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# A Hybrid Bulk Algorithm to Predict Turbulent Fluxes over Dry and Wet Bare Soils --Manuscript Draft--

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#### A Hybrid Bulk Algorithm to Predict Turbulent **Fluxes over Dry and Wet Bare Soils** ANDREY A. GRACHEV<sup>a, b, \*</sup>, CHRISTOPHER W. FAIRALL<sup>a</sup>, BYRON W. BLOMQUIST<sup>a, b</sup>, HARINDRA J. S. FERNANDO<sup>c</sup>, LAURA S. LEO<sup>c, d</sup>, SEBASTIÁN F. OTÁROLA-BUSTOS<sup>c</sup>, JAMES M. WILCZAK<sup>a</sup>, KATHERINE L. MCCAFFREY<sup>a, b, \*</sup> <sup>a</sup> NOAA Physical Sciences Laboratory, Boulder, CO, USA <sup>b</sup> Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, CO, USA <sup>c</sup> Department of Civil & Environmental Engineering & Earth Sciences, Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN, USA <sup>d</sup> Department of Physics and Astronomy, Alma Mater Studiorum-University of Bologna, Bologna, Italv \*Current affiliation: Boundary Layer Research Team/Atmospheric Dynamics & Analytics Branch, DEVCOM Army Research Laboratory, WSMR, NM, USA \* Current affiliation: S & P Global Market Intelligence, Boulder, CO, USA Corresponding author: Andrey A. Grachev, Andrey.Grachev@colorado.edu Journal of Applied Meteorology and Climatology Manuscript submitted: October 11, 2020 Revised: October 25, 2021

43 ABSTRACT

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45 Measurements made in the Columbia River Basin (Oregon) in an area of irregular terrain during 46 the second Wind Forecast Improvement Project (WFIP 2) field campaign are used to develop an 47 optimized hybrid bulk algorithm to predict the surface turbulent fluxes from readily measured or modelled quantities over dry and wet bare or lightly vegetated soil surfaces. The hybrid 48 49 (synthetic) algorithm combines (i) an aerodynamic method for turbulent flow which is based on 50 the transfer coefficients (drag coefficient and Stanton number), roughness lengths, and Monin-51 Obukhov similarity and (ii) a modified Priestley-Taylor (P-T) algorithm with physically based 52 ecophysiological constraints which is essentially based on the surface energy budget (SEB) 53 equation. Soil heat flux in the latter case was estimated from measurements of soil temperature 54 and soil moisture. In the framework of the hybrid algorithm, bulk estimates of the momentum 55 flux and the sensible heat flux are derived from a traditional aerodynamic approach, whereas the 56 latent heat flux (or moisture flux) is evaluated from a modified P-T model. Direct measurements 57 of the surface fluxes (turbulent and radiative) and other ancillary atmospheric/soil parameters 58 made during WFIP 2 for different soil conditions (dry and wet) are used to optimize and tune the 59 hybrid bulk algorithm. The bulk flux estimates are validated against the measured eddy-60 covariance fluxes. We also discuss the SEB closure over dry and wet surfaces at various 61 timescales based on the modelled and measured fluxes. Although this bulk flux algorithm is optimized for the data collected during the WFIP 2, a hybrid approach can be used for similar 62 63 flux-tower sites and field campaigns.

64

## **1. Introduction**

67	Determination of momentum, heat, and mass exchange between the atmosphere and the
68	underlying surface is a central problem of atmospheric boundary-layer (ABL) research.
69	Understanding and proper parameterization of the surface turbulent fluxes (e.g., flux-profile
70	relationships) is of obvious relevance for the modelling of the coupled atmosphere-land/ocean
71	system, including climate modelling, weather forecasting, environmental impact studies, and
72	many other applications. It should be noted that with the exception of direct numerical
73	simulations the surface fluxes are always subgrid- scale processes that cannot be explicitly
74	resolved and must be parameterized, regardless of how high the resolution of a numerical model
75	is. At present, in almost all numerical models, from local and mesoscale to global models (i.e., in
76	weather prediction and climate models), turbulence fluxes are parametrized using Monin-
77	Obukhov similarity theory (MOST) or/and a bulk flux algorithm.
78	A direct application of the turbulent energy fluxes is the net surface energy budget (SEB).
79	An accurate determination of energy balance closure and all components of the SEB at the air-
80	surface interface are required in a wide variety of applications including atmosphere-land/snow
81	simulations and validation of the surface fluxes predicted by numerical models over
82	representative spatial and temporal scales.
83	Recently, progress has been made in our understanding of the turbulent mixing and
84	development of bulk schemes over, more or less, horizontally homogeneous surfaces such as the
85	open ocean (e.g., the COARE bulk flux algorithm by Fairall et al. 1996, 2003) and snow covered
86	sea ice (e.g., the SHEBA bulk turbulent flux algorithm by Andreas et al. 2010a, 2010b). Because
87	of the complexity of vegetated and bare (or lightly vegetated) surfaces, an equivalent progress in

development of simplified bulk algorithms over land is not as straightforward as in the case of
the over water or snow/ice, but appears feasible in this case. In this study, surface fluxes
(turbulent and radiative) and other ancillary atmospheric and soil data collected in the Columbia
River Gorge area near Wasco, Oregon, during 2016-2017 within the second Wind Forecast
Improvement Project (WFIP 2), are used to develop a hybrid bulk flux algorithm utilizing the
available WFIP 2 experimental data.

94 The novelty of the present study is to develop a hybrid or synthetic (in the sense of 95 "combination") bulk approach to predict the surface turbulent fluxes from tower-based 96 measurements. Traditional bulk flux schemes (e.g., the COARE and SHEBA algorithms) derive 97 all three turbulent fluxes (momentum, sensible, and latent heat) in the same way. The hybrid bulk 98 flux algorithm developed in this study derives the turbulent fluxes of momentum and sensible 99 heat from the traditional aerodynamic method for the turbulent flow (similar to the COARE and 100 SHEBA algorithms), whereas the latent heat flux is estimated from a method which is essentially 101 based on the conservation of energy principle (i.e., the surface energy balance at the surface-102 atmosphere interface). Although our bulk flux algorithm is based on the WFIP 2 data, the hybrid 103 approach developed here can be applied to similar tower-based measurements over land to 104 predict the turbulent fluxes.

105 The paper is organized as follows. The following section contains information about the 106 observation site, instrumentation and dataset collection. Section 3 provides a formal background 107 for measuring and modelling surface fluxes including the SEB closure problem and traditional 108 bulk flux approach. In Section 4, we develop and verify a hybrid bulk flux algorithm for 109 computing surface fluxes from readily measured or modelled during WFIP 2 bulk quantities. The 110 conclusions are summarized in Section 5. Some material presented in the current study, e.g.,

111	associated with the description of the observation site, instrumentation, and data (Section 2), is
112	partially repeated here from Grachev et al. (2020). Both studies use the same WFIP 2 dataset but
113	for different problems.
114	
115	2. Observation Site, Instrumentation, and Data
116	
117	This study analyzes and discusses the data collected during a 10-month long portion of
118	the second Wind Forecast Improvement Project (WFIP 2) field campaign (see Bianco et al.
119	2019; Olson et al. 2019; Shaw et al. 2019; Wilczak et al. 2019 for details). Grachev et al. (2020)
120	described the measurement site, instruments, various observations, data processing etc. in detail.
121	Here we provide some relevant information about the turbulent and profile measurements in the
122	near-surface atmosphere and soil layer during the WFIP 2 project.
123	The WFIP 2 field campaign took place in an area of irregular terrain along the Columbia
124	River Gorge in eastern Oregon and Washington states (Fig. 1). Here we use measurements of 30-
125	min averaged surface fluxes and basic meteorological/soil parameters from the Physics Site 1
126	tower (PS01) located near Wasco (Oregon). The PS01 study area encompasses relatively flat
127	plain (e.g. Fig. 2) and a ridge (e.g. Grachev et al. 2020, their Fig. 2) sited in irregular terrain of
128	moderate complexity. The ridge is aligned approximately in a W-E direction. The instruments at
129	the PS01 site (Figs. 1 and 2) were deployed in an area similar to a high-resolution model grid cell
130	for observing subgrid-scale turbulent processes (Shaw et al. 2019). According to Grachev et al.
131	(2020, their Fig. 3b), prevailing winds observed at PS01 site have a bimodal distribution with the

- 132 two dominant wind directions  $\approx 180^{\circ}$  apart (easterly and westerly winds). These predominant
- 133 winds generally blow parallel to the ridge and not frequent southerly wind directions are

