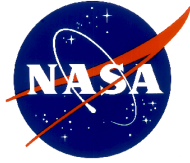


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ECOSystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS)



Level-3 Evapotranspiration L3 (JET) Algorithm Theoretical Basis Document

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List of Acronyms

ALEXI	Atmosphere–Land Exchange Inverse
ATBD	Algorithm Theoretical Basis Document
Cal/Val	Calibration and Validation
CONUS	Contiguous United States
ECOSTRESS	ECOSystem Spaceborne Thermal Radiometer Experiment on Space Station
ET	Evapotranspiration
ESI	Evaporative Stress Index
EVI-2	Earth Ventures Instruments, Second call
FLiES	Forest Light Environmental Simulator
GEO	Group on Earth Observations
GEWEX	Global Energy and Water Cycle Exchanges Project
GLEAM	Global Land-surface Evaporation: the Amsterdam Methodology
GMAO	Global Modeling and Assimilation Office
HypIRI	Hyperspectral Infrared Imager
IGBP	International Geosphere-Biosphere Program
iLEAPs	International Land Ecosystem-Atmospheric Processes Study
ISS	International Space Station
L-2	Level 2
L-3	Level 3
LE	Latent heat flux
LST	Land Surface Temperature
MERRA	Modern Era Retrospective-Analysis for Research and Applications
METRIC	Mapping EvapoTranspiration at high-Resolution with Internalized Calibration
MODIS	MODerate-resolution Imaging Spectroradiometer
MPI-BGC	Max Planck Institute for Biogeochemistry
NSE	Nash-Sutcliffe Efficiency
PHyTIR	Prototype HypIRI Thermal Infrared Radiometer
PM-MOD16	Penman-Monteith MOD16
PMBL	Penman-Monteith-Bouchet-Lhomme
PT-JPL	Priestley-Taylor Jet Propulsion Laboratory
RMSD	Root Mean Squared Difference
SDS	Science Data System
SEBS	Surface Energy Balance System
STIC	Surface Temperature Initiated Closure
TIR	Thermal Infrared
VIC	Variable Infiltration Capacity
VIIRS	Visible Infrared Imaging Radiometer Suite
WUE	Water Use Efficiency

Contents

1	Introduction.....	5
	1.1 Purpose.....	5
	1.2 Scope and Objectives.....	5
2	Parameter Description and Requirements	5
3	Ancillary Variables	6
	3.1 STARS NDVI and Albedo.....	6
	3.2 Downscaled Meteorology and Soil Moisture	9
4	Evapotranspiration Retrieval: Jet Propulsion Laboratory EvapoTranspiration (JET)	
Ensemble.....		11
	4.1 PT-JPL _{SM} : General Form	11
	4.1.1 Diurnal cycling.....	Error! Bookmark not defined.
	4.1.2 Spatial resolution improvements	14
	4.2 STIC: General Form	14
	4.3 MOD16: General Form.....	16
	4.4 BESS: General Form.....	17
	4.5 Daily Ensemble Value	18
5	Calibration/Validation.....	18
	5.1 ET evaluation.....	18
	5.2 WUE Evaluation	19
	5.3 ESI Evaluation	20
	5.4 Ancillary variable evaluation.....	20
6	Mask/Flag Derivation	21
7	Metadata	22
8	Acknowledgements	22
9	References.....	23

1 Introduction

1.1 Purpose

Evapotranspiration (ET) is one of the main science outputs from the ECOSystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS) mission (Fisher et al., 2020). ET is a Level-3 (L-3) product constructed from a combination of the ECOSTRESS Level-2 (L-2) Land Surface Temperature (LST) product (Hulley et al., 2022) and ancillary data sources. The rate of ET is controlled by many environmental and biological controls including: incoming radiation, the atmospheric water vapor deficit, soil water availability, and vegetation physiology and phenology (Brutsaert, 1982; Monteith, 1965; Penman, 1948). Therefore, to accurately model ET, it remains important to consider these variables. Scientists have been able to form models that ingest satellite observations that capture environmental and biological controls on ET across the globe. Because LST holds the unique ability to capture when and where plants experience stress, as observed by elevated temperatures, LST can inform which areas have a reduced capacity to evaporate or transpire water to the atmosphere (Allen et al., 2007). Version 1 of Level-3 ET data from ECOSTRESS provided a ET data from the Priestley-Taylor Jet Propulsion Laboratory (PT-JPL) model and uncertainty in ET from a 3 model ensemble (Fisher et al., 2020). The L-3 product revealed promising comparison to in situ data, but was limited by the latency in observations of vegetation and LST, the ability to provide consistent meteorological forcing in lieu of cloud cover, and only utilized one model to resolve ET. In this Algorithm Theoretical Basis Document (ATBD), we describe the new Jet Propulsion Laboratory ET (JET) Ensemble approach taken to resolve ET globally and new ancillary data products with application to the ECOSTRESS mission.

1.2 Scope and Objectives

In this ATBD, we provide:

1. Description of the ET parameter characteristics and requirements;
2. Description of the general form of the ET algorithms in the JET ensemble;
3. Required algorithm-specific adaptations specific to the ECOSTRESS mission;
4. Required Ancillary data products with potential sources and back-up sources;
5. Plan for the calibration and validation (Cal/Val) of the ET retrieval.

2 Parameter Description and Requirements

Attributes of the ET data produced by the ECOSTRESS mission include:

- Spatial resolution of 70 m x 70 m;
- Diurnally varying temporal resolution to match the overpass characteristics of the International Space Station (ISS);
- Latency as required by the ECOSTRESS Science Data System (SDS) processing system;
- Includes all geographic terrestrial regions visible by the ECOSTRESS instrument from the ISS, limited only by bandwidth to the ISS.

