 \text{ ‰}$ ) summarized by Gat (1996) and  
 413 based on data of the International Atomic Energy Agency (IAEA) network. Rearranging

414 Equation 9, observed  $\delta_{FT}$  can be calculated using  $\delta_{FTIR}$ ,  $\delta_{atm}$  and  $f_{ET}$ . The mean observed ET  
 415 isotopic compositions were well captured by the model (e.g., mean observed and modeled  
 416  $\delta^{18}O$  both equalled -4.8 ‰). Such estimate is simplified calculations and involves  
 417 assumptions of constant  $\delta_{atm}$  and constant  $f_{ET}$ . The isotopic budget method used here  
 418 (equation 9) could lead to large varying  $\delta_{ET}$  values when the advected moisture source  
 419 isotopic composition changes.

420 To further investigate the origin of air masses arriving at Lucas Heights during the  
 421 observational period, the wind observations and back trajectories were analysed. The wind  
 422 observations were taken from 10 m, which is the same heights as the FTIR intake, and wind  
 423 roses were calculated for the whole time period. Hourly back trajectories were calculated  
 424 with the Hybrid Single Particle Lagrangian Integrated Trajectory Model (HYSPLIT v4.0)  
 425 (Draxler and Rolph, 2003) forced with the Global Data Assimilation System (GDAS)  
 426 meteorological dataset that has a horizontal resolution of  $0.5^\circ$  and 55 hybrid sigma-pressure  
 427 levels. The trajectories were calculated back in time for 3 days and were released from a  
 428 height of 100 m at the site. Only 3 day trajectories were calculated as we were interested in  
 429 only the recent air mass origin (whether the air mass had come directly off the ocean or not).  
 430 The footprint for these trajectories over the course of the observational period was calculated  
 431 by first creating a  $2^\circ \times 2^\circ$  horizontal grid between latitudes of  $-25^\circ$  and  $-50^\circ$  and longitudes of  
 432  $140^\circ$  and  $180^\circ$ . The total number of points from all trajectories that were positioned in a grid  
 433 space was counted, shown by

$$434$$

$$435 \quad N_{x,y} = \sum_{t=0}^n T_{i,t}, \quad (10)$$

436 where  $N_{x,y,t}$  is the total number of trajectory points that pass through grid point  $(x, y)$  for all  
 437 the hourly trajectories  $t$ . Each back trajectory consists of  $n$  points (72 hourly points for 3  
 438 days).  $T_{i,t}$  is either 1 or 0 depends on point  $i$  on the back trajectory released at time  $t$  being

439 inside grid point  $x,y$  or not.  $N_{x,y}$ , was calculated for all grid points over the specified domain.  
440 The more frequently a trajectory passes through a certain grid space the higher  $N_{x,y}$  and the  
441 calculation then determines the most common air mass origin. As shown in Figure 5A, the  
442 predominant wind direction was from the northeast and south. Figure 5B show back  
443 trajectory origin for the period of the observational period and confirm the predominant air  
444 mass origin and therefor moisture source is the ocean.

445 Based on the results of wind observations and back trajectory analyses, variations in  
446 the observed isotopic composition of water vapor therefore tend to be driven by larger scale  
447 processes such as precipitating weather systems. As the passing of weather patterns is  
448 generally random, the signals associated with these events generally cancel out for the diurnal  
449 composites. This indicates that for this particular site, *in-situ* vapor measurements at one  
450 height may not inform local land atmosphere exchange especially at the temporal resolution  
451 of 10 min. A better alternative method to quantify  $\delta_{ET}$  is to use temporal (with relatively  
452 higher temporal resolution) and spatial (with relatively lower temporal resolution) Keeling  
453 plot approach to capture the dynamic nature of  $\delta_{ET}$  (Good et al., 2012). In addition, how best  
454 to incorporate the isotopic compositions of advected air into ISOLSM in order to better  
455 reproduce the observed isotopic dynamics requires further investigations.

456

### 457 **3.4. Process insight into water cycle components**

458 After evaluating the ISOLSM total ET fluxes, the simulated ET flux was partitioned  
459 into T, E and CE (Figure 6). Modeled T and E exhibit a strong diurnal cycle (Figure 6) that  
460 correlates with solar radiation. The modeled T values had the highest magnitude among the  
461 three water fluxes, reaching a daily maximum of up to  $2.0 \times 10^{-3}$  mm/s: more than three times  
462 E (Figure 6b). The model suggests that transpiration was the dominant flux (T is typically  
463 about 70% of total ET), which has been demonstrated by previous studies in similar

464 ecosystems (Blanken et al., 1997; Unsworth et al., 2004; Wang et al., 2014). Though the  
465 simulated transpiration ratio is a reasonable estimate, we note that the ratio is not validated  
466 using the isotope measurements for this study. The transpiration ratio could be quantified  
467 using a combined tower measurements and chamber-based isotopic partitioning methods for  
468 further studies (e.g., Good et al., 2012; Wang et al., 2012; Wang et al., 2013).