134 generally associated with lights winds. Turbulent fluxes and other ancillary atmospheric data at 135 the PS01 site were measured continuously on a 10-m meteorological tower at 3 m and 10 m 136 levels (Fig. 2) from 24 June 2016 to 01 May 2017, Year Days (YD) 176-487 with respect to 137 January 1, 2016 UTC. Each level was instrumented with identical fast response three-axis sonic 138 anemometers sampling wind velocity and sonic temperature at 20 Hz (R.M. Young Model 139 81000) and Rotronics HC2S3 temperature and relative humidity probes (T/RH, sampling 140 frequency = 1 Hz). The HC2S3 probes were housed in ventilated radiation shields. A fast-141 response (20 Hz) infrared gas analyzer (LI-7500) was collocated at 3-m height with the lower 142 sonic anemometer. The mean wind speed and wind direction were derived from the sonic 143 anemometers using the ordinary planar-fit method rotation of the coordinate system proposed by 144 Wilczak et al. (2001). Several data-quality indicators based on objective and subjective methods 145 have been applied to the original flux data to remove spurious or low-quality records (e.g., 146 Bariteau et al. 2010; Grachev et al. 2011, 2015; Blomquist et al. 2014 and references therein). 147 Specifically, turbulent data have been edited for unfavorable relative wind direction for which 148 the tower was upwind of the sonic anemometers, non-stationarity, minimum or/and maximum 149 thresholds for the turbulent statistics, etc. In particular, sonic anemometer data based on the 150 planar-fit procedure were flagged as bad if the mean vertical velocity component differed by more than 0.2 m s<sup>-1</sup> from the plane. For example, after data-quality control screening, the number 151 152 of data-points for sensible heat  $H_S$  and latent heat  $H_L$  fluxes measured at the level 3m during the 153 entire WFIP 2 field campaign decreased to  $\approx 90.2\%$  and  $\approx 79.6\%$  of the original amount 154 respectively.

Measurements of soil temperature and moisture were made at five levels located
nominally at 5, 10, 20, 50, and 100 cm depths below the ground surface approximately 5 m from

157	the flux tower. Note that no direct measurements of surface soil heat flux with a heat flux plate
158	were performed at this site. The soils at the WFIP 2 Physics Site PS01 are primarily well-drained
159	silt (73%), with minor components of sand (14%), and clay (13%) and average 152 cm in depth
160	before reaching harder rock. In general, the underlying surface at the PS01 site can be described
161	as bare and/or short vegetation surface (cf. Cuxart and Boone 2020, their Fig. 1). The
162	downwelling and upwelling shortwave and infrared radiation was measured from two radiation
163	masts located near the flux tower by Eppley pyranometers and pyrgeometers respectively (Fig.
164	2). The 'slow'-response data used in this study (T/RH, solar radiation, soil temperature and
165	moisture) are based on 1 Hz raw measurements which were averaged over 1-min time intervals.
166	The time series of half-hour averaged surface fluxes and basic meteorological variables to
167	describe weather and soil conditions, surface fluxes, and other relevant variables as observed
168	during the entire WFIP 2 field campaign for the period 24 June 2016 to 01 May 2017 (YD 176-
169	487 with respect to January 1, 2016 UTC) can be found in Grachev et al. (2020, Figs. 3-6).
170	Similar to Grachev et al. (2020, Sect. 4.1), in this study we sort the data into dry and wet
171	categories (the soil moisture content below is the volumetric soil moisture):
172	(i) Dry bare (or lightly vegetated) soil surfaces, if the soil temperature at 5 cm depth is $> 1^{\circ}$ C
173	and the volumetric soil moisture at 5 cm depth is $\leq 0.07$ ;
174	(ii) Wet bare (or lightly vegetated) soil surfaces, if the soil temperature at 5 cm depth is $> 1^{\circ}$ C
175	and the volumetric soil moisture at 5 cm depth is $> 0.07$ .
176	According to our data, dry and wet surfaces for this location and for the considered time
177	intervals are generally associated with the volumetric soil moisture at 5 cm depth under 0.05 and
178	above 0.15 respectively (Grachev et al. 2020, Fig. 4b). Range between 0.05 and 0.15 can be
179	considered as a transition interval. However our data show that the surface soil moisture

180 increases rapidly during approximately two days around YD 291 with the onset of the rainy 181 season (Grachev et al. 2020, Fig. 4b-d). Thus, transition from the dry-soil case to the wet-soil 182 case has occurred within a fairly short period of time and, for this reason, the choice of any value 183 from the transition range as a threshold (e.g., 0.07) has little or no effect on the final results. 184 The original 10-month long in situ data often contain gaps (Grachev et al. 2020, Figs. 3-185 6). To calibrate and verify the bulk flux algorithm over different soil conditions, we use in this 186 study a 30-day long uninterrupted time series of relatively good data separately for dry and wet 187 soil conditions (WFIP 2 "golden files") described by Grachev et al. (2020, Sect. 4.4). Data 188 collected during year days 240–270 (27 August-26 September 2016) provide an illustrative 189 example of surface meteorology and surface fluxes observed at the WFIP 2 Physics site PS01 for 190 dry soils. Similarly the 30-day long time period from 25 March to 24 April 2017 (YD 450-480 191 with respect to 1 January 2016) was selected to analyze data over wet soil surfaces. 192 Figures 3-6 show continuous monthly (30-day long) records of the surface fluxes and 193 surface meteorology for dry and wet soils respectively. The data presented in Figs. 3-6 and some 194 other ancillary information for these time periods are used in this study to test the bulk algorithm. 195 Additionally, the time-series of the SEB components (the net radiation, the sum of the sensible 196 and latent heat fluxes, the SEB residual) over dry and wet soils for the same time periods as in 197 Figs. 3-6 in the current study can be found in Grachev et al. (2020, Figs. 10 and 11). Thereby, we 198 use a subset of the data analyzed in our previous study (Grachev et al. 2020), though of a higher 199 quality. 200 As expected, variations of the air temperature, topsoil temperature, and the turbulent 201 energy fluxes,  $H_S$  and  $H_L$ , have a pronounced diurnal cycle (Figs. 3-6). We note different

202 behavior of  $H_S$  and  $H_L$  for different soil conditions. According to Fig. 4a and Fig. 6a, values of

203 the half-hourly  $H_S$  at local noon are generally larger for drier than for wetter soils, whereas the 204 situation with  $H_L$  is obviously opposite. The turbulent flux of the latent heat shown in Fig. 4b is 205 small over dry soil surfaces indicating that evaporation is negligible for drier than for wetter soils 206 (cf. Fig. 6b). Furthermore, diurnal variations of  $H_L$  are much less evident in the case of dry soil 207 conditions (Fig. 4b). Note also that in general the soil moisture increases with increasing depth 208 for dry soils (Fig. 3d) and vice versa for wet soils (Fig. 5d). 209 Other details regarding the observation site, the instrumentation, and the data can be 210 found in Grachev et al. (2020). 211 212 3. Measuring and Modeling Surface Fluxes 213 The turbulent fluxes of momentum  $\tau$  (or magnitude of the wind stress), sensible heat  $H_S$ , 214 and latent heat  $H_L$  can be estimated by the eddy-correlation method according to 215  $\tau = \rho u_*^2$ 216 (1) $H_{\rm S} = c_n \rho \overline{w'\theta'} = -c_n \rho u_* \theta_*$ 217 (2)  $H_L = \mathcal{L}_e \rho \overline{w'q'} = -\mathcal{L}_e \rho u_* q_*$ 218 (3) 219 where  $\rho$  is the mean air density,  $\theta$  is the air potential temperature, q is the air specific humidity, 220  $c_p$  is the specific heat capacity of air at constant pressure,  $\mathcal{L}_e$  is the latent heat of evaporation of water,  $u_*^2 = \sqrt{(\overline{w'u'})^2 + (\overline{w'v'})^2}$  ( $u_*$  is the friction velocity),  $\theta_* = -\overline{w'\theta'}/u_*$  and  $q_* =$ 221  $-\overline{w'q'}/u_*$  are the temperature and the specific humidity scales respectively. Here w is the 222 223 vertical velocity component, the prime ['] denotes fluctuations about the mean value, and an 224 overbar is an averaging operator (half an hour in this study). Note that in Eq. (1),  $\tau$  is based on

the both longitudinal (or downstream),  $\tau_x = -\rho \overline{w'u'}$ , and the lateral (or crosswind),  $\tau_y = -\rho \overline{w'v'}$ , components of wind stress (see Grachev et al. 2011 for discussion).