3 Ancillary Variables

Ancillary variable	Equation	Source
Normalized difference vegetation index (NDVI)	STARS	Harmonized Landsat Sentinel (HLS) 2.0 product and daily, moderate spatial resolution images from the Suomi NPP Visible Infrared Imaging Radiometer Suite (VIIRS) VNP09GA product
Albedo (α)	STARS	Harmonized Landsat Sentinel (HLS) 2.0 product and daily, moderate spatial resolution images from the Suomi NPP Visible Infrared Imaging Radiometer Suite (VIIRS) VNP09GA product
Near-surface air temperature (T_a)	L3G MET	GEOS-5 FP tavg1_2d_slv_Nx product
Near surface dew point temperature (T_d)	Net radiation	GEOS-5 FP tavg1_2d_slv_Nx product
Relative humidity (RH)	L3G MET	GEOS-5 FP tavg1_2d_slv_Nx product
Soil moisture (SM)	L3G SM product	GEOS-5 FP tavg1_2d_lnd_Nx product

Table 1. Showing ancillary variables and their respective equations, and data sources

3.1 STARS NDVI and Albedo

In ECOSTRESS Collection 1, the normalized difference vegetation index (NDVI) and albedo required for ET processing were produced using the most recent Landsat scenes covering the ECOSTRESS scene. Landsat often provides only partial coverage, so NDVI and albedo were gap-filled with daily 1 km MODIS. The temporal gap between the most recent Landsat scene and the ECOSTRESS scene caused the collection 1 workflow to not capture short-term changes in vegetation conditions, such as harvest, that occurred during that lag period. ECOSTRESS Collection 2 addresses this by producing coincident, gapfilled NDVI and albedo estimates at 70 m ECOSTRESS standard resolution for each daytime ECOSTRESS overpass through data fusion of temporally sparse but fine spatial resolution images from the Harmonized Landsat Sentinel (HLS) 2.0 product with daily, moderate spatial resolution images from the Suomi NPP Visible Infrared Imaging Radiometer Suite (VIIRS) VNP09GA product. The data fusion is performed using a variant of the Spatial Timeseries for Automated high-Resolution multi-Sensor data fusion (STARS) methodology (Johnson et al., 2022). STARS is a state-space timeseries methodology that provides streaming data fusion and uncertainty quantification through efficient Kalman filtering.

Prior to data fusion, a pixelwise, lagged 16-day implementation of the VNP43 algorithm (Schaaf, 2017) is used for a near-real-time bi-directional reflectance function (BRDF) correction on the VNP09GA products to produce VIIRS nadir BRDF-adjusted red and near-infrared reflectance at 500 m resolution for NDVI, and 1 km estimates of black-sky albedo (a_{black}) and white-sky albedo (a_{white}) for VIIRS M-bands 1, 2, 3, 4, 5, 7, 8, 10, and 11. Blue-sky albedo (a_{blue}) for each of these bands is calculated as in (Schaaf, 2017)

$$a_{blue} = SKYL * a_{white} + (1 - SKYL)a_{black} \tag{1}$$

where SKYL is the fraction of diffuse skylight read from a look-up table according to solar zenith angle and aerosol optical depth (AOD) retrieved from GEOS-5 FP `tavg3_2d_aer_Nx`. The broadband blue-sky albedo is calculated by a weighted sum of the VIIRS M-band blue-sky albedo estimates using the near-to-broadband coefficients described in (Schaaf, 2017) described in Table 2.

VIIRS M-Band	NTB Coefficient
1	0.2418
2	-0.201
3	0.2093
4	0.1146
5	0.1146
7	0.1348
8	0.2251
10	0.1123
11	0.0860
Offset	-0.0131

Table 2. Near-to-Broadband (NTB) coefficients for VIIRS M-band albedo (Schaaf, 2017)

A near-to-broadband albedo is estimated for HLS using the Sentinel-2a/b coefficients in Table 3 and Landsat 8 coefficients in Table 4. HLS 30 m NDVI and albedo estimates are upsampled to the 70m ECOSTRESS standard resolution.

Band	NTB Coefficient
2	0.1324
3	0.1269
4	0.1051
5	0.0971
6	0.0890
7	0.0818
8	0.0722
11	0.0167
Offset	0.0002

Table 3. Near-to-Broadband (NTB) coefficients for Sentinel-2a/b albedo (Vanino, 2018)

Landsat 8 Band	NTB Coefficient
2	0.356
3	0.13
4	0.373
5	0.085
6	0.072
Offset	-0.018

Table 4. Near-to-Broadband coefficients for Landsat 8 albedo (Liang, 2001)

For ECOSTRESS Collection 2, the STARS method is implemented as described below. Let $x_{i,t}$ represent NDVI or albedo to be estimated in the i^{th} 70 m ECOSTRESS resolution pixel on day t , and likewise, let $Y_{i,t}^H$ be the corresponding HLS measurement at the i^{th} 70 m pixel. Note that $Y_{i,t}^H$ is assumed to be missing if there is no HLS overpass on day t . Then, let $Y_{j,t}^V$ represent the VIIRS measurement at the j^{th} cell in the VIIRS resolution grid (490m and 980m for VIIRS NDVI and albedo, respectively) and let A_j be the set of all 70m pixels overlapped by the VIIRS pixel. The STARS model for ECOSTRESS Collection 2 has the following form

$$Y_{j,t}^V = \alpha_t(A_j) + \frac{1}{|A_j|} \sum_{i \in A_j} x_{i,t} + \epsilon_{j,t}^V \quad \epsilon_{j,t}^V \sim \text{Normal}(0, \sigma_v^2) \quad (2a)$$

$$Y_{i,t}^H = x_{i,t} + \epsilon_{i,t}^H \quad \epsilon_{i,t}^H \sim \text{Normal}(0, \sigma_h^2) \quad (2b)$$