469         Following the precipitation in the wet period, the moisture in the top soil layer  
470 increased from 7 to 30 mm (Figure 7), and was accompanied by decreases in soil water  $\delta^2\text{H}$   
471 (70 to 20‰) and  $\delta^{18}\text{O}$  (7‰ to 2.5‰). When soil moisture started to decrease from the end of  
472 the wet period, the isotopic values of the soil were shown to increase, as light isotopes were  
473 preferentially removed from the soil water pool via E. The isotopic values then decreased  
474 again in the middle of the dry period, likely due to the water moving up through the soil  
475 column as the top layer dries. The isotopic composition of E followed the same trend as the  
476 first layer soil water isotopic compositions (Figure 6d, 7b and c), suggesting that water vapor  
477 fluxes from E were mainly derived from the top soil layer. Figure 5 and Figure 6 also provide  
478 useful information about the water source of T. The precipitation had only a small influence  
479 on T in comparison to E, and T was supported by the second layer soil water dynamics. The  
480 second layer soil water decreased slowly with time, which was caused by plant water  
481 extraction (Figure 7). The evidence of this was shown by the fairly constant isotopic  
482 compositions of the second layer soil water where soil water uptake by plants does not  
483 fractionate (Ehleringer and Dawson, 1992). At the same time, the depth distribution of root  
484 water uptake affects the predicted isotopic composition of transpiration, since deeper water  
485 tends to be isotopically lighter (Riley et al., 2002). It can be concluded that the water source  
486 of T depends on the distribution of the rooting system, highlighting the importance of  
487 accurate rooting depth characterization in land surface model simulation. Zhang et al. (2011)  
488 showed that the soil water fractionation can be observed in the layer as deep as 20-30 cm in a

489 crop field. In this study, the isotope components in the second layer (10-20 cm) were relative  
490 stable (Figure 7), this is likely due to different soil and rainfall conditions, which limits the  
491 depth of evaporation front.

492

#### 493 **4. CONCLUSION**

494 An isotope-enabled land surface model was forced for a period of one month with  
495 meteorological data from the ANSTO measurement facility near Sydney, Australia.

496 A sensitivity analysis was undertaken to test the impact of uncertainties in model  
497 parameterization on the simulation of the isotopic composition of various processes. It was  
498 demonstrated that isotopic compositions of the first and second layer (0-20 cm) soil water, E  
499 and T responded linearly to the isotopic compositions of precipitation input. In particular, the  
500 isotopic composition of E was approximately twice as sensitive to the isotopic composition of  
501 precipitation relative to T, which drew moisture from deeper in the soil column. Both T and E  
502 were equally sensitive to the isotopic composition of the initial soil water. Though the  
503 experiment run through both dry and wet periods, the dataset is relatively short and more  
504 diverse settings of meteorological conditions could enhance evaluation of the model  
505 performance.

506 The study showed that ISOLSM, when driven by high-resolution (10 min)  
507 meteorological measurements, was able to adequately reproduce observed surface heat  
508 fluxes. Better agreement in modeled LE and H was observed during the dry analysis period,  
509 while the sensible heat flux was poorly simulated when the top soil moisture layer was very  
510 wet. Four performance metrics (RMSE, I, bias and R) were adopted to investigate ISOLSM  
511 energy simulation, indicating that the model provided more accurate measures of LE and H  
512 during the dry period, whereas the accuracy of G was similar for both wet and dry periods.

513 The issue of model evaluation in wet or humid environments using eddy covariance data  
514 requires continued research effort, but highlights the importance of introducing multiple  
515 sources of observations to better constrain models. Using ISOLSM we showed that T was the  
516 dominant source in total ET (~70%) at this evergreen coastal site and both T and E showed  
517 strong diurnal variations. Different soil layers affected T and E dynamics, e.g., only first layer  
518 affected E while both first and second layers affected T.

519 One of the important findings from this work was related to the comparison of the *in-*  
520 *situ* isotopic water vapor measurements and the modeled isotope composition of ET. It was  
521 observed that due to the coastal location of the site and the inherent large moisture source, the  
522 local ET contribution to the atmospheric vapor was very small. As ISOLSM only simulates  
523 the local ET flux isotopic composition, it was not easy to fully utilize the *in-situ* isotope data  
524 for model evaluation. The results do show that utilizing an isotope-enabled land surface  
525 model allows for a clearer discrimination between different hydrological components and  
526 increased insight into hydrological processes. The isotopes provided a constraint to partition  
527 E and T and illustrated the different water sources for E and T. They also enabled the  
528 capacity to introduce new measures to assist in constraining model predictions (e.g., soil  
529 water isotopic compositions or rooting depth).

530

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536

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Table 1. Measured variable which are used in the model simulation at ANSTO (34.05°S, 150.98°E). The site was covered with evergreen forest vegetation with soil texture of sand, silt and clay: 48%, 28% and 24% respectively.