228 a. SEB Closure

229

Knowledge of the surface energy fluxes (2) and (3) is considered fundamental to the surface energy budget (SEB). Typically, the SEB equation accounts for energy inputs and outputs at the infinitesimal interface between atmosphere and land and it is assumed that the energy budget must balance; that is, the SEB equation is a balance equation. Thus, the classical formulation of the SEB equation is:

235

$$H_S + H_L + G = R_{net} \tag{4}$$

where *G* is the soil heat flux,  $R_{net}$  is the net radiation defined as the balance between downwelling and upwelling SW and LW radiation:

$$238 R_{net} = SW_{down} - SW_{up} + LW_{down} - LW_{up} (5)$$

Note that unlike the momentum flux  $\tau$  (1), the turbulent energy fluxes  $H_S$  and  $H_L$  are 239 highly correlated with the net radiation  $R_{net}$  due to the SEB equation (e.g., Grachev et al. 2020, 240 241 Fig. 8), providing an objective approach for a land-surface model or numerical models of the 242 climate system to estimate missing terms (e.g.,  $H_S$  or  $H_L$ ) as the residual of the others based on 243 (4) which is traditionally considered to have to be closed (e.g., Cuxart et al. 2015 and references 244 therein). A similar approach is used in soil-vegetation-atmosphere transfer schemes where the 245 surface energy fluxes are estimated from thermal infra-red data (i.e. radiometric surface 246 temperature) and SEB, Eq. (4) (e.g., Priestley and Taylor 1972; Su 2002; Kustas et al. 1993,

247 2004; Yao et al. 2015 and references therein). In the next section, we develop a method of 248 estimating  $H_L$  on the basis of the surface energy balance.

In practice, the soil heat flux *G* in (4) can be measured at some reference depth *z* below the ground surface by a heat flux plate or estimated from soil temperature profile measurements using Fourier's Law of Heat Conduction (gradient method):

252 
$$G(z) = -\lambda \frac{\partial T_S}{\partial z}$$
(6)

~ ~

where  $\lambda$  is the thermal conductivity of the soil and  $\partial T_S / \partial z$  is the vertical temperature gradient of the soil temperature,  $T_S$ . Traditionally,  $\partial T_S / \partial z$  in the soil layer  $\Delta z$  is replaced by  $\Delta T_S / \Delta z$  and Eq. (6) reduces to  $G(z) \approx -\lambda \Delta T_S / \Delta z$ .

256 Surface energy balance closure (4) is a formulation of the conservation of energy 257 principle at the interface and Eq. (4) assumes an ideal case, when all the fluxes are measured at 258 the infinitesimal interface between the atmosphere and the soil and it is a statement of how the 259 net radiation (5) is balanced by turbulent sensible (2), latent (3), and soil (6) heat fluxes in the 260 absence of other energy sources and sinks. However, many studies reported that the surface 261 energy balance (4) is difficult to close at temporal scales less than several hours (e.g., Wilson et 262 al. 2002; Foken et al. 2006; Mauder et al. 2007, 2020; Cava et al. 2008; Foken 2008; Jacobs et al. 263 2008; Higgins 2012; Leuning et al. 2012; Stoy et al. 2013; Cuxart et al. 2015; Majozi et al. 2017; 264 Gao et al. 2017a; Grachev et al. 2020 and references therein). Direct measurements of energy 265 budget at these time scales (in particular, at half-hourly and hourly averaged time scales) showed 266 that in most cases the sum of the turbulent fluxes of sensible and latent heat plus the ground heat 267 flux systematically is lower than the net radiation by around 20-30% during daytime and 268 generally is higher than the net radiation at night.

Because the fluxes cannot be measured at the surface and the energy balance often cannot be closed based on experimental data, the SEB equation (4) is re-formulated for a control volume instead of at the interface of the two media (e.g., Foken et al. 2006; Mauder et al. 2020):

(7)

 $H_{S} + H_{L} + G + Res = R_{net}$ 

273 where *Res* is a residual term. Note, that Eq. (7) implies now a two-layer (atmosphere and soil) 274 column of finite thickness (e.g., Foken 2008, his Fig. 1) where the turbulent fluxes (1)-(3) and 275 the net radiation (5) are measured at the upper boundary plane whereas the soil flux is measured 276 at the lower boundary plane of the total layer respectively. In the general case, Res can be 277 partitioned as the sum of an additional transport (vertical and horizontal) term through all 278 boundary planes, a total storage term in the two-layer column (air and soil), and all other reasons 279 unaccounted in (4) which can be also responsible for the SEB imbalance. The storage term in 280 turn can be partitioned as a sum of storage of energy in the air column due to radiative and/or 281 sensible heat flux divergence (the air enthalpy change), ground heat storage above a near-surface 282 reference point, radiation consumed in photosynthesis (the photosynthesis flux), canopy heat 283 storage in biomass (the rate change in enthalpy of the vegetation), as well as all other storage 284 terms (e.g., Meyers and Hollinger 2004, Jacobs et al. 2008; Leuning et al. 2012, Masseroni et al. 285 2014).

A variety of factors (except of  $H_S$ ,  $H_L$ ,  $R_{net}$ , and G) may be responsible for the lack of SEB closure. For example, failure to close the energy balance may be associated with storage of energy in the air column due to radiative and/or sensible heat flux divergence (the air enthalpy change), the ground heat storage above a heat flux plate measurement level, the radiation consumed in photosynthesis (the photosynthesis flux), the canopy heat storage in biomass (the rate change in enthalpy of the vegetation), and other storage terms, e.g. the atmospheric moisture

292 change and the canopy dew water enthalpy change (e.g., Mauder et al. 2020). In addition, 293 another complexity of the SEB closure is associated with non-stationarity (diurnal variations), 294 even during a half-hour averaging period (e.g., Garratt 1992). The diurnal cycle of solar radiation 295 modulates a sinusoidal variation in the ground surface heat flux and diurnal thermal waves in the 296 top soil layer. The impact of the hysteresis effect in diurnal cycles and the effect of the wave 297 phase difference between different atmospheric and/or soil variables on the SEB closure are 298 discussed in number of studies (e.g., Gao et al. 2017a and references therein). It is generally 299 accepted that the underestimation of the sensible and latent heat fluxes is associated with large-300 scale non-turbulent transport mechanisms at low-frequencies such as boundary-layer scale eddies 301 under convective conditions, mesoscale and sub-mesoscale transport, secondary circulations etc. 302 (Foken 2008; Mauder et al. 2020). According to Grachev et al. (2020), extending the averaging 303 time consistently from half-hourly to daily, weekly, monthly, seasonal, and sub-annual 304 timescales (311-day averaging for the entire WFIP 2 field campaign) significantly reduces the 305 SEB imbalance on average. Increasing the averaging time to daily and longer time intervals 306 substantially reduces averaged ground heat flux and storage terms, because energy locally 307 entering the soil, air column, and vegetation in the morning and during the first half of the day is 308 released in the afternoon, evening, and night.

309

### 310 b. Traditional Bulk Turbulent Flux Algorithm

311

In almost all numerical weather prediction and climate models the turbulent fluxes of momentum  $\tau$ , sensible heat  $H_S$ , and latent heat  $H_L$ , Eqs. (1)-(3), are estimated using MOST or/and a bulk flux algorithm. In this study, we will use a bulk formulation, which is in part based on the COARE bulk flux algorithm derived for open ocean (Fairall et al. 1996, 2003), and the SHEBA bulk flux algorithm developed for sea ice conditions (Andreas et al. 2010a, 2010b). We will use observations from the WFIP 2 Physics Site PS01 to evaluate bulk representations of the turbulent and ground fluxes, including the turbulent surface stress,  $\tau$ , because  $u_*$  is required for surface layer similarity theory that forms the basis of bulk turbulent flux algorithms.

- The turbulent fluxes are parameterized by bulk aerodynamic relationships, which relate fluxes to mean properties of the flow through the height-dependent transfer coefficients:  $C_D$  (the drag coefficient),  $C_H$  (the Stanton number), and  $C_E$  (the Dalton number):
- 323  $\tau = C_D \rho S U , \qquad (8)$

$$H_S = C_H c_p \rho S \Delta \theta , \qquad (9)$$

 $H_L = C_E \mathcal{L}_e \rho S \Delta q , \qquad (10)$ 

Here  $\Delta \theta = (\theta_0 - \theta_a)$  and  $\Delta q = (q_0 - q_a)$ , where subscripts 'zero' and a for the potential 326 327 temperature  $\theta$  and the air specific humidity q denote their surface ('skin', z = 0) and atmospheric 328 reference height values respectively. It is often assumed that the water vapor and other scalars 329 (e.g. carbon dioxide and methane) are transported similarly to the temperature, i.e. with the same efficiency (the Lewis analogy) and, therefore,  $C_H = C_E$ . Note, that accurate estimation of the 330 331 transfer coefficients in (8)–(10) is a crucial problem of air-sea/land interaction. The transfer 332 coefficients depend on stratification (atmospheric stability) and roughness lengths (e.g., Fairall et 333 al. 1996, 2003). Scalar averaged wind speed S in (8)–(10) is defined and discussed in the 334 Appendix.

335

## 336 4. Hybrid Bulk Algorithm and Analysis of the WFIP 2 Data

338 Following the discussion in the Section 3 and in the Appendix, turbulent fluxes are 339 computed from (8) - (10) and (A4) via an iteration because the transfer coefficients depend on 340 the MOST stability parameter z/L which is computed from the fluxes (see Fairall et al. 1996, 341 2003). The forms of (8)–(10) apply well to reasonably statistically homogeneous surfaces where 342 an interfacial value of  $q_0$  can be unambiguously established - oceans, lakes, ice, snow covered 343 surfaces, or water-saturated soils where we can assume  $q_0$  is the water saturation value at temperature  $\theta_0$ . For dry and wet bare soils or simple ground-hugging plant canopies, Eq. (8) and 344 345 (9) still work but in general case (10) does not apply because the surface is not near saturation. 346 Kondo et al (1990) show that application of Eq. (10) for parameterization of evaporation from 347 bare soil surfaces requires coupling with a special model of molecular diffusion of water vapor in 348 the surface soil pore with the vapor being carried from the interior of the soil pore to the land 349 surface.