$$x_{i,t} = x_{i,t-1} + \omega_{i,t} \quad \omega_{i,t} \sim \text{GP}(0, \tau^2, \mathcal{K}(\cdot)) \quad (3)$$

where equations (2a,b) describe the instrument measurements as noisy, aggregate in the case of VIIRS, observations of the target high resolution image values, $x_{i,t}$. The terms $\alpha_t(A_j)$ model a dynamic additive offset between VIIRS and HLS measurements, and measurement errors are assumed to be mean-zero and normally distributed with standard deviations σ_v, σ_h for VIIRS and HLS, respectively. Equation 3 describes day-to-day temporal dependence in NDVI/albedo through a first-order Markov chain where the magnitudes of pixel-level changes between days ($\omega_{i,t}$) follow a Gaussian process (GP) with covariance function $\mathcal{K}(\cdot)$, modelling spatial correlation of day-to-day changes between pixels. The standard deviation parameter, τ , constrains the expected magnitude of change. To achieve scalability, STARS is implemented in a block, moving window where blocks are defined by the coarse resolution grid plus a spatial buffer region.

For $\mathbf{x}_t = (\dots, x_{i,t}, \dots)$ the vector of the n target image pixels within a block on day t , and \mathbf{y}_t the stacked vector of available coarse and fine measurements, the timeseries model above induces the full state space model

$$\mathbf{y}_t = \boldsymbol{\alpha}_t + \mathbf{F}_t \mathbf{x}_t + \boldsymbol{\epsilon}_t \quad \boldsymbol{\epsilon}_t \sim \text{MultivariateNormal}(0, \mathbf{V}) \quad (4)$$

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \boldsymbol{\omega}_t \quad \boldsymbol{\omega}_t \sim \text{MultivariateNormal}(0, \mathbf{W}) \quad (5)$$

where \mathbf{V} is a diagonal matrix with elements σ_v^2 , σ_h^2 for VIIRS and HLS observations, respectively. The matrix, \mathbf{F}_t , is the aggregation matrix analog to the linking of VIIRS and HLS observations to the target resolution grid in equation (2a,b). The estimation of the target 70m NDVI or albedo image on day t is inferred through the posterior distribution of \mathbf{x}_t given all considered past and current HLS and VIIRS observations up to day t . This distribution is known to be Gaussian with mean, \mathbf{m}_t , and covariance, \mathbf{C}_t . The mean provides the estimated imagery, while the covariance provides quantified uncertainties characterizing uncertainty due to spatial and temporal downscaling. Estimates of \mathbf{m}_t and \mathbf{C}_t are obtained recursively through the well-known Kalman filtering equations (Kalman, 1960). Specifically, given estimates of \mathbf{m}_t , \mathbf{C}_t , and any new observations from VIIRS or HLS on day $t + 1$ (\mathbf{y}_{t+1}), the updated estimates of \mathbf{m}_{t+1} , and \mathbf{C}_{t+1} are calculated as

$$\mathbf{m}_{t+1} = \mathbf{m}_t + \mathbf{K}_{t+1}(\mathbf{y}_{t+1} - \mathbf{F}_{t+1}\mathbf{m}_t) \quad (6)$$

$$\mathbf{C}_{t+1} = (\mathbf{I} - \mathbf{K}_{t+1}\mathbf{F}_{t+1})(\mathbf{C}_t + \mathbf{W}) \quad (7)$$

where $\mathbf{K}_{t+1} = (\mathbf{C}_t + \mathbf{W})\mathbf{F}_{t+1}^T(\mathbf{F}_{t+1}(\mathbf{C}_t + \mathbf{W})\mathbf{F}_{t+1}^T + \mathbf{V})^{-1}$ is the Kalman gain matrix. If neither VIIRS nor HLS measurements are available on day $t + 1$, the mean estimate is propagated forward ($\mathbf{m}_{t+1} = \mathbf{m}_t$) but the covariance is increased ($\mathbf{C}_{t+1} = \mathbf{C}_t + \mathbf{W}$) quantifying increased uncertainty in fused NDVI and albedo estimates due to lack of available data. By leveraging a timeseries approach to data fusion, STARS provides automated spatial and temporal gapfilling, uncertainty quantification, and the capability to provide estimates of coincident NDVI/albedo with any ECOSTRESS overpass. The pixel-wise uncertainties of the NDVI and albedo estimates are distributed as data layers in the STARS product.

Near-real-time STARS NDVI/albedo products corresponding to each daytime L2T_LSTE product are produced by loading the set of STARS means and covariances saved from the day of the previous ECOSTRESS overpass, downloading any available VIIRS and HLS measurements between overpasses, and Kalman filtering forward the NDVI/albedo estimates to the current target day. The latency of this operation depends on the approximately two day latency of HLS and VIIRS. The coincident STARS NDVI and albedo products are recorded in the L2T_STARS product.

3.2 Downscaled Meteorology and Soil Moisture

Near-surface air temperature (Ta) and relative humidity (RH) are sourced from the GEOS-5 FP tavg1_2d_slv_Nx product. Soil moisture (SM) is sourced from the GEOS-5 FP tavg1_2d_lnd_Nx product.

The Ta, RH, and SM inputs of the ET models are retrieved at low latency from the GEOS-5 FP dataset at coarse resolution, approximately a third of a degree. To improve the spatial fidelity of evapotranspiration processing, these coarse meteorological estimates are spatially downscaled to the fine spatial structure of the ECOSTRESS surface temperature and STARS NDVI and albedo. Future versions of this product will include a more robust method.