Names	Units	Measurement Frequency (min)	Data descriptions
Air temperature	K	10	Meteorological measurement
Wind speed	m/s	10	Meteorological measurement
Air pressure	Pa	10	Meteorological measurement
Incoming visible direct radiation	W/m <sup>2</sup>	10	Derived from shortwave incoming radiation measurement
Incoming visible diffuse radiation	W/m <sup>2</sup>	10	Derived from shortwave incoming radiation measurement
Incoming near-infrared direct radiation	W/m <sup>2</sup>	10	Derived from shortwave incoming radiation measurement
Incoming near-infrared diffuse radiation	W/m <sup>2</sup>	10	Derived from shortwave incoming radiation measurement
Incoming longwave solar radiation	W/m <sup>2</sup>	10	Derived from shortwave incoming and net solar radiation measurement
Specific humidity (H <sub>2</sub> <sup>16</sup> O)	kg/kg	10	Meteorological measurement
Specific humidity (H <sub>2</sub> <sup>18</sup> O)	kg/kg	10	Derived from specific humidity (H <sub>2</sub> <sup>16</sup> O) measurement
Specific humidity (HD <sup>16</sup> O)	kg/kg	10	Derived from specific humidity (H <sub>2</sub> <sup>16</sup> O) measurement
Latent heat	W/m <sup>2</sup>	30	Eddy covariance measurement
Sensible heat	W/m <sup>2</sup>	30	Eddy covariance measurement
Ground heat	W/m <sup>2</sup>	30	Soil heat flux plates
Water vapor concentration	%	10	FTIR measurement
Oxygen isotopic composition δ <sup>18</sup> O	‰	10	FTIR isotopic measurement
Hydrogen isotopic composition δD	‰	10	FTIR isotopic measurement

Table 2. The results of four performance measures RMSE, I, bias and  $R^2$  calculated for LE, H and G in a wet period (Jan 5-15, 2011) and a dry period (Jan 16-25, 2011). The observed energy fluxes were adjusted to achieve energy balance closure.

	RMSE ( $W/m^2$ )		I		bias ( $W/m^2$ )		$R^2$	
	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry
LE	88.94	58.06	0.82	0.93	66.67	28.15	0.69	0.81
H	107.35	70.16	0.65	0.82	-84.90	-52.00	0.43	0.71
G	21.85	23.31	0.91	0.92	3.11	7.04	0.82	0.86