350 Various techniques to represent  $H_L$  over land surfaces have been reported in the literature 351 (see Garratt 1992; Foken 2017 for background). The most widely used model is the physically-352 based Penman-Monteith (hereinafter P-M) model (Penman 1948; Monteith 1965; De Bruin and 353 Holtslag 1982) which combines the SEB and aerodynamic transport equations, assuming that 354 surface meteorological observations are available. An alternative approach, the Priestley-Taylor 355 (hereinafter P-T) algorithm is relatively simple, and can be considered as a simplified P-M 356 method that avoids parameterizations of aerodynamic and surface resistance without decreasing the accuracy of the  $H_L$  estimates (Priestley and Taylor 1972). Both the P-M and P-T methods 357 358 have been shown to give relatively low biases, particularly in comparison with the relatively 359 poor accuracy of other methods (Fisher et al. 2008).

360	The SEB equation (4), which is assumed to be closed, is the starting point in the P-T
361	model. The Bowen-ratio method and the Clausius-Clapeyron equation are also used in the
362	derivation of the P-T relationship (e.g., Foken 2017). Although the original P-T method
363	(Priestley and Taylor 1972) was developed for saturated surfaces, it has been widely extended to
364	unsaturated surfaces. Different modified P-T models are based on parameters that relate the
365	saturated and unsaturated surfaces and parameterization of the atmospheric and resistance
366	variables ("constraint functions"). Further discussion regarding various modifications of the P-T
367	model can be found in De Bruin (1983), Fisher et al. (2008), Venturini et al. (2011), Yao et al.
368	(2013, 2014, 2015), and Hao et al. (2019) among others. The P-T model stands for its simplicity
369	and low data requirements (e.g., where ground observations of aerodynamic and surface
370	resistance is not available) and for this reason the P-T approach is widely used as a satellite-
371	based $H_L$ -algorithm and remote sensing technology that enables estimation of the terrestrial $H_L$ at
372	regional or global scales (e.g., Fisher et al. 2008; Li et al. 2009; Venturini et al. 2011; Yao et al.
373	2013, 2014, 2015). Further discussion, the state of the art, and perspectives on determining
374	evapotranspiration by various methods (including MOST, P-M and P-T approaches) can be
375	found in a review paper by Cuxart and Boone (2020).

In this study, we follow a modified P-T model by Yao et al. (2015) to estimate  $H_L$  over dry and wet bare soils during the WFIP 2 field campaign. The approach by Yao et al. (2015) combines the P-T method which avoids the uncertainty associated with the Dalton transfer coefficient and an effective surface relative humidity in (10) with physically based ecophysiological constraints. According to a modified P-T model by Yao et al. (2015), the latent heat flux  $H_L$  can be expressed as:

382 
$$H_L = \alpha \frac{\Delta_s}{\Delta_s + \gamma} f(e) (R_{net} - G)$$
(11)

383 where  $\Delta_s$  is the temperature derivative from the saturated vapor pressure relationship (see 384 Priestley and Taylor 1972 for detail),  $\gamma$  the psychrometric constant, f(e) the sum of the weighted 385 ecophysiological constraints, and  $\alpha$  the P-T parameter. According to Priestley and Taylor (1972), 386 the empirical parameter  $\alpha$  in (11) equal to 1.26 on average for saturated surfaces. In general, the 387 P-T parameter  $\alpha$  varies with soil moisture, the canopy resistance, thermal stratification, etc. and 388 has a diurnal cycle (e.g., De Bruin 1983; Lhomme 1997; Pereira 2004; Cristea et al. 2013; 389 Assouline et al. 2016; Cuxart and Boone 2020). In particular, the P-T parameter  $\alpha$  increases as 390 the surface resistance to the evapotranspiration decreases; i.e.,  $\alpha$  increases with increasing the 391 soil moisture (Cristea et al. 2013) and, according to De Bruin (1983),  $\alpha > 1$  for well-watered 392 surfaces and  $\alpha < 1$  under dry conditions. 393 The value of f(e) in (11) varies from 0 to 1. According to Yao et al. (2015, Eq. 11), the 394 ecophysiological constraint function f(e) in (11) can be expressed as  $f(e) = k_0 + k_1\theta_a + k_2RH^{VPD} + (k_3NDVI - k_4)VPD$ 395 (12)396 where VPD is the air vapor pressure deficit  $e_{sat}(\theta) - e$ , RH the relative humidity (0 to 1), and NDVI the normalized difference vegetation index. The  $k_i$  (i = 0, ..., 4) are empirical coefficients 397 398 given in Table 1 of Yao et al. (2015) for nine different surface types. We have chosen a type 399 'GRA' (Yao et al. 2015, their Table 1), which includes grassland and barren or sparsely vegetated 400 soil (soil at the PS01 tower site is essentially a plowed fallow field with little vegetation). 401 In order to calculate  $H_L$  from a P-T type model, the soil heat flux G in (11) needs to be 402 estimated. As mentioned earlier, we do not have direct measurements of the soil heat flux G at 403 the WFIP 2 Physics Site PS01. There are numerous approaches to compute the soil heat flux, that 404 use different input data from in situ measurements (e.g., see Liebethal et al. 2005; Liebethal and 405 Foken 2007; Gao et al. 2017b). Different methods for evaluating G can use various in situ

406 measurements such as soil temperature, soil moisture, net radiation, etc. Furthermore, some 407 parameterization approaches can be suitable for different times of the day. Here, we use 408 measurements of soil temperature,  $T_S(z)$ , and soil moisture,  $Q_S(z)$ , to estimate *G* in (11) based 409 on (6). Eq. (6) can be now integrated for the interface down to some reference depth  $\Delta z$ . Near the 410 surface we can linearly approximate G(z), so

411 
$$\int_{0}^{\Delta z} \left( G + z \frac{\partial G}{\partial z} \right) dz = G \Delta z + \frac{1}{2} \frac{\partial G}{\partial z} \Delta z^{2} = \lambda [\theta_{0} - T_{S}(\Delta z)]$$
(13)

412 In this notation G in (13) is the value at the interface z = 0 where also  $T_S(0) = \theta_0$  (cf. Eq. 8).

413 The gradient term in (13) is estimated from the temporal change of the soil temperature

414 
$$\rho_S c_{pS} \frac{\partial T_S}{\partial t} = -\frac{\partial G}{\partial z}$$
(14)

415 where  $\rho_S$  is the soil density and  $c_{pS}$  is the soil specific heat. Thus, *G* can be estimated as the sum 416 of a gradient and storage term (Garratt 1992)

417 
$$G = \frac{\lambda}{\Delta z} [\theta_0 - T_s(\Delta z)] + \frac{1}{2} \rho_s c_{ps} \frac{\partial T_s}{\partial t} \Delta z$$
(15)

The system of the hybrid bulk flux computations is summarized in Table 1. Execution of these requires specification of certain coefficients which we have determined by tuning to agree with direct measurements at the PS01 site. Some other properties, such as  $\Delta_s$  and  $\gamma$  in Eq. (11), or atmospheric stability functions, are considered universal and we take them from the literature. For the turbulent fluxes, we need to determine the transfer coefficients  $C_H$  and  $C_D$ . Following the discussion in the Appendix, we can estimate the 10-m neutral coefficients directly via

424 
$$C_{X10n} = \frac{\overline{w'x'}}{U_{10n}\Delta X_{10n}G_f}$$
(16)

425 where x = u,  $\theta$ , or q, X = U,  $\theta$ , or q, and  $\Delta X = X_0 - X_a$  is the difference between the surface 426 value (zero for wind speed *U*) and the value at reference height *z* in the atmosphere,  $G_f$  is the gustiness factor (see the Appendix). Application of (16) is problematic when  $U_{10n}$  and/or  $\Delta X_{10n}$ are small. We can set minimum thresholds  $U_{th}$  and  $\Delta X_{th}$  for  $U_{10n}$  and  $\Delta X_{10n}$  respectively and average (16) for a subset of the data restricted to conditions where  $U_{10n} > U_{th}$  and  $|\Delta X_{10n}| >$  $\Delta X_{th}$ . A variation on this approach is to do a linear regression of the form