The ST, NDVI, and albedo are spatially aggregated to the GEOS-5 FP spatial resolution. A linear regression is calculated from these three variables as independent variables to the GEOS-5 FP variable as the dependent variable for each of the GEOS-5 FP variables. The coefficients from this regression are applied to the fine resolution ECOSTRESS surface temperature and STARS NDVI and albedo to produce a fine resolution estimate of air temperature, humidity, or soil moisture. This fine scale estimate is bias corrected by spatially aggregating to the GEOS-5 FP scale, measuring the bias against the GEOS-5 FP estimate, and spatially interpolating this coarse scale bias to the 70 m ECOSTRESS grid, and subtracting this interpolated bias. Cloud-obstructed areas of are filled in with bi-cubically resampled GEOS-5 FP. The meteorology variables Ta and RH are recorded in the L3T MET and mosaicked into the L3G MET. The SM data is recorded in the L3T SM product and mosaicked into the L3G SM product.

3.3 Net Radiation

The generation of net radiation (R_n) involves the integrated retrieval of individual radiation balance components: downwelling shortwave radiation (R_{SD}), upwelling shortwave radiation (R_{SU}), downwelling longwave radiation (R_{LD}), and upwelling longwave radiation (R_{LU}) [Verma *et. al*, 2016]:

$$R_N = (R_{SD} - R_{SU}) + (R_{LD} - R_{LU}) \quad (8)$$

where a is the surface albedo.

NETRAD	Equations	Data Variable & Sources
R_{SD}	FLiES	Cloud Optical Thickness and Aerosol Optical Thickness (GEOS-5 FP)
R_{SU}	$R_{SU} = \alpha R_{SD}$	Land Surface Albedo (STARS)
R_{LD}	$R_{LD} = \sigma \epsilon_A T_a^4$	Near Surface Air Temperature and Vapor Pressure (GEOS-5 FP)
R_{LU}	$R_{LU} = \sigma \epsilon_S T_S^4$	Land Surface Temperature and Emissivity (ECO2LSTE)

Table 5. Showing radiation balance components and their respective equations, variables, and data sources

R_{SD} is calculated from an atmospheric radiative transfer model, the Forest Light Environmental Simulator (FLiES) [Iwabuchi, 2006; Kobayashi and Iwabuchi, 2008; Ryu *et al.*, 2011; Ryu *et al.*, 2012]. To speed processing, a neural network machine learning algorithm was trained on to generate R_{SD} from solar zenith angle, aerosol optical thickness, cloud optical thickness, land surface albedo, atmospheric profile height, aerosol type, and cloud height. R_{SU} is calculated from R_{SD} and land surface albedo as:

$$R_{SU} = \alpha R_{SD} \quad (9)$$

R_{LD} is calculated from Stefan-Boltzmann's Law:

$$R_{LD} = \sigma \varepsilon_A T_a^4 \quad (10)$$

$$\varepsilon_A = 1 - \left(1 + .467 \frac{E_a}{T_a}\right) \cdot e^{-\sqrt{1.2+3 \cdot \frac{4.65 \cdot E_a}{T_a}}} \quad (11)$$

$$E_a = 2.171 \cdot 10^{10 \cdot e^{-\frac{4157}{T_d} - 33.91}} \quad (12)$$

where σ is the Stefan-Boltzmann constant ($5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$), ε_A is the atmospheric emissivity calculated from total atmospheric precipitable water (ζ) [Prata, 1996], T_a is near surface air temperature, E_a is the vapor pressure, and T_d is the near surface dew point temperature. T_a and T_d ($^{\circ}\text{C}$) are available from GEOS-5 [Verma et. al, 2016]:

R_{LU} is calculated from Stefan-Boltzmann's Law [Verma et. al, 2016]:

$$R_{LU} = \sigma \varepsilon_S T_S^4 \quad (13)$$

where ε_S is the broadband surface emissivity sourced from the ECOSTRESS Level 2 emissivity ECO2LSTE, and T_S is LST available from ECOSTRESS Level 2 ECO2LSTE.

We emphasize these data products provide data at unprecedented scales. Therefore, we solicit feedback on the quality and utility of these variables in their ability to advance science and scientific applications. A preliminary evaluation of the ancillary data accuracy is presented in Section 5.

4 Evapotranspiration Retrieval: Jet Propulsion Laboratory EvapoTranspiration (JET) Ensemble

The JPL EvapoTranspiration (JET) data ensemble provides a robust estimation of ET from multiple ET models. The JET ensemble incorporates ET data from four algorithms: Priestley Taylor-Jet Propulsion Laboratory model with soil moisture (PT-JPL_{SM}), the Penman Monteith MODIS Global Evapotranspiration Model (MOD16), Soil Temperature Initiated Closure (STIC) model, and the Breathing Earth System Simulator (BESS) model.

4.1 PT-JPL_{SM}: General Form

The PT-JPL_{SM} model relies on the Priestley-Taylor [1972] equation to resolve potential ET (PET). This formulation is removed from the need to parameterize stomatal and aerodynamic resistances and instead multiples the α coefficient (1.26) to the rate of equilibrium ET:

$$PT = \alpha \frac{\Delta}{\Delta + \gamma} R_N - G \quad (14)$$

where Δ is the slope of the saturation-to-vapor pressure curve (dependent on near surface air temperature, T_a , and atmospheric vapor pressure, e_a), γ is the psychrometric constant, and R_N is net radiation (W m^{-2}) and G is the ground heat flux (W m^{-2}). PET is given in units of R_N , or W

m^{-2} , and is therefore considered as an energy variable, i.e., LE. To convert LE to ET, one can divide LE by the latent heat of vaporization (MJ kg^{-1}).

