JPL D-96969

ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS) Mission

Level 2 Land Surface Temperature and Emissivity (LST&E) Algorithm Specification Document

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1.0 INTRODUCTION

1.1 Identification

This is the Algorithm Specification Document (ASD) for Level 2 data for the ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS) project. The Level 2 (L2) product provides Land Surface Temperature and Emissivity (LST&E) data produced using the Temperature Emissivity Separation (TES) algorithm described in the L2 Algorithm Theoretical Basis Document (ATBD) (JPL D-94644). This document applies to the Level 2 LST&E product produced from thermal infrared data acquired by the ECOSTRESS radiometer instrument.

1.2 Purpose and Scope

This Algorithm Specification Document describes the Level 2 process used to generate the LST&E product with the TES algorithm. This includes an outline of the software used to compute LST&E, and a description of the workflow to assimilate ECOSTRESS data products and the various ancillary data sets required for the L2 product.

The purpose of this ASD is to describe, in computer-science terms, the remote sensing algorithms that produce the ECOSTRESS end-user L2 data products. The science basis of an algorithm is not covered in an ASD, but is described in a corresponding ATBD (see section 1.4).

The ASD provides a software description of those algorithms as implemented in the operational ground system, the Science Data Operations System (SDOS). The intent of an ASD is to capture the "as-built" operational implementation of the algorithm. An individual ASD describes the process used in the creation of a single level of data product.

1.3 Mission Overview

The ECOSTRESS instrument measures the temperature of plants and uses that information to better understand how much water plants use and how they respond to stress.

ECOSTRESS addresses three overarching science questions:

- How is the terrestrial biosphere responding to changes in water availability?
- How do changes in diurnal vegetation water stress impact the global carbon cycle?
- Can agricultural vulnerability be reduced through advanced monitoring of agricultural water consumptive use and improved drought estimation?

The ECOSTRESS mission answers these questions by accurately measuring the temperature of plants. Plants regulate their temperature by releasing water through pores on their leaves called stomata. If they have sufficient water, they can maintain their temperature. However, if there is insufficient water, their temperatures rise. This temperature rise can be measured with a sensor in space. ECOSTRESS uses a multispectral thermal infrared (TIR) radiometer to measure the surface temperature from the International Space Station. The instrument will measure radiances at 5 spectral bands in the 8-12.5 μm range with a spatial resolution of approximately 70 by 70 meters on the ground.

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1.4 Applicable and Reference Documents

"Applicable" documents levy requirements on the areas addressed in this document. "Reference" documents are identified in the text of this document only to provide additional information to readers. Unless stated otherwise, the document revision level is Initial Release. Document dates are not listed, as they are redundant with the revision level.

1.4.1 Applicable Documents

ECOSTRESS Project Level 2 Science Data System Requirements (JPL D-94088).

ECOSTRESS Science Data Management Plan (JPL D-94607)

423-ICD-005 ICD Between ECOSTRESS SDS and LPDAAC

ECOSTRESS Level 1 Algorithm Theoretical Basis Documents (JPL D-94641, D-94642)

ECOSTRESS Level 1 Algorithm Specification Document (JPL D-94643)

ECOSTRESS Level 2 Algorithm Theoretical Basis Documents (JPL D-94643, D-94644)

ECOSTRESS Level 2 Algorithm Specification Document (JPL D-96969)

ECOSTRESS Level 2 Product Specification Document (JPL D-94635)

1.4.2 Reference Documents

n/a

1.5 ECOSTRESS Data Products

The ECOSTRESS mission will generate 13 different distributable data products. The products represent four levels of data processing, with data granules defined as an image scene. Each image scene consists of 44 scans of the instrument mirror, each scan taking approximately 1.181 seconds, and each image scene taking approximately 52 seconds. Each image scene starts at the beginning of the first target area encountered during each orbit. Each orbit is defined as the equatorial crossing of an ascending International Space Stations (ISS) orbit.