Figure1

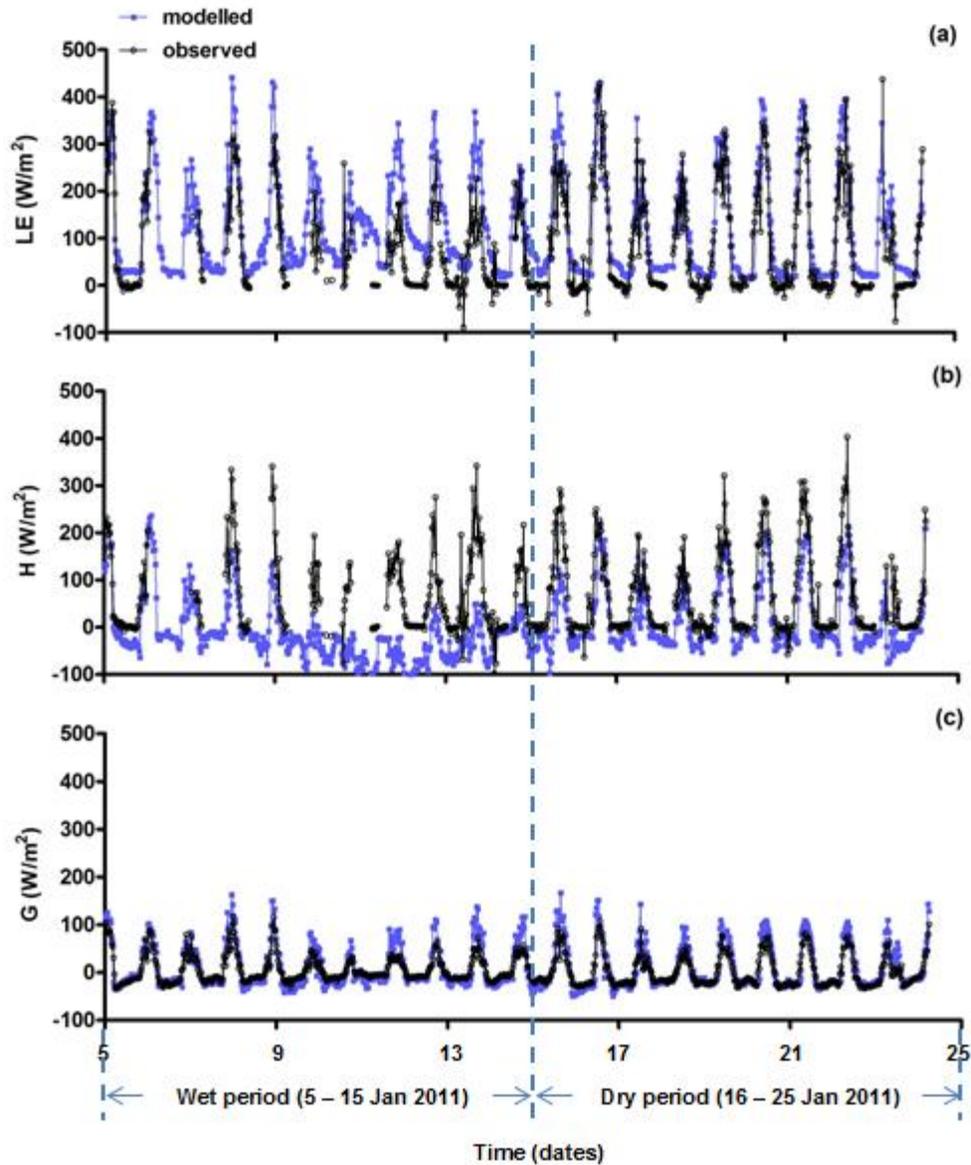


Figure 1. Half-hourly observed (black dotted line) and modelled (blue dotted line) energy fluxes (LE – top, H – middle and G – bottom) comparison for a wet period (5-15 Jan, 2011 – left) and a dry period (16-25 Jan, 2011 – right). The observed energy fluxes were adjusted to achieve energy balance closure.

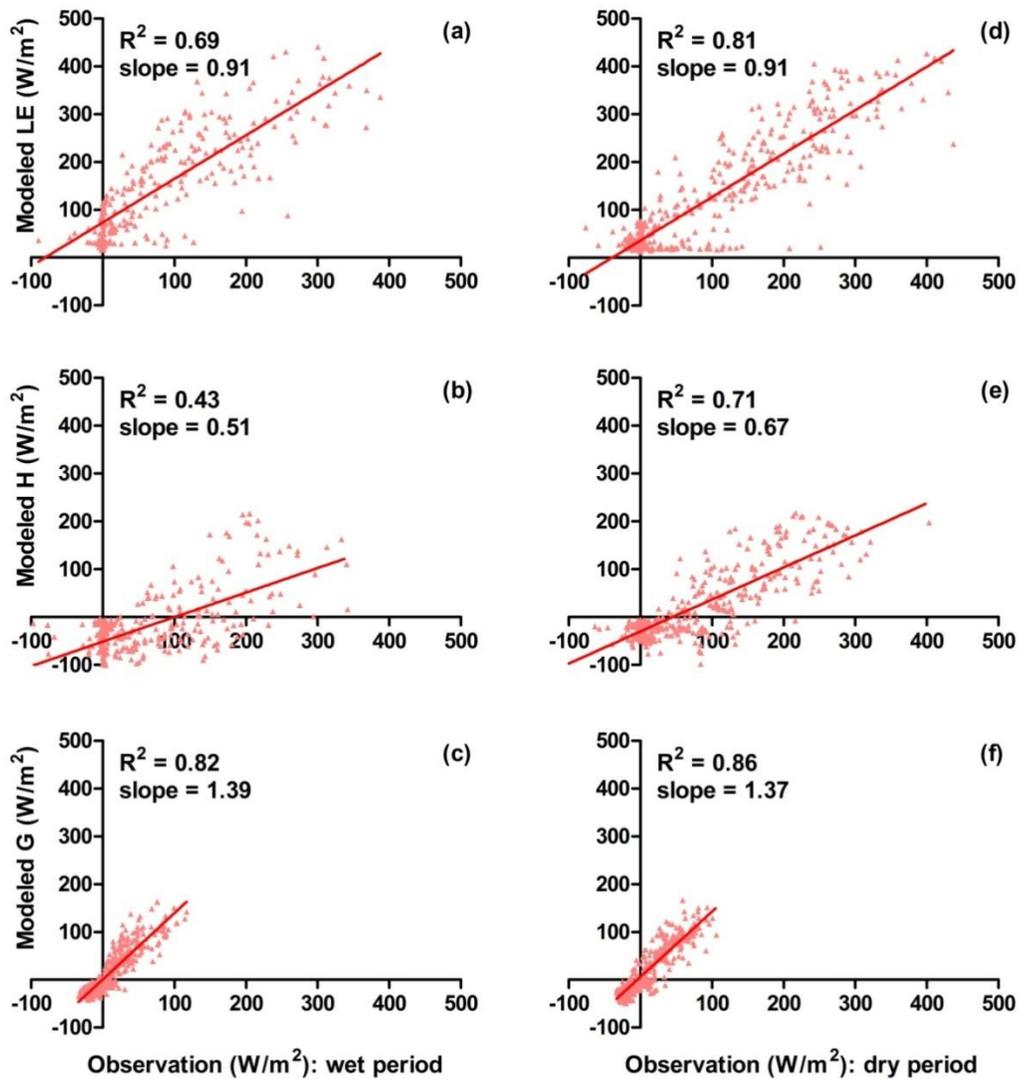


Figure 2. Half-hourly observed (x axis) vs. modelled (y axis) energy fluxes (LE – top, H – middle and G – bottom) for a wet period (Jan 5-15, 2011 – left) and a dry period (Jan 15-25, 2011 – right). The observed energy fluxes were adjusted to achieve energy balance closure.