To reduce PET to actual ET (AET), *Fisher et al.* [2008] applied ecophysiological constraint functions (f -functions, unitless multipliers, 0-1) based on atmospheric moisture (vapor pressure deficit, VPD; and, RH) and vegetation indices (normalized difference and soil adjusted vegetation indices, NDVI and SAVI, respectively). While this model has been demonstrated to perform well at large scales in space and time, certain model assumptions of land-atmosphere equilibrium fall apart at finer spatial and temporal frequencies. As a result, the PT-JPL formulation from *Fisher et al.* [2008] has been shown to overestimate ET in arid regions. To overcome these limitations *Purdy et al.* [2018] modified the algorithm to incorporate explicit constraint from soil water availability. The driving equations in the PT-JPL_{SM} algorithm are:

$$AET = ET_s + ET_c + ET_i \quad (15)$$

$$ET_s = (f_{wet} + f_{rew}(1 - f_{wet}))\alpha \frac{\Delta}{\Delta + \gamma} (R_{ns} - G) \quad (16)$$

$$ET_c = (1 - f_{wet})f_{trm}f_gf_t\alpha \frac{\Delta}{\Delta + \gamma} R_{nc} \quad (17)$$

$$ET_i = f_{wet}\alpha \frac{\Delta}{\Delta + \gamma} R_{nc} \quad (18)$$

where ET_s , ET_c , and ET_i are evaporation from the soil, canopy and intercepted water, respectively, each calculated explicitly and summing to total AET . f_{wet} is relative surface wetness (RH^4) [*Stone et al.*, 1977] representing the fraction of soil and canopy that delivers water to the atmosphere potential rate. f_{rew} is the relative extractable water defined as the difference between observed soil moisture (θ_{obs}) and soil moisture at the plant wilting point (θ_{wp}) divided by the difference of soil moisture at field capacity (θ_{fc}) and soil moisture at the plant wilting point ($\frac{\theta_{obs} - \theta_{wp}}{\theta_{fc} - \theta_{wp}}$). Canopy constraints include the fraction of green canopy ($f_g = f_{APAR}/f_{IPAR}$) [*Zhang et al.*, 2005], plant temperature constraints ($f_t = \exp(-((T_{max} - T_{opt})/T_{opt})^2)$) [*Potter et al.*, 1993; *June et al.*, 2004], and plant and soil moisture controls (f_{trm}) [*Purdy et al.*, 2018]. f_{APAR} is absorbed photosynthetically active radiation (PAR), f_{IPAR} is intercepted PAR, T_{max} is maximum air temperature, T_{opt} is T_{max} at $\max(R_n T_{max} \frac{SAVI}{VPD})$, G is the soil heat flux, and R_{nc} , R_{ns} are the net radiation ('c' for canopy and 's' for soil). f_{trm} combines both f_m the plant moisture control and soil moisture control on transpiration (f_{rew}) by weighting each constraint by the relative humidity as:

$$f_{trm} = (RH^{4(1-VWC)(1-RH)})f_m + (1 - RH^{4(1-VWC)(1-RH)})f_{rew} \quad (19)$$

During periods of high humidity, plant moisture is a stronger control than soil water control. During periods of low humidity, soil water control is greater (Figure 1).

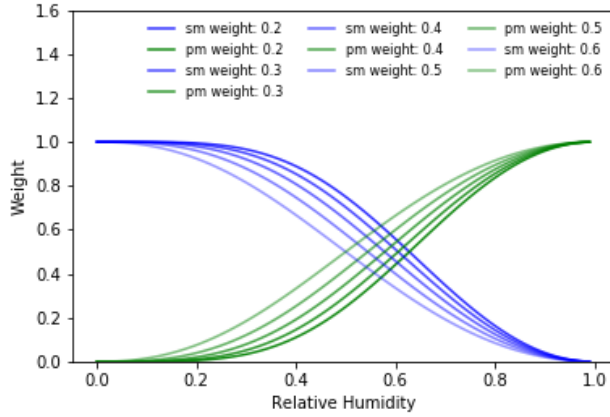


Figure 1) Plant moisture (green) and soil water control (blue) weight by relative humidity (x-axis) and VWC (legend values: 0.2-0.6). During periods of high relative humidity periods higher weights on plant moisture indicate more control from this scalar. During low humidity more weight is placed on soil water control.

The individual plant moisture and soil water constraints on transpiration are derived as:

$$f_m = \frac{f_{APAR}}{f_{APARmax}} \quad (20)$$

$$f_{trew} = 1 - \left(\frac{\theta_{cr} - \theta_{obs}}{\theta_{cr} - \theta_{wpch}} \right)^{CH_{scalar}} \quad (21)$$

where CH_{scalar} is a canopy height scalar that impacts the sensitivity of vegetation to soil water availability equal to \sqrt{CH} and capped between 1 and 5, θ_{cr} is the critical soil moisture at which soil water availability begins to constrain ET and computed as:

$$\theta_{cr} = \left(1 - \left(\frac{1}{1 + PET} - 0.1 \frac{1}{1 + CH} \right) \right) \left(\theta_{fc} - \frac{\theta_{WP}}{CH_{scalar}} \right) + \frac{\theta_{WP}}{CH_{scalar}} \quad (22)$$

The adjustment of θ_{fc} to θ_{cr} is removed from the dependence on land classification datasets and facilitates continuously mapping when soil water availability begins to limit transpiration within f_{trew} (Figure 2).

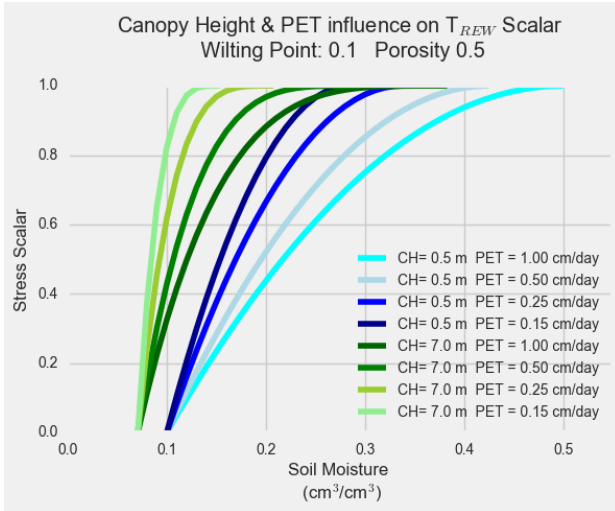


Figure 2) Supplemental figure from Purdy et al., 2018. f_{rew} on canopy height and PET (see legend). During high PET conditions soil water control begins sooner than during low PET conditions. Canopy height impacts when soil water control begins with taller canopies (greens) being less sensitive to surface soil water control than shorter canopies (blues).