431 
$$\frac{\overline{w'x'}}{U_{10n}G_f} = a_x + b_x \Delta X_{10n} \tag{17}$$

432 so that  $C_{X10n} = b_x$ . This has advantages for the heat flux because we do not have to restrict 433  $\Delta \theta_{10n}$  and the offset coefficient  $a_x$  in (17) gives an indication of relative bias between  $\theta_0$  and 434  $\theta_a$ . If there is no bias, the regression should pass through the origin; a temperature bias would be indicated as  $\delta X = -a_x/b_x$ . An example of half-hourly averaged covariance sensible heat flux 435 normalized by  $c_p \rho U_{10n} G_f$  versus 10-m neutral surface-air temperature difference for the 436 437 uninterrupted 30-day time series ("golden files" periods) is shown in Fig. 7 separately for dry 438 soils (upper panel) and for wet soils (lower panel). In this case we examined fits where we have ignored observations with low wind speed (thresholds of  $U_{th} = 1 \text{ ms}^{-1}$  and  $4 \text{ ms}^{-1}$  are used). 439 440 These thresholds were selected based on a visual analysis of the data scatter in Fig. 7 and similar plots. The obvious outliers occur for winds less than 4 ms<sup>-1</sup> but the fits yield about the same 441 value for the Stanton number  $C_{H10n}$ , about  $2.20 \cdot 10^{-3}$  using (16) and  $2.15 \cdot 10^{-3}$  using (17) for 442 443 dry soils (the uninterrupted 30-day time series, YD 240-270, 27 August-26 September 2016; see 444 Fig. 3 and Fig. 4). For wet soils (the uninterrupted 30-day time series, YD 450–480, 27 25 March-24 April 2017; see Fig. 5 and Fig. 6), the corresponding values of  $C_{H10n}$  are 2.30  $\cdot$  10<sup>-3</sup> 445 using (16) and  $2.39 \cdot 10^{-3}$  using (17). Similarly, results for the drag coefficient  $C_{D10n}$  are 2.76 · 446  $10^{-3}$  (16) and  $2.29 \cdot 10^{-3}$  (17) for dry soil "golden files" (YD 240–270) and  $3.63 \cdot 10^{-3}$ (16) and 447  $3.21 \cdot 10^{-3}$  (17) for wet soil "golden files" (YD 450–480) for the thresholds of  $U_{th} = 1 \text{ ms}^{-1}$  and 448

449 4 ms<sup>-1</sup> (plots for  $C_{D10n}$  similar to Fig. 7 are not shown here). Note that the number of data-points 450 for the sensible heat measured during the dry soil "golden files" period (Fig. 7a) decreased to  $\approx$ 451 97% of the original amount for wind speed greater than 1 ms<sup>-1</sup> and  $\approx$  59% of the original amount 452 for wind speed greater than 4 ms<sup>-1</sup> respectively. Similar values for the wet soil "golden files" 453 period (Fig. 7b) were  $\approx$  94% and  $\approx$  48% respectively.

454 A similar approach can be used to determine the ground flux; for Eq. (15) we do a linear 455 regression of the form

456 
$$G_{res} - \frac{1}{2}\rho_S c_{pS} \frac{\partial T_S}{\partial t} \Delta z = a_g + b_g [\theta_0 - T_S(\Delta z)]$$
(18)

457 so that  $\lambda/\Delta z = b_g$ . Because we do not have direct measurements of *G*, we have substituted the 458 residual from an assumed energy balance

 $G_{res} = R_{net} - H_S - H_L \tag{19}$ 

460 Thus, the residual term *Res* (all storage and transport contributions as well as other unspecified

461 processes) in Eq. (7) is attributed in our model to the ground heat flux, i.e., by  $G_{res} = G + Res$ .

462 Based on this assumption, we apply a linear fit in Eq. (18) to calibrated the model. Note that

463 Mauder et al. (2020, Section 4) recently surveyed different methods when *Res* is attributed to  $H_S$ 

464 or  $H_L$  in order to to close energy balance.

An example for the dry soil "golden files" period (YD 240–270) and the wet soil "golden files" period (YD 450–480) is shown in Fig. 8. Here we have plotted the individual half-hourly values (Fig. 8) and, to reduce the noise, values from the mean diurnal cycle (Fig. 9). The fit yields a value of  $\lambda/\Delta z = 2.859$  Wm<sup>-2</sup>K<sup>-1</sup> and 7.034 Wm<sup>-2</sup>K<sup>-1</sup> for dry and wet soils respectively. We have done these fits for 15-day increments throughout the entire experimental period (311day dataset from 24 June 2016 to 01 May 2017, YD 176–487) and found that the thermal 471 conductivity of the soil,  $\lambda$ , varies considerably but with a strong correlation to soil moisture (see 472 discussion in Appendix 4 of Garratt 1992). This correlation is illustrated in Fig. 10. Thus, based 473 on the data presented in Fig. 10 for the entire field campaign, we estimate  $\lambda$  via 474  $\lambda = 0.180 + 1.09Q_{S5}$ (20)where  $Q_{S5}$  is the soil moisture measured at 5 cm depth. Of course, by tuning the coefficients to 475 the residual flux, we are forcing our parameterization to, on average, produce a reasonable total 476 477 energy balance. 478 We also examined the use of (11) and (12) to estimate the latent heat flux  $H_L$ . We chose 479 coefficients appropriate for bare soil from Yao et al (2015). However, we found that a constant 480 value for the P-T coefficient  $\alpha$  gave poor results. So we adjusted  $\alpha$  in (11) to give a reasonable 481 estimate of the mean flux and, as with the soil conductivity, we fit the values to soil moisture:  $\alpha = 0.4 + 50_{ss}$ 482 (21)483 This is in good agreement with the values reported in literature for dry and well-watered surfaces 484 (e.g., De Bruin 1983; Cristea et al. 2013; Assouline et al. 2016). Note, however, that Eq. (21) for 485 the P-T parameter derived from the WFIP 2 data is not a universal formula. 486 An example comparing direct covariance and bulk estimates of the sensible and latent 487 heat fluxes for the dry and wet soil "golden files" is shown in Fig. 11. According to our half-488 hourly averaged data for the sensible heat flux  $H_S$ , the linear regression forced through the origin is y = 1.02x with the correlation coefficient  $R^2 = 0.99$  in the case of the dry soil "golden files" 489 (Fig. 11a) and the regression is y = 0.97x with  $R^2 = 0.98$  in the case of the wet soil "golden" 490 files" (Fig. 11b) respectively. Thus, on average, the scatter plots for  $H_S$  (Fig. 11a and Fig. 11b) 491 492 show a fairly good agreement between direct covariance and bulk estimates. The scatter in the 493 sensible heat flux is about what we expect for covariance sampling error over half-hour averages

494	(at least possible biases associated with the bulk flux algorithm are within the accuracy of the
495	field turbulence data of $\approx$ 20-30%, see Yaglom, 1974). The scatter and bias between bulk and
496	direct half-hour values of latent heat flux for the dry period (Fig. 11c) is considerably greater
497	than that obtained for sensible heat flux but comparable to that for $H_S$ for the wet period (Fig.
498	11d). According to our data, the linear regression forced through the origin is $y = 0.57x$ with the
499	correlation coefficient $R^2 = 0.56$ in the case of the dry soil "golden files" (Fig. 11c) and the
500	regression is $y = 0.93x$ with $R^2 = 0.88$ in the case of the wet soil "golden files" (Fig. 11d)
501	respectively. The scatter plots of the measured turbulent fluxes versus their bulk counterparts
502	(Fig. 11) can be considered as a validation test for our hybrid bulk flux algorithm.
503	One further point to consider is the nature of tuning coefficients in the context of
504	imperfect observations. If we examine (9) we see one primary coefficient $C_{H10n}$ and three
505	observational variables S, $\theta_0$ , and $\theta_a$ . In principle, we could tune the transfer coefficient to give
506	the correct observed mean flux for some period. Alternatively, we could look for inconsistencies
507	in the observables and perhaps apply a correction. It is clear that $\theta_0$ is subject to significant error,
508	on the order of 1°C, because it is computed from upward and downward radiative fluxes which
509	are each uncertain by roughly 5 Wm <sup>-2</sup> (e.g., see specifications for Eppley PIR pyrgeometer).
510	Also, note that both G and $LW_{up}$ contain $\theta_0$ , so adjusting $\theta_0$ will affect their mean values.
511	Another factor is that for time periods of a few weeks, the variance of each of the fluxes is
512	dominated by the diurnal cycle. A summary of flux statistics (monthly mean and standard
513	deviation) for the dry and wet soil "golden files" periods is given in Tables 2 and 3 respectively.
514	Values in Tables 2 and 3 are based on the data presented in Fig. 11. So, if we take the mean
515	diurnal cycle of one of the fluxes (e.g., Fig. 9), we can diagnose the relevant errors in transfer
516	coefficients or conductivity versus biases in the observed temperatures. The strength of the