Figure3

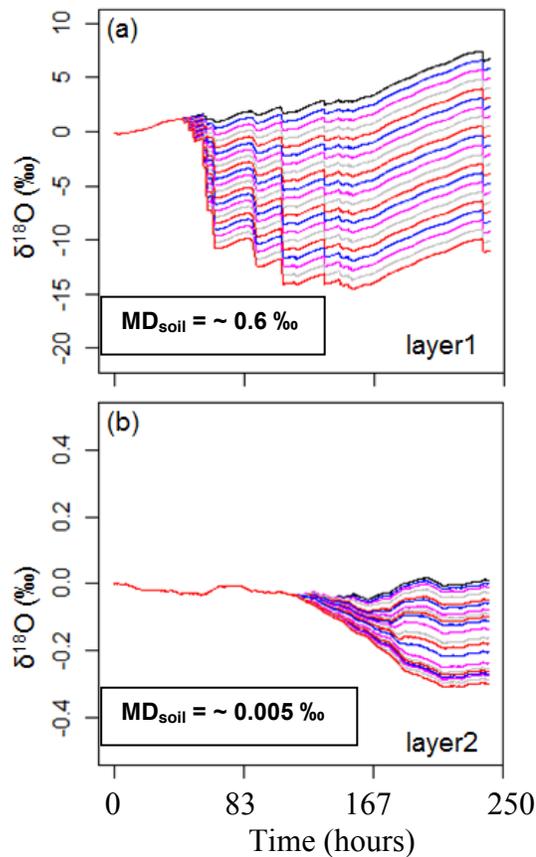


Figure 3. Simulated soil water  $\delta^{18}\text{O}$  (initial value 0 ‰) during wet period with input  $\delta^{18}\text{O}$  of precipitation varying from -20 ‰ to 0 ‰ (1‰ increment) for the top two soil layers. This is an analysis of the sensitivity of the ISOLSM model's soil water isotopic composition to rainfall isotopic composition for several rainfalls (total rainfall is ~45 mm starting at hour 50) over the course of 250 hours. There are 21 different simulated rainfall compositions values corresponding to the 21 lines on each graph. The layer1 (0-0.1 m deep, a) and layer2 (0.1-0.2 m deep, b) showed plotted lines (21 tests) being almost equally spaced. The difference between adjacent lines at each time step was calculated and then averaged to obtain mean difference ( $\text{MD}_{\text{soil}}$ ) for the entire testing period. The mean difference between modeled  $\delta^{18}\text{O}$  of soil water for every 1‰ increment of  $\delta^{18}\text{O}$  of input precipitation varied from -20 ‰ to 0 ‰ were calculated for soil layer1 ( $\text{MD}_{\text{soil}} = \sim 0.6 \text{ ‰}$ ) and layer2 ( $\text{MD}_{\text{soil}} = \sim 0.005 \text{ ‰}$ ).