To integrate PT-JPL_{SM} for use in the ECOSTRESS mission include a need existed to adapt resolve ET across the diurnal cycle (1) and refine the spatial resolution (2).

4.1.1 Spatial resolution improvements

To maintain continuity with other ECOSTRESS data products, ET from PT-JPL_{SM} is produced at 70 m. This required generating ancillary variables such as NDVI, albedo (α), air temperature (T_a), relative humidity (RH), soil moisture (SM), canopy height, and soil properties at the same spatial resolution. Section 3 details how NDVI, albedo, air temperature, relative humidity, soil moisture, and net radiation were resampled or downsampled to fill this need. Soil properties and canopy height data were sourced from X and Y. As with the earlier versions of ECOTRESS ET data we advise caution to users interested in highly heterogeneous land surfaces and meteorological conditions at length scales less than 1 km.

4.2 STIC: General Form

The Surface Temperature Initiated Closure (STIC) (latest version 1.3) is a one-dimensional SEB model treating soil-vegetation as a single unit [Mallick et al., 2015; 2018; 2022]. STIC directly integrates LST into the Penman-Monteith Shuttleworth-Wallace system of ET equations [Penman, 1965; Shuttleworth and Wallace, 1985] to solve the aerodynamic temperature, which is the most critical temperature for ET modeling. STIC assumes a first-order dependence of aerodynamic conductance (g_a) and canopy conductance (g_{cs}) on LST (through soil moisture availability and aerodynamic temperature (T_0)). Surface moisture availability (also called surface wetness) is first estimated as a function of LST, and then constrains g_a and g_{cs} conductances through the surface wetness in an analytical framework. In addition to LST, the inputs to STIC1.3 include radiation (net radiation), emissivity, albedo, fractional vegetation cover (FVC) (derived from NDVI), and meteorological inputs (air temperature, relative humidity, and incoming solar radiation).

The general approach to STIC is (and see flow diagram in Figure 1):

- (1) STIC solves the state equations to find analytical solution of T_0 , and the conductances (g_a and g_{cs}).
- (2) There are more unknowns in the state equations (e.g., aerodynamic vapor pressure components), these unknowns are initialized as a function of LST.
- (3) The additional unknowns are estimated iteratively by combining Penman-Monteith and Shuttleworth-Wallace equations

The state equations solved in Step 1 are as follows:

$$F_E = \frac{2\alpha s}{2s + 2\gamma + \gamma(1 + I_{SM}) \frac{g_a}{g_{cs}}} \quad (23)$$

$$T_0 = T_a + \frac{(e_0 - e_a)}{\gamma} \frac{(1 - F_E)}{F_E} \quad (24)$$

$$g_a = \frac{R_N - G}{\rho c_p [(T_0 - T_a) + \frac{(e_0 - e_a)}{\gamma}]} \quad (25)$$

$$g_{cs} = g_a \frac{(e_0 - e_a)}{(e_0^* - e_0)} \quad (26)$$

Where F_E is the evaporative fraction (defined as the fractional contribution of ET from total available energy), α is the Priestley-Taylor coefficient [Priestley & Taylor, 1972], s is the slope of the saturation vapor pressure at air temperature (T_a) (hPa/°C), γ is the psychrometric constant (hPa/°C), e_0^* and e_0 are the saturation vapor pressure and ambient vapor pressure at the canopy-air stream, also called source-sink height (hPa), R_N and G are net radiation and ground heat flux (W/m^2), e_a is the atmospheric vapor pressure (hPa) at the level of T_a measurement, ρ is the air density (kg/m^3), and c_p is the specific heat of air at constant pressure (j/kg/K).

I_{SM} describes the relative wetness or the intensity of water stress on a surface. This variable controls the transition from potential to actual evaporation, with I_{SM} tending to 1 on a unstressed wet surface, and 0 on a stressed dry surface. Since LST is extremely sensitive to surface water stress variations, it is used directly to estimate I_{SM} . For further details, refer to Mallick et al. [2018, 2022].

In Step 1, initial estimates of an initial estimate of e_0^* , e_0 , I_{SM} , and surface dew point temperature (T_{sd}), are obtained. The initial I_{SM} and R_N are used for an initial estimate of G . In Step 2, initial estimates of the conductances, T_0 , F_E and sensible heat (H) and latent heat flux (LE) are

obtained. In Step 3, the process is iterated by updating e_0^* , e_0 , I_{SM} , and α , and used to recalculate G , g_a , g_{cs} , T_0 , F_E , H , and LE until convergence of LE is obtained (10 – 15 iterations).

The major differences of version 1.3 [Mallick *et al.*, 2022] from the previous version concern the calculation of G , which is calculated according to Santanello and Friedl [2003] with the following function:

$$\frac{G}{R_N} = c_g \left[\frac{2\pi(t_{g0} + 10800)}{t_g} \right] \quad (27)$$

Where c_g is the maximum proportion of G/R_N ; t_{g0} is time in seconds relative to solar noon, t_g is the factor that minimizes the deviation between G/R_N and governs the phase difference between G and R_N . c_g and t_g are linked to surface wetness I_{SM} with:

$$c_g = (1 - I_{SM})c_{gmax} + I_{SM}c_{gmin} \quad (28)$$

$$t_g = (1 - I_{SM})t_{gmax} + I_{SM}t_{gmin} \quad (29)$$

Using the values of c_{gmax} (0.35), c_{gmin} (0.05), t_{gmax} (100000 s), and t_{gmin} (74000 s). With the initial estimate of I_{SM} , initial G is estimated, and then updated in the iterative process. Further details are available in the supporting information of [Mallick *et al.* 2022].