517 diurnal cycle is principally proportional to  $C_{H10n}$  or  $\lambda$ . If the difference in the day-night 518 excursions of the bulk fluxes matches the observed fluxes, then the coefficients are about right. Offsets in the mean diurnal cycles can be reduced by 'correcting'  $\theta_0$ ,  $T_S$ , or  $\theta_a$ . For sensible heat 519 520 the slope from (17) yields the transfer coefficient that will match the diurnal cycle and the 521 intercept indicates if there is a mismatch between  $\theta_0$  and  $\theta_a$ . The small intercept bias in Fig. 7 gives an indication of relatively good correlation between the sensible heat flux  $H_S$  and  $\Delta \theta_{10n}$ 522 under the assumption that  $\theta_0$  and  $\theta_a$  were accurately measured. Both Figs. 7 and 8 indicate 523 524 reasonable compatibility of  $\theta_0$  and  $T_{S5}$ . Although in general, the bulk flux estimates provide 525 reasonable renditions of the mean and standard deviation of the fluxes and the mean diurnal 526 cycles (Fig. 12), the bulk estimates of the latent heat flux are somewhat higher than the measured 527 ones during the daytime for dry soils (Fig. 12a). The sum of the three bulk fluxes yields a 528 reasonable balance of the net radiation at half-hour time scales (Fig. 13). According to Fig. 13, 529 the linear regression forced through the origin for the half-hourly data is y = 1.10x for the dry soil "golden files" and y = 0.98x for the wet soil "golden files". 530 531 As mentioned earlier, direct measurements of the soil heat flux G with a heat flux plate

532 were not available during the field campaign WFIP 2. However, we use model estimates of G 533 from the bulk flux algorithm described in this section to make estimates of the SEB closure (4). 534 Figure 14 shows the net surface energy balance based on the measured sensible and latent heat 535 fluxes  $H_S + H_L$  and bulk estimates of the ground heat flux  $G_b$  versus the net solar radiation  $R_{net}$ . Two upper panels (a, b) show incomplete energy balance equation,  $H_S + H_L$  vs.  $R_{net}$ , whereas 536 537 two lower panels (c, d) are based on Eq. (4),  $H_S + H_L + G_b$  vs.  $R_{net}$ . Plots in the left panels (a, c)538 represent the dry soil "golden files" (YD 240-270, 27 August-26 September 2016) and the right 539 panels (b, d) represent the wet soil "golden files" period (YD 450–480, 25 March-24 April 2017).

540	According to the data presented in Fig. 14, the SEB imbalance in the case of the incomplete
541	energy balance equation, that is; $H_S + H_L$ vs. $R_{net}$ , is about 20% for dry soils (Fig. 14a), and is
542	about 27% for wet soils (Fig. 14b) for half-hourly averaged fluxes. However, including the bulk
543	estimates of the ground heat flux $G_b$ in the SEB closure equation, that is; $H_S + H_L + G_b$ vs. $R_{net}$ ,
544	substantially reduces the SEB imbalance for each specific soil condition, (to about 5%, Fig. 14c,
545	and 3%, Fig. 14d, respectively). The SEB imbalance is also reduced for 30-day averaged data
546	(cf. Figs. 14a, 14b and Figs. 14c, 14d respectively). Note that plots of monthly means in Grachev
547	et al. (2020, Fig. 13) (triangular symbols for dry and wet soils) and in Fig. 14 (blue and pink six-
548	pointed star symbols) are based on the data presented in Tables 2 and 3.
549	Although the entire 311-day experimental period (YD 176-487) is used for regression fit
550	of the soil thermal conductivity soil in Fig. 10, the model is calibrated based on the data collected
551	during two 30-day "golden files" time periods separately for dry (YD 240-270) and wet (YD
552	450-480) soils (Figs. 3-6). In the same time, the "golden files" periods are used for model
553	verification (Fig. 11-14) what may not look quite correct. Therefore, for the independent model
554	verification we tested our model beyond the calibration periods (the "golden files" periods). We
555	have selected two additional 15-day test periods for dry (YD 270-285) and wet (YD 435-450)
556	soil conditions and then apply the model without further tuning. The choice of is these time
557	intervals associated with the availability of uninterrupted time series of relatively good data (see
558	Grashev et al. 2020, Figs. 4–6). The results are shown in Figs. 15 and 16 and, as expected, they
559	did not change significantly as compared to the calibration "golden files" periods (cf. linear
560	regressions and correlation coefficients for pairs Fig. 15 – Fig. 11 and Fig. 16 – Fig. 13).
561	

## **5. Summary and Discussion**

564	While progress has been made in studying and in parameterizations turbulent fluxes of
565	momentum, heat, and water vapor over horizontally homogeneous surfaces such as open ocean
566	(Fairall et al. 1996, 2003) and sea ice or snow covered surfaces (e.g., Andreas et al. 2010a,
567	2010b), an equivalent level of progress in the development of simple bulk algorithms over land is
568	not practical because of the complexity of the surface. Here we examine a land case that is just
569	one step more complex than a water surface – relatively flat land with low vegetation. The
570	parametrization of the turbulent fluxes for terrestrial sites and their representation in numerical
571	models is a challenging problem because of the spatial complexity of the underlying surface
572	especially in the case of heterogeneous or patched terrain (e.g., when bare and vegetated surfaces
573	coexist) or for non-saturated conditions, which are common in arid and semi-arid climates, and
574	in complex terrain (e.g. Bou-Zeid et al. 2020; Cuxart and Boone 2020). Myriad different types of
575	climates, soils, and vegetation add extra complexity in the problem. Another issue of the flux
576	estimates from routine meteorological measurements over land is associated with the availability
577	of the relevant model input parameters and their related uncertainties. This implies a need to use
578	non-traditional synthetic methods and to work in an interdisciplinary framework.
579	Using the data from the second Wind Forecast Improvement Project (WFIP 2) field
580	campaign collected in the Columbia River Gorge area of irregular terrain near Wasco, Oregon,
581	during 2016-2017, we have developed and tested an optimized hybrid bulk flux algorithm for
582	predicting the turbulent surface fluxes of momentum, sensible, and latent heat (1)-(3) over dry
583	and wet bare or lightly vegetated soil surfaces. The bulk flux algorithm combines (i) the
584	traditional COARE bulk flux algorithm (Fairall et al. 1996, 2003) adopted for over-land
585	situations for estimation of the turbulent fluxes of momentum $\tau$ and the sensible heat $H_S$ (Section

586	3 and as described in the Appendix), and (ii) a modified Priestley-Taylor (P-T) model (11) with
587	physically based ecophysiological constraints (12) by Yao et al. (2015) to estimate the latent heat
588	flux $H_L$ (or moisture flux) (Section 4). Whereas bulk estimates of $\tau$ and $H_S$ are derived from a
589	traditional approach, which is based on the transfer coefficients (drag coefficient and Stanton
590	number), aerodynamic and scalar roughness lengths, and MOST flux-profile relationships,
591	modeled values of $H_L$ are evaluated from a modified P-T approach, which is essentially based on
592	the SEB equation (4) (i.e., on the conservation of energy principle). Note also, that a MOST-
593	based flux-profile approach or a bulk flux algorithm requires measurements of the relevant
594	variables (e.g., wind speed and T/RH) at two different levels whereas a SEB-type model needs
595	data (e.g., radiative fluxes) from a single level only. One may classify this approach as a hybrid
596	or synthetic (composite) approach because it uses different physical principles for
597	parameterization of the turbulent fluxes. Our hybrid bulk flux approach is summarized in Table
598	1.

599 Thus, the novelty in our bulk flux algorithm for a terrestrial tower site is associated with 600 the use of a hybrid approach to predict the turbulent fluxes, when even the turbulent energy fluxes,  $H_S$  and  $H_L$ , are estimated from two completely different physical principles. As 601 602 mentioned above, a two-level aerodynamic method for a turbulent flow in the case of  $\tau$  and  $H_S$ 603 estimates (i.e., a traditional bulk approach) and the first law of thermodynamics at the interface for  $H_L$  estimates (one may say that these two approaches are "apples and oranges"). In addition, a 604 hybrid approach is characterized by flexible logic. For example,  $H_L$  can be estimated from 605 another model based on the SEB equation (4), whereas  $\tau$  and  $H_S$  can be derived from a gradient 606 607 method (requiring meteorological measurements at two atmospheric levels) rather a traditional 608 bulk approach (requiring meteorological measurements at one atmospheric level and estimation

609 of  $\theta_0$ ,  $z_{0x}$  at the surface–atmosphere interface, see Section 4). Obviously other options for the 610 flux estimates are also possible in the framework of a hybrid approach (e.g., see Basu 2019 for 611 discussion).