Figure4

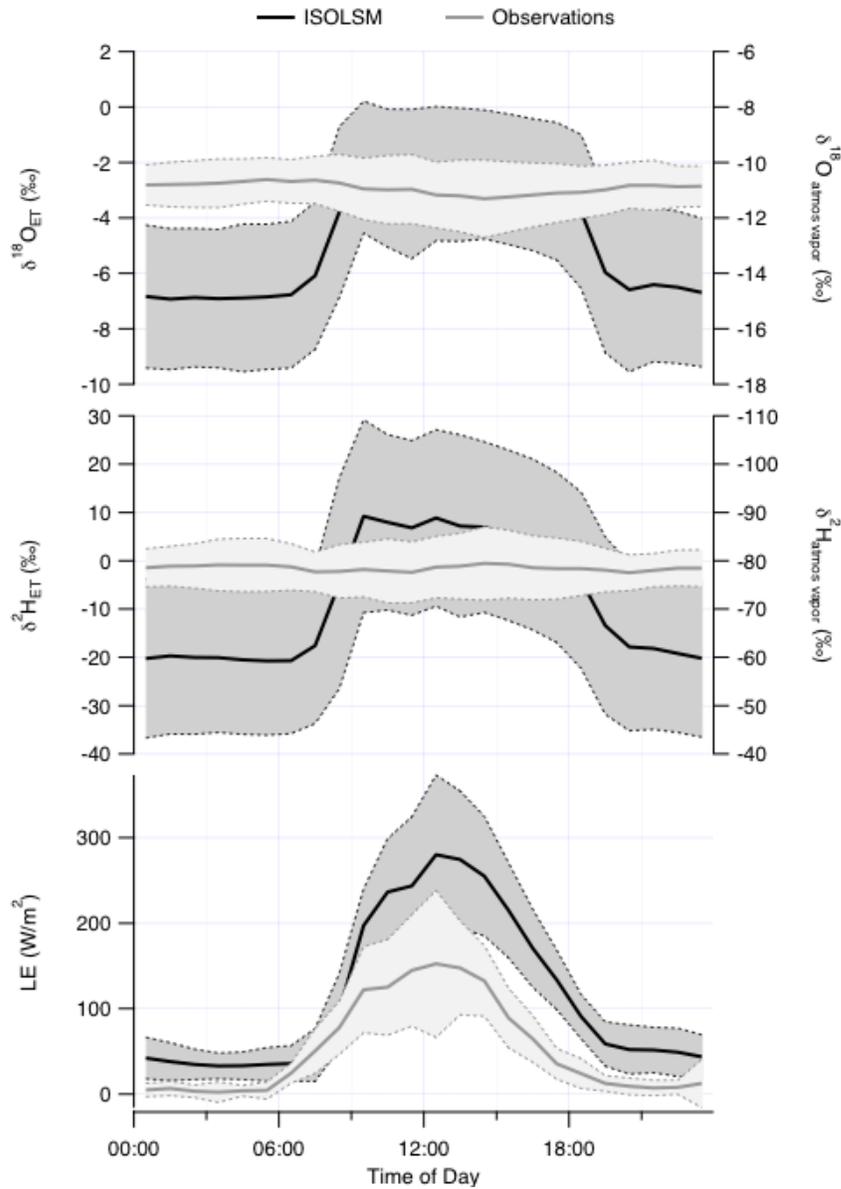


Figure 4. The *in-situ* measured isotopic compositions of atmospheric water vapor (gray line) against simulated isotopic composition of evapotranspiration (black line) as well as observed (gray line) and simulated (black line) latent heat flux. All the results are the mean composite values across the whole study period. The shaded areas are the standard deviations. The stable water vapor isotopic compositions of oxygen and hydrogen data were measured between December 22, 2010 and January 26, 2011, using a Fourier Transform Infrared spectrometer deployed at Lucas Heights, which sampled air through heated sampling lines from a height of 10 m. FTIR measurements were averaged to

present 10 minute values.