ECOSTRESS Level 0 data include spacecraft packets that have been pre-processed by the Ground Data System (GDS). Level 1 products include spacecraft engineering data, the time-tagged raw sensor pixels appended with their radiometric calibration coefficients, the black body pixels used to generate the calibration coefficients, geolocated and radiometrically calibrated at-sensor radiances of each image pixel, the geolocation tags of each pixel, and the corrected spacecraft attitude data. Level 2 products include the land surface temperature and emissivity of each spectral band retrieved from the at-sensor radiance data, and a cloud mask. Level 2 products also appear in image scene granules. Level 3 products contain evapotranspiration data derived from Level 2 data. Level 4 products contain evaporative stress index and water use efficiency derived from Level 2 data.

The ECOSTRESS products are listed in Table 1-1. This document will discuss only the Level 2 LST&E product.

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Table 1-1: ECOSTRESS Distributable Standard Products

Product type	Description
L0	Level 0 “raw” spacecraft packets
L1A_ENG	Spacecraft and instrument engineering data, including blackbody gradient coefficients
L1A_RAW_ATT	Uncorrected spacecraft ephemeris and attitude data
L1A_PIX	Raw pixel data with appended calibration coefficients
L1B_RAD	Calibrated at-sensor radiances
L1B_GEO	Geolocation tags, sun angles, and look angles, and calibrated, resampled at-sensor radiances
L1B_ATT	Corrected spacecraft ephemeris and attitude data
L2_LSTE	Land Surface temperature and emissivity
L2_CLOUD	Cloud mask
L2_ET_LST&E	Evapotranspiration retrieved from L2_LSTE
L2_ET_ALEXI	Evapotranspiration generated using the ALEXI/DisALEXI Algorithm
L4_ESI_LST&E	Evaporative Stress Index generated with LST&E
L4_ESI_ALEXI	Evaporative Stress Index generated with ALEXI/DisALEXI
L4_WUE	Water Use Efficiency (WUE)
L2_L4_QA	Quality Assessment fields for all ancillary data used in L2 and L4 products

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2.0 ALGORITHM AND DATA DESCRIPTION

2.1 Overview of L2 algorithm and role in ECOSTRESS SDS

The ECOSTRESS Level-2 algorithm derives its heritage from the ASTER Temperature Emissivity Separation (TES) algorithm and the MODIS and VIIRS atmospheric correction schemes. Details of these processes can be found in the L2 ATBD. Level 2 processes operate primarily on input L1B radiances and geolocation information to produce LST and emissivity products. The L2 process also ingests ancillary emissivity data from the ASTER Global Emissivity Dataset (GED), meteorological fields from GEOS5, and DEM information from SRTM. These L2 products are then used as input to create Level 3 and Level 4 products consisting of evapotranspiration, evaporative stress index, and water use efficiency.

2.2 Input data sets

2.2.1 Requirements on inputs

All input data for the L2 product must be geolocated and time-ordered, and therefore have latitude, longitude, and time associated with each pixel. We do not pose strict requirements on the input products regarding format, projection, and spatiotemporal range. Table 1 gives a brief description of information required to generate the L2 products. The L2 product requires a combination of ECOSTRESS L1 data and external agency data available in-house at JPL. The details of these products are described in Table 2.

2.2.2 Attributes of ECOSTRESS input products

ECOSTRESS input data products used for the L2 data product are:

- L1B_GEO – Geolocation
- L1B_RAD – Calibrated radiance

2.2.3 Attributes of ancillary input products

Other ancillary input data products used for the L2 data product are:

- ASTER GED v3
- GEOS5-FP atmosphere

See Table 2-1 below for more detailed information.