612 In this study, we use two 30-day long uninterrupted time series of the data separately for 613 dry and wet soil conditions (WFIP 2 "golden files"). Time periods from 27 August to 26 614 September 2016 (YD 240-270) and 25 March to 24 April 2017 (YD 450-480 with respect to 1 615 January 2016) were selected to calibrate and verify parameterizations for the surface fluxes over 616 dry and wet soil surfaces respectively (see Grachev et al. 2020 for further detail). We sorted the 617 data into dry and wet categories based on the soil temperature and soil moisture measured at 5 618 cm depth (Section 2). The direct measurements of the surface fluxes (turbulent and radiative) and 619 other ancillary atmospheric/soil parameters made during WFIP 2 for different soil conditions 620 (dry and wet) are used to optimize and tune the hybrid bulk algorithm. In particular, our results 621 suggest that the P-T coefficient  $\alpha$  varies with soil moisture according to (21). Because direct 622 measurements of the soil heat flux G (e.g., with a heat flux plate) were not available during the 623 field campaign WFIP 2, G in the P-T model (11) was estimated from the Fourier's Law of Heat 624 Conduction (6) based measurements of soil temperature and soil moisture. Dependence of the 625 thermal conductivity of the soil  $\lambda$  in (6) versus soil moisture content at 5 cm depth for the entire 626 field campaign (Fig. 10) was estimated via. Eq. (21).

The bulk flux estimates have been validated against the eddy-covariance fluxes (Fig. 11). According to linear regression slopes for the scatter plots shown in Fig. 11, the bulk flux estimates for  $H_S$  and  $H_L$  predicted by the hybrid bulk flux algorithm provide reasonable agreement on average (within a few percent except  $H_L$  for the dry period) with the measured half-hourly averaged flux values (see also Tables 2 and 3). In this study we also discuss the SEB
closure over dry and wet surfaces at various timescales (from half-hourly to monthly averages)
based on the modelled and measured fluxes for the dry and wet soil "golden files" periods (Figs.
13 and 14). In addition, we tested the model beyond the 30-day "golden files" calibration periods
without further tuning (Figs. 15 and 16). The bulk flux algorithm described in Section 4 is
optimized for the data collected at the WFIP 2 Physics Site PS01. However, our model and its
modifications can be used for other similar flux-tower sites and similar field campaigns.

638 It can be assumed that our approach is applicable to other similar sites in which 639 advection, heterogeneity etc. is considered not to be relevant. This is because our approach is 640 based on the first principles; that is, on the aerodynamic method for a turbulent mixing in the 641 case of  $\tau$  and  $H_S$  estimates and the first law of thermodynamics at the interface for  $H_L$  estimates. 642 To apply our approach to other locations, the tunable model parameters associated with surface 643 properties and soil type (e.g.,  $z_0$  and  $\lambda$ ) must be changed. However, it is necessary to keep in 644 mind that our approach as well as other land-surface models and remote-sensing applications 645 assume a closed energy balance only for four main terms (4), allowing to compute explicitly 646 missing terms as the residual of the others (e.g., Cuxart et al. 2015; Mauder et al. 2020 and 647 references therein). The limitation of this approach is associated with neglecting of all storage 648 and transport contributions, and other unspecified processes. This can lead to systematic bias in 649 estimates of the energy fluxes (in our case  $H_L$ ). Mauder et al. (2020) recently survey different 650 methods of estimating the magnitude of the SEB residual imbalance, which can improve the 651 predictability of the energy fluxes.

652

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- 658
- 659

# 661

#### APPENDIX

#### **Turbulent Bulk Flux Algorithm**

662

### In a traditional bulk turbulent flux algorithm in Eq. (8)–(10), we make a distinction

between the scalar averaged wind speed (i.e., the mean wind speed), S, and the vector averaged

wind speed (i.e., the magnitude of the mean wind vector), U, at reference height z (see Grachev

et al. 1998, Section 3.1, and Akylas et al. 2003, Section 2a, for discussion). The vector averaging

of the wind speed first takes the average of the longitudinal and lateral wind speed components,

668 u and v respectively, and then takes the square,

$$U = \left(\overline{u}^2 + \overline{v}^2\right)^{1/2} \tag{A1}$$

670 whereas the scalar averaging firstly takes the square and then average,

671 
$$S = \left(\overline{u^2} + \overline{v^2}\right)^{1/2}$$
(A2)

672 Combining (A1) and (A2) with the definition of variance leads to a relationship between U and673 S:

674 
$$S^2 - U^2 = \left(\overline{u^2} - \overline{u}^2\right) + \left(\overline{v^2} - \overline{v}^2\right) = \sigma_u^2 + \sigma_v^2 \tag{A3}$$

where  $\sigma_u$  and  $\sigma_v$  are the horizontal velocity variances. Relationship (A3) is also known as the gustiness assumption (e.g., Fairall et al. 1996; Grachev et al. 1998). According to (A3), *S* in such conditions is the vector sum *U* and the convective gustiness velocity,  $U_G = (\sigma_u^2 + \sigma_v^2)^{1/2}$ :

678 
$$S^2 = U^2 + U_G^2 = (UG_f)^2$$
(A4)

679 where  $G_f = S/U$  is called the gustiness factor. In convective conditions, large-scale circulations 680 embracing the entire convective boundary layer (CBL) create random gusts that crucially affect 681 the surface fluxes. In the COARE bulk algorithm, for unstable stratification  $U_G = \beta w_*$  where  $\beta \approx 1.25 \text{ (Fairall et al. 1996) and } w_* = \left(\overline{w'\theta_v'}gh/\theta_v\right)^{1/3} \text{ is the Deardorff (1970) convective}$ velocity scale ( $\theta_v$  is the virtual temperature, and *h* is the CBL height). A key point of (*A*4) is
employment of  $\sigma_u, \sigma_v \sim w_*$  (Panofsky et al. 1977); that is, a convective gust is proportional to
the Deardorff (1970) velocity scale  $w_*$ , which is added to the mean wind speed *U*. Thus, under
light wind conditions (in the free-convection limit)  $U \rightarrow 0$  whereas  $S \rightarrow w_*$ . Note that variances
of the horizontal wind components in the convective surface layer are practically independent of
height and, therefore, do not follow the traditional surface layer scaling.

689 It is obvious that vector or scalar averaging can be applied to the turbulent stress as well 690 since the instantaneous vector of the wind stress has the same direction as the wind vector 691 (Grachev et al. 1998; Akylas et al. 2003). Similar to S defined by Eqs. (A2)–(A4), the scalar averaged stress,  $\tau_S$ , has a finite limit as U approaches zero. In this case, random CBL-scale 692 693 coherent structures produce a local log-profile in the layer attached to the bottom of the large 694 eddies. This local velocity profile generates a local stress (the 'minimum friction velocity'). Thus, 695 the concept of gustiness immediately leads to a 'minimum friction velocity' assumption (e.g. 696 Businger 1973; Schumann 1988; Sykes et al. 1993; Akylas et al. 2003) also referred as the 697 convection-induced stress regime (Grachev et al. 1997, 1998; Zilitinkevich et al. 1998, 2005, 698 2006). In fact, free convection can be considered as a particular case of forced convection. 699 Zilitinkevich et al. (1998, 2005, 2006) developed a more detailed theoretical model for the non-700 local momentum and heat transfer. The vector or scalar averaging of the turbulent stress is 701 related in particular to the time averaging procedure. Mahrt et al. (1996) reported a substantial 702 difference of the drag coefficient in light winds for different averaging times and vector/scalar 703 wind speed averaging procedures. According to Mahrt et al. (1996), higher values of the drag 704 coefficient occur for a 10-min time averaging period compared to 60-min averaged values. The

vector averaging of the surface stress would be appropriate for determination of the average, net

706 large scale force acting on a surface (e.g., for description of the surface currents for

707 measurements over sea surface). Note that both the COARE and SHEBA bulk flux algorithms as

- 708 well as Eq. (8) are based on the vector averaging of the turbulent stress when  $\tau = \rho u_*^2 \propto SU$
- 709 whereas the scalar averaged wind stress assumes  $\tau_s = \rho u_{*s}^2 \propto S^2$  (where  $u_{*s}$  is the friction
- 710 velocity based on the scalar averaging).
- The COARE bulk flux algorithm is described in detail by Fairall et al. (1996, 2003) but it is sketched here. The transfer coefficients in (8)–(10) are partitioned into individual profile
- 713 components (Fairall et al. 1996, Eq. 5):

714 
$$C_D = c_d^{1/2} c_d^{1/2}, \qquad C_H = c_d^{1/2} c_h^{1/2}, \qquad C_E = c_d^{1/2} c_e^{1/2}$$
 (A5)

The bulk variables are used to compute so-called Monin-Obukhov (MO) scaling
parameters (Fairall et al. 1996, Eq. 9):

717 
$$u_*^2 = C_D SU, \qquad \theta_* = -c_h^{\frac{1}{2}} \Delta \theta, \quad q_* = -c_e^{\frac{1}{2}} \Delta q \qquad (A6)$$

Traditionally, the transfer coefficients (*A*6) are adjusted to neutral conditions using MO
similarity theory via (e.g., Fairall et al. 1996, Eq. 6)