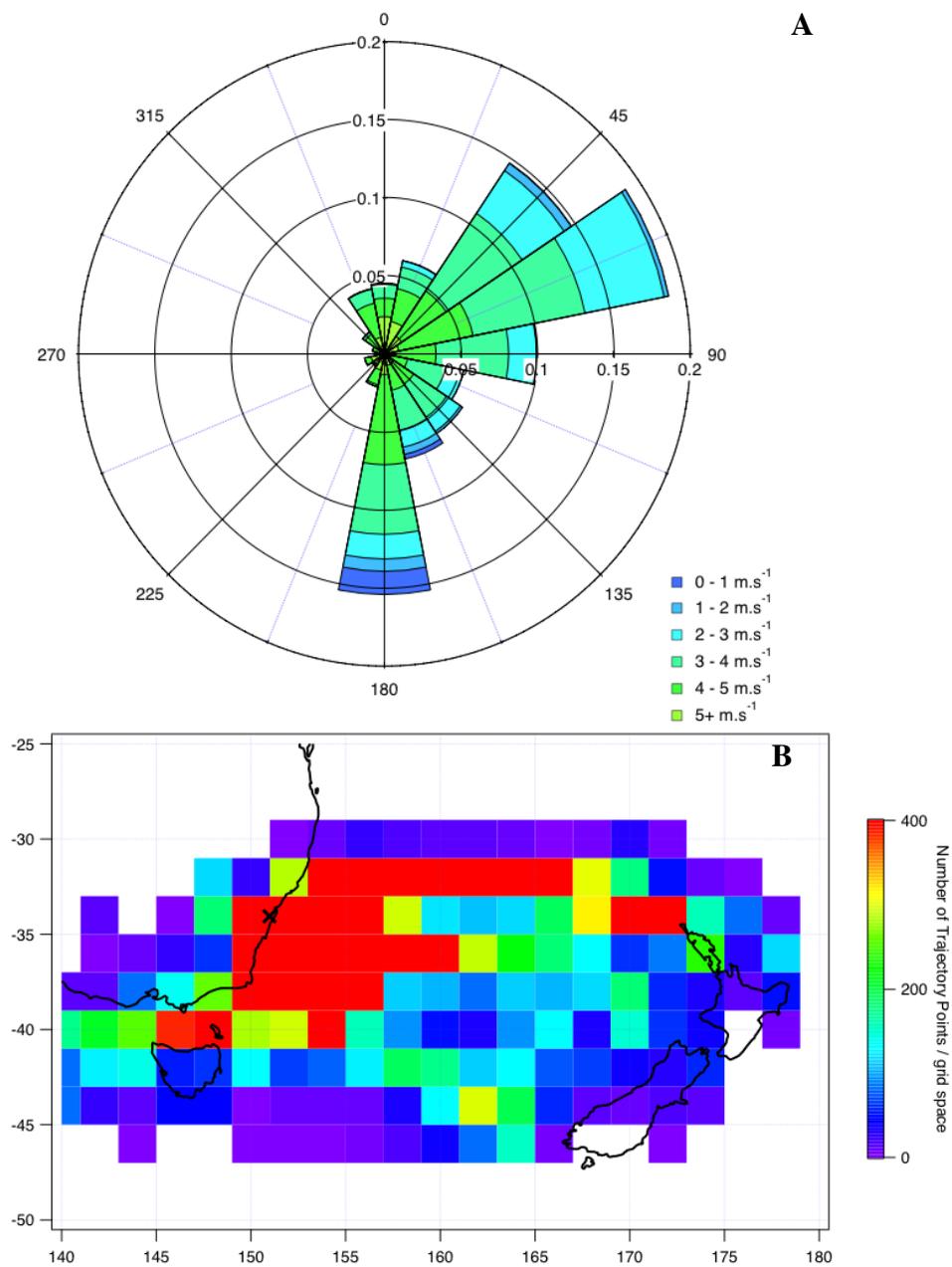


Figure 5: Wind rose of the wind observations from 10 m high (A), and hourly back trajectory footprint (B) for the whole observation period at the study site. Hourly back trajectories were calculated with the Hybrid Single Particle Lagrangian Integrated Trajectory Model (HYSPLIT v4.0).

Figure6

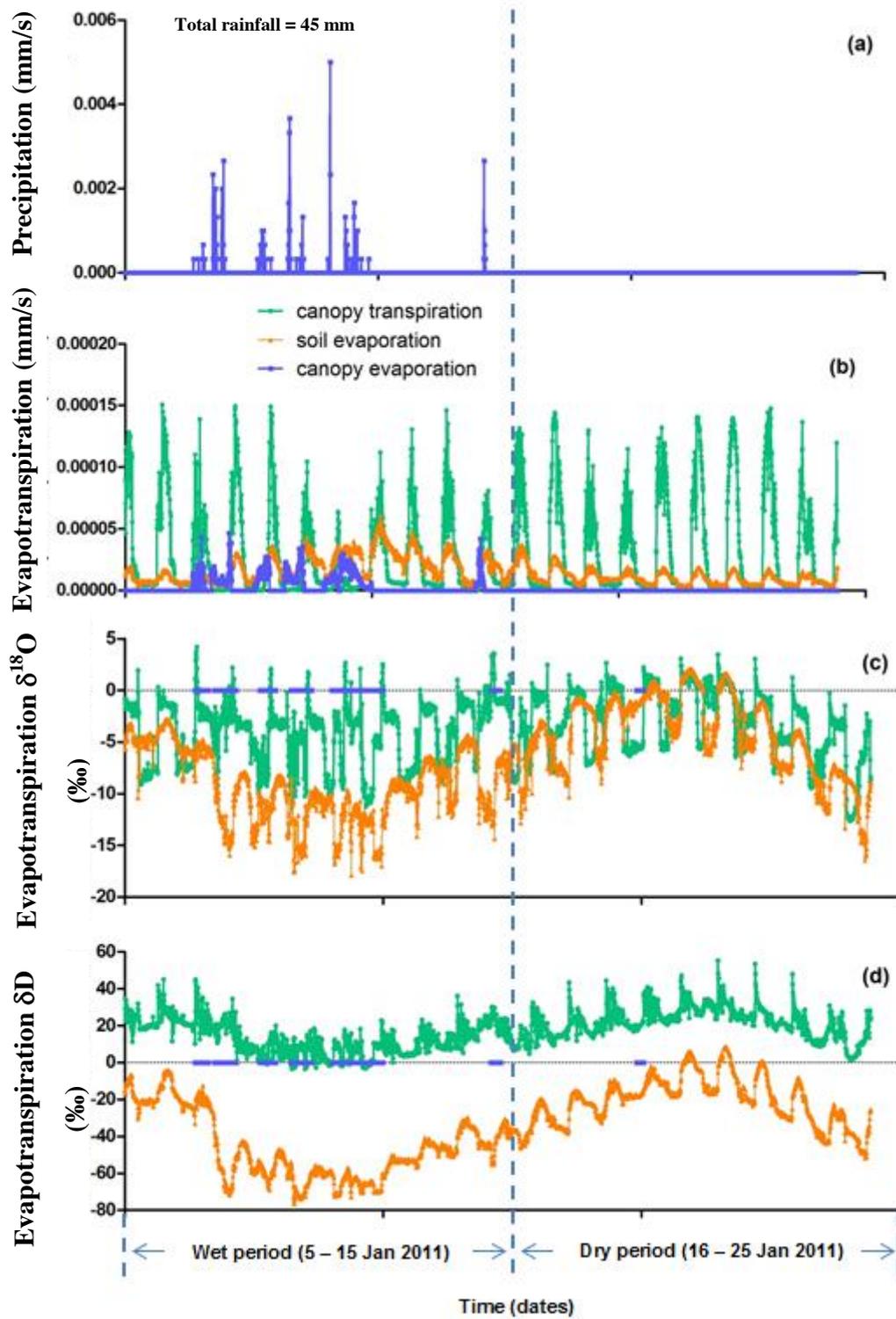


Figure 6. Half-hourly water budget model simulation (precipitation – (a, blue dotted line)