For its implementation in ECOSTRESS Collection 2, here we modified the STIC version 1.3 equation in the following ways:

- We use a different method to calculate dew point temperature (T_d) with relative humidity (RH) and air temperature (T_a):

$$T_d = T_a - \frac{100 - RH * 100}{5} \quad (30)$$

- The inputs R_N , albedo, emissivity, NDVI, relative humidity, air temperature and incoming solar radiation are the same as used for other models in the JET ensemble. This is done in order to have more consistency in the input data.

4.3 MOD16: General Form

The MOD16 algorithm is rooted in the Penman Monteith equation with environmental constraints from vegetation cover, temperature, and atmospheric moisture deficits (Mu *et al.*, 2011). Similar to the PT-JPLSM model, the MOD16 algorithm resolves evaporative fluxes from the soil, canopy, and intercepted water separately.

$$AET = ET_s + ET_c + ET_i \quad (31)$$

$$ET_S = \left(f_{wet} + (1 - f_{wet})RH^{\frac{e_{sat}-e}{\beta}} \right) \frac{sA_C + \frac{\rho Cp(e_{sat} - e)}{r_{a_s}}}{\Delta + \gamma \left(1 + \frac{r_{S_s}}{r_{a_s}} \right)} \quad (32)$$

$$ET_S = (1 - f_{wet})f_c \frac{sA_C + \frac{\rho Cp(e_{sat} - e)}{r_{a_s}}}{\Delta + \gamma \left(1 + \frac{r_{S_s}}{r_{a_s}} \right)} \quad (33)$$

$$ET_S = f_{wet}f_c \frac{sA_C + \frac{\rho Cp(e_{sat} - e)}{r_{a_s}}}{\Delta + \gamma \left(1 + \frac{r_{S_s}}{r_{a_s}} \right)} \quad (34)$$

Where f_{wet} is fraction of wet surface, RH is the relative humidity, s is the slope of saturated water vapor pressure to temperature ($d(e_{sat})/dT$); A is the available energy with subscripts to distinguish differences between the soil and canopy; ρ is the air density; Cp is the specific heat capacity of air; γ is the psychrometric constant; e is the actual water vapor pressure; r_a is the aerodynamic resistance; and r_s is the surface resistance. Vegetation-dependent environmental constraints on stomatal conductance are incorporated through the surface resistance in the formulation above.

4.4 BESS: General Form

BESS is a coupled biophysical modeling system that couples atmospheric and canopy radiative transfer processes with photosynthesis, stomatal conductance, and transpiration using (Ryu et al., 2011). BESS applies an equilibrium evaporation representation to resolve soil evaporation and solves a quadratic representation of the Penman Monteith model to estimate transpiration [Jiang et. al, 2016]:

$$AET = ET_s + ET_c \quad (35)$$

$$ET_s = \frac{s}{(s + \gamma)} (R_{ns} - G) RH^{VPD} \quad (36)$$

$$aET_c^2 + bET_c + c = 0 \quad (37)$$

$$a = \frac{r_a^2}{2[\rho_a C_p \gamma (r_a + r_c)]} \frac{d^2 e_{sat}(T_a)}{dT_a^2} \quad (38)$$

$$b = -1 - r_a \frac{de_{sat}(T_a)}{d(T_a)} \frac{1}{\gamma(r_a + r_c)} - \frac{R_{nj} r_a^2}{\rho_a C_p \gamma (r_a + r_c)} \frac{d^2 e_{sat}(T_a)}{dT_a^2} \quad (39)$$

(40)

$$c = \frac{\rho_a C_p D}{\gamma(r_a + r_c)} + \frac{r_a R_{nj}}{\gamma(r_a + r_c)} \frac{de_{sat}(T_a)}{dT_a} + \frac{1}{2} \frac{(r_a R_{nj})^2}{\rho_a C_p \gamma(r_a + r_c)} \frac{d^2 e_{sat}(T_a)}{dT_a^2}$$

where r_a is the aerodynamic; r_c is the canopy resistance; R_{nj} is the net radiation; ρ_a is the air density; γ is the psychrometric constant; $e_{sat}(T_a)$ is the saturated water vapor pressure at temperature T_a .

4.5 Daily Ensemble Value

Differences in model structure provide a range in ET estimates to consider for each 70m pixel. Previous studies have shown the combination of an ensemble of modeled values provides improved or equal accuracy to any one given model [Kirtman et al., 2014]. Due to the limited number of models used within the JET algorithm, we adopt a simplified approach by taking the median value of the instantaneous ET ensemble (PT-JPL_{SM}, MOD16, STIC, TSEB, & BESS). The ensemble median value is used to provide a daily estimate of ET for each 70 m pixel. Additionally, the uncertainty is estimated as the standard deviation of the ensemble for each pixel.

5 Calibration/Validation

5.1 ET evaluation

To evaluate remote sensing ET datasets requires ground observations at similar length scales and temporal frequencies. Eddy covariance (EC) towers provide year-round observations at frequencies (~30 minutes) and spatial scales (10's-100's m) that capture exchanges of water vapor from the land surface to the atmosphere necessary to evaluate the JET ensemble. Here, we employ EC observations from the Ameriflux network due to their data collection standards, availability, and distribution across various land uses in North and South America. We only include EC towers in our analysis that are within ECOSTRESS observations (<58°N & > 58°S), have data during ECOSTRESS mission (2018-Present), and have a long-term closure ration of greater than 0.70. This filtering resulted in 74 towers across 11 land uses for the JET ensemble comparison (Figure 3).