720 
$$c_d^{1/2} = \frac{c_{dn}^{1/2}}{1 - \frac{c_{dn}^{1/2}}{\kappa} \Psi_m(\zeta)}, \quad c_h^{1/2} = \frac{c_{hn}^{1/2}}{1 - \frac{c_{hn}^{1/2}}{\kappa} \Psi_h(\zeta)}, \quad c_e^{1/2} = \frac{c_{en}^{1/2}}{1 - \frac{c_{en}^{1/2}}{\kappa} \Psi_h(\zeta)}$$
 (A7)

Here 
$$\Psi_m(\zeta)$$
 and  $\Psi_h(\zeta)$  are the MO profile functions for mean profiles of wind speed and scalars  
in the surface layer,  $\kappa \approx 0.4$  is the von Kármán constant. In neutral conditions ( $\zeta \equiv 0$ ) the  $\Psi$ -  
functions obey  $\Psi_m(\zeta) = \Psi_h(0) = 0$ . Subscript *n* in  $c_{dn}$ ,  $c_{hn}$ , and  $c_{en}$  in (*A*7) denotes the value  
in neutral conditions. The MO stability parameter  $\zeta = z/L$  (*L* is the Obukhov length) is defined  
by

$$\zeta = \frac{\kappa g z}{\theta_a} \frac{\theta_{\nu*}}{u_*^2} \tag{A8}$$

Here *g* is the acceleration due to gravity and, historically, the von Kármán constant is included in the definition of *L* and  $\zeta$  simply by convention. Subscript *v* in  $\theta_{v*}$  in (*A*8) denotes the virtual temperature. The neutral transfer coefficients in (*A*7) are uniquely related to the aerodynamic,  $z_0$ , and scalar,  $z_{0\theta}$  and  $z_{0q}$ , roughness lengths through

731 
$$c_{dn}^{1/2} = \frac{\kappa}{\log(z/z_0)}, \quad c_{hn}^{1/2} = \frac{\kappa}{\log(z/z_{0\theta})}, \quad c_{en}^{1/2} = \frac{\kappa}{\log(z/z_{0q})}$$
 (A9)

The transfer coefficients depend on height via (A9) but the roughness lengths are fixed for a given surface. Traditionally the transfer coefficients for operational or practical considerations are also represented at a standard reference height of 10 m and neutral conditions and denoted as  $C_{D10n}, C_{H10n}$ , and  $C_{E10n}$ . These 10-m neutral transfer coefficients are computed from  $U_{10n}$ ,  $\Delta\theta_{10n}$  and  $\Delta q_{10n}$  (see Fairall et al. 2003, Eqs. 31 and 32).

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6	TABLE 1.	The hybrid	bulk flux	algorithm	parameters	and equations.
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Flux Variables	Equations	Coefficients	Input Variables
$ au$ , $H_S$	( <i>A</i> 1), ( <i>A</i> 2), (A7)	$C_D, C_H$	$U, \theta_0, \theta_a, q_a$
$H_L$	(8), (9)	α, k <sub>i</sub>	R <sub>net</sub> , G
G	(12)	$\lambda, \rho_S, c_{pS}$	$\theta_0, T_{S5}$

TABLE 2. Summary of flux statistics (monthly averages and standard deviations) for the dry soil "golden files" (year days 240–270). 

Flux Variables	<bulk></bulk>	<direct></direct>	$\sigma$ Bulk	$\sigma$ Direct
$G[Wm^{-2}]$	-2.4		58.9	
$H_S [Wm^{-2}]$	71.5	69.9	131.2	126.9
$H_L [Wm^{-2}]$	9.0	7.4	20.0	22.3
$\tau [Nm^{-2}]$	0.10	0.12	0.11	0.13
$R_{net} \left[ Wm^{-2} \right]$		72.8		173.0

TABLE 3. Summary of flux statistics (monthly averages and standard deviations) for the wet soil "golden files" (year days 450-480). 

Flux Variables	<bulk></bulk>	<direct></direct>	$\sigma$ Bulk	$\sigma$ Direct
$G[Wm^{-2}]$	7.4		66.4	
$H_S [Wm^{-2}]$	40.0	40.2	87.4	88.0
$H_L [Wm^{-2}]$	45.7	53.3	68.1	61.2
$\tau [Nm^{-2}]$	0.13	0.15	0.16	0.19
$R_{net} \left[ Wm^{-2} \right]$		108.9		201.9







Fig. 2. View of the 10-m PS01 flux tower showing the lower (3 m) measurement level during
summer conditions (23 June 2016). The two radiation masts for measurements of the
downwelling and upwelling radiation are located right behind the flux tower in this photo.







998 temperature, and (d) volumetric soil moisture observed at the WFIP 2 Physics site PS01 during

999 year days 240–270 (27 August-26 September 2016). The data are based on half-hour averaging.





latent heat (water vapor) flux measured at 3 m, (c) short-wave (SW) downwelling and upwelling
radiation, and (d) long-wave (LW) downwelling and upwelling radiation observed at the WFIP 2
Physics site PS01 during year days 240–270 (27 August-26 September 2016). The data are based
on half-hour averaging.



1011 Fig. 5. Same as Fig. 3 but for wet soils observed at the WFIP 2 Physics site PS01 during year







1017 days 450–480 (25 March-24 April 2017). The data are based on half-hour averaging.





**Fig. 7.** Linear regression fit of half-hourly averaged covariance sensible heat flux normalized by  $c_p \rho U_{10n}G_f$  versus 10-m neutral surface-air temperature difference for (*a*) the dry soil "golden files" (year days 240–270, 27 August-26 September 2016) and (*b*) the wet soil "golden files" period (year days 450–480, 25 March-24 April 2017). The green ×-symbols are data for 10-m neutral wind speed greater than 1 ms<sup>-1</sup>; for blue +-symbols only wind speed greater than 4 ms<sup>-1</sup> are considered. The cyan solid lines are regressions based on the half-hourly averaged values for wind speed greater than 1 ms<sup>-1</sup>.



**Fig. 8.** The adjusted ground flux (residual) storage term versus temperature difference between surface ( $\theta_0$ ) and soil at 5 cm depth ( $T_{S5}$ ) for (*a*) the dry soil "golden files" period (year days 240– 270) and (*b*) the wet soil "golden files" period (YD 450–480). The green ×-symbols are halfhourly averaged values; blue circles are derived from the mean diurnal cycle. The magenta solid lines are regressions with  $\lambda/\Delta z = 2.859 \text{Wm}^{-2} \text{K}^{-1}$  for the dry soils and  $\lambda/\Delta z = 7.034 \text{Wm}^{-2} \text{K}^{-1}$  for the wet soils based on the half-hourly averaged values.



1037



1039 240–270) and (b) the wet soil "golden files" period (YD 450–480). The blue lines are the

1040 residual estimate of G and the red lines are G computed via (15) based on the half-hourly

1041 averaged values. Magenta dotted lines show standard deviations for the gradient estimates of the

- 1042 ground flux (15).
- 1043





1046 Fig. 10. Regression fit of the thermal conductivity of the soil  $\lambda$  versus soil moisture content at 5



1048 dataset from 24 June 2016 to 01 May 2017, YD 176–487).



**Fig. 11.** Scatter plots of the bulk estimates of (a, b) sensible heat flux  $H_S$  and (c, d) latent heat flux  $H_L$  versus their measured (direct covariance) counterparts based on the half-hourly and monthly averaged data using (11) and (12) with  $\alpha = 0.4 + 5Q_{S5}$  ( $\alpha$  not to exceed 1.45). Plots in the left panels (a, c) represent the dry soil "golden files" (YD 240–270) and the right panels (b,d) represent the wet soil "golden files" period (YD 450–480). Correlation coefficients:  $(a) R^2 =$ 0.99,  $(b) R^2 = 0.98$ ,  $(c) R^2 = 0.56$ , and  $(d) R^2 = 0.88$ .





1065 fluxes respectively.



1068 Fig. 13. Net surface energy balance from bulk flux calculations for (a) the dry soil "golden files"

- 1069 (YD 240–270) and (b) the wet soil "golden files" period (YD 450–480). Observed net radiation
- $R_{net}$  versus the sum of the sensible, latent and ground fluxes as yielded by (9), (11), and (15).
- 1071 Correlation coefficients: (a)  $R^2 = 0.99$  and (b)  $R^2 = 0.99$ .



**Fig. 14.** Scatter plots of the net surface energy balance for (a, b) the sum of the measured sensible and latent heat fluxes  $H_S + H_L$  and (c, d) the sum of the measured  $H_S + H_L$  and bulk estimates of the ground heat flux  $G_b$  versus the net solar radiation  $R_{net}$  based on the half-hourly and monthly averaged data. Plots in the left panels (a, c) represent the dry soil "golden files" (YD 240–270) and the right panels (b, d) represent the wet soil "golden files" period (YD 450–480).





1084 soils). Correlation coefficients: (a)  $R^2 = 0.98$ , (b)  $R^2 = 0.98$ , (c)  $R^2 = 0.79$ , and (d)  $R^2 = 0.92$ . 







1089 Correlation coefficients: (a) 
$$R^2 = 0.97$$
 and (b)  $R^2 = 0.99$ .

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