and evapotranspiration – including transpiration (green dotted line), soil evaporation (orange dotted line) and canopy evaporation (blue dotted line)) for H<sub>2</sub>O (b), δ<sup>18</sup>O (c) and δD (d).

Figure7

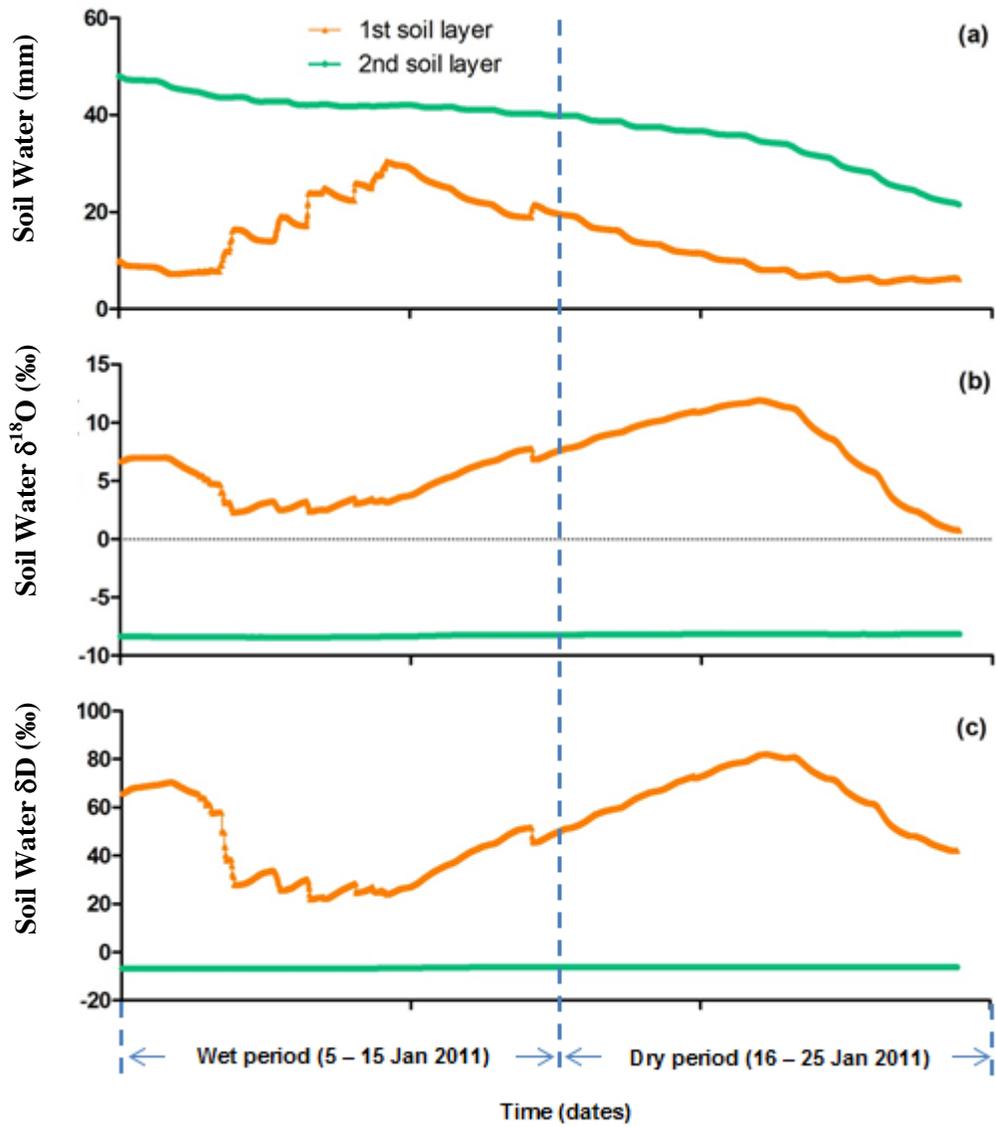


Figure 7. Half-hourly soil water simulation for  $\text{H}_2\text{O}$  (a),  $\delta^{18}\text{O}$  (b) and  $\delta\text{D}$  (c) for the top two soil layers. The assumed isotopic composition of precipitation and soil water are 0 ‰.