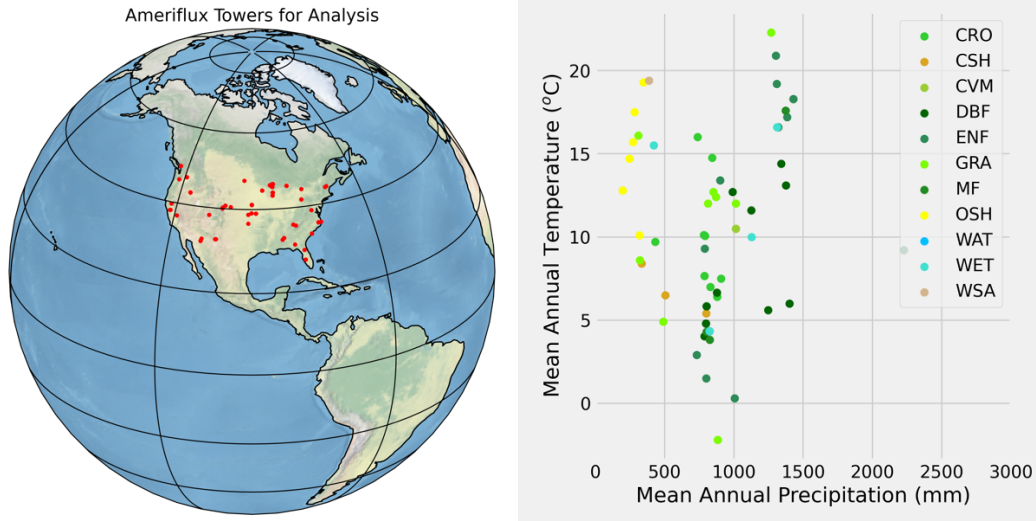


Figure 3) Left: Distribution of filtered Ameriflux towers across North America within ECOSTRESS view. Right: Range in EC towers' mean annual precipitation (x-axis), temperature (y-axis) by vegetation class (color).

EC data from Ameriflux are post-processed for quality and to ensure surface energy budget closure. Surface energy balance variables including sensible heat, latent heat, ground heat flux, and net radiation were filtered for outliers according to a median of absolute deviation about the median approach [Papale et al., 2006]. Next, the surface energy budget was closed while preserving the Bowen Ratio, the ratio of sensible heat to latent heat, following the EBC_CF Method 1 and EBC_CF Method 2 procedures of the OneFLUX processing [Pastorello et al., 2020]. This closure approach yields energy closures according to the 25th, 50th, and 75th percentiles for dates spanning plus or minus 15 and 5 days respectively. Only cloud-free ECOSTRESS observations are utilized in this analysis. Due to uncertainties and on-going debate about the surface energy imbalances from EC observations, we compute the statistics computed based on the best comparison across the raw observation and the closed budget options. We compute statistics of unbiased root mean square error, mean absolute bias, and the correlation coefficient.

5.2 WUE Evaluation

BESS uses a carbon-water-coupled model to separately evaluate C3 and C4 species provided by a global map [Still et al., 2003] a given pixel, the sum of that relative proportion of C3 and C4 in that pixel determines the GPP [Jiang et al., 2016]. The GPP product in kilograms of carbon per square meter estimated by BESS is ingested operationally into the data production stream to estimate water use efficiency (WUE). Process-based approaches like BESS have an advantage to represent the interaction between the soil system, plants, and atmosphere as an organic integration rather than ingesting GPP semi-empirically [Jiang et al., 2016]. The carbon uptake is divided by the daily ET in kilograms per square meter to determine the ratio of grams of carbon fixed to kilograms of water lost in units of ET. This ratio describes the WUE, higher values indicate more plant productivity, lower values indicate less productive plants.

$$WUE = \frac{GPP}{ET} \quad (42)$$

5.3 ESI Evaluation

The Evaporative Stress Index (ESI) is used as a climate indicator of agricultural drought and plant stress by comparison of ET to PET to determine anomalous reduction in ET relative to potential ET. PET is already calculated internally in the PT-JPL algorithm and can be used directly to compute the ESI without ancillary information.

$$ESI = \frac{ET}{PET} \quad (42)$$

5.4 Ancillary variable evaluation

EC towers commonly measure Ta, RH, and SM in addition to capturing exchanges of radiative energy, carbon, and water from the Earth's surface and atmosphere. We utilize the same Ameriflux data source. Instead of screening for surface energy balance closure, we only consider the quality of each variable when considering data for use in this evaluation. For soil moisture, we only utilize EC towers data from the National Ecological Observation Network (NEON) due to the number of soil moisture observations. Recently, the NEON towers provided a great comparison to evaluate the utility of remotely sensed soil moisture in forested and non-forested regions [Ayres et al., 2022]. For each variable we compute statistics of unbiased root mean square error, mean absolute bias, and the correlation coefficient.

6 Mask/Flag Derivation

For T_s and e_s , the ECOSTRESS L2 flags are used to provide quality information for the L3 ET product.

7 Metadata

- unit of measurement: Watts per square meter (W m^{-2})
- range of measurement: 0 to 3000 W m^{-2}
- projection: ECOSTRESS swath
- spatial resolution: 70 m x 70 m
- temporal resolution: dynamically varying with precessing ISS overpass; instantaneous throughout the day, local time
- spatial extent: all land globally, excluding poleward $\pm 60^\circ$
- start date time: near real-time
- end data time: near real-time
- number of bands: not applicable
- data type: float
- min value: 0; ET, WUE, ESI
- max value: 3000; ET, WUE, ESI
- no data value: NaN
- bad data values: NaN

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