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Table 2-1: L2 LST&E Ancillary Input Products

ECOSTRESS L1B Radiance	Description	Calibrated and geolocated radiances
	Format	HDF5
	Projection	Swath
	Resolution	70×70m, 5 TIR bands
	Location	ECOSTRESS SDS at JPL
GEOS5-FP	Description	GEOS5-FP atmospheric profiles from NASA GMAO
	Format	Netcdf4
	Projection	Global Grid
	Resolution	Spatial: 1/3×1/4 degree longitude, latitude Temporal: 3 hourly UTC
	Location	ECOSTRESS SDS at JPL
ASTER GED v3	Description	ASTER Global Emissivity Database v3
	Format	HDF5
	Projection	Gridded, 1×1 degree
	Resolution	100 m
	Location	TIR server at JPL
ECOSTRESS L1 Geolocation	Description	Geolocation and satellite viewing geometry data
	Format	HDF5
	Projection	Swath
	Resolution	70×70m
	Location	ECOSTRESS SDS at JPL

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2.3 Output data sets

2.3.1 Attributes of output products

The ECOSTRESS Level 2 output product fields are described in the table below:

Table 2-2: L2 LST&E Output fields

ECOSTRESS_L2_LSTE_<ORBIT>_<SCENE>_<SCENETIME>_<BUILD>_<VERSION>.h5

SDS	Long Name	Data type	Units	Valid Range	Fill Value	Scale Factor	Offset
Group	**SDS (per pixel, 5400 * 5632)**						
LST	Land Surface Temperature	uint16	K	7500-65535	0	0.02	0.0
QC	Quality control for LST and emissivity	uint16	n/a	0-65535	0	n/a	n/a
Emis1	Band 1 emissivity	uint8	n/a	1-255	0	0.002	0.49
Emis2	Band 2 emissivity	uint8	n/a	1-255	0	0.002	0.49
Emis3	Band 3 emissivity	uint8	n/a	1-255	0	0.002	0.49
Emis4	Band 4 emissivity	uint8	n/a	1-255	0	0.002	0.49
Emis5	Band 5 emissivity	uint8	n/a	1-255	0	0.002	0.49
LST_Err	Land Surface Temperature error	uint8	K	1-255	0	0.04	0.0
Emis1_Err	Band 1 emissivity error	uint16	n/a	0-65535	0	0.0001	0.0
Emis2_Err	Band 2 emissivity error	uint16	n/a	0-65535	0	0.0001	0.0
Emis3_Err	Band 3 emissivity error	uint16	n/a	0-65535	0	0.0001	0.0
Emis4_Err	Band 4 emissivity error	uint16	n/a	0-65535	0	0.0001	0.0
Emis5_Err	Band 5 emissivity error	uint16	n/a	0-65535	0	0.0001	0.0
EmisWB	Wideband emissivity	uint8	n/a	1-255	0	0.002	0.49
PWV	Precipitable Water Vapor	uint16	cm	0-65535	0	0.001	0.0

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Table 2-3: L2 Cloud Output fields

ECOSTRESS_L2_CLOUD_<ORBIT>_<SCENE>_<SCENETIME>_<BUILD>_<VERSION>.h5

Bit Field	Long Name	Result
0	Cloud Mask Flag	0 = not determined 1 = determined
1	Cloud, either one of bits 2, 3, or 4 set.	0 = no 1 = yes
2	Thermal Brightness Test	0 = no 1 = yes
3	Band 4-5 Thermal Difference test	0 = no 1 = yes
4	Band 2-5 Thermal Difference test	0 = no 1 = yes
5	land/water mask	0 = land 1 = water

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3.0 SOFTWARE DESIGN

3.1 Overview

The L2 algorithm has four primary modules that operate within the Production Generation Executable (PGE). First the atmospheric correction module is run using the RTTOV radiative transfer software, followed by the cloud mask algorithm with input calibrated radiances and water vapor information from the atmospheric correction, DEM, and geolocation parameters, then the atmospheric correction module is run with input GEOS5 atmospheric data. Lastly the TES algorithm is run with input surface radiance, and atmospheric correction data from the previous modules. The entire L2 code is written in C with input options and settings controlled via a RunConfig file and a PGERunParameters file. The RunConfig file. contains unique identifiers used to track instances of a PGE run, versions of science software, product input files and their location. The PGERunParameters file contains internal algorithm settings and thresholds.

3.2 Description of major code sections

The following sections will provided a description of each subprocess identified in the main L2 PGE as detailed in the schematic in Figure 3-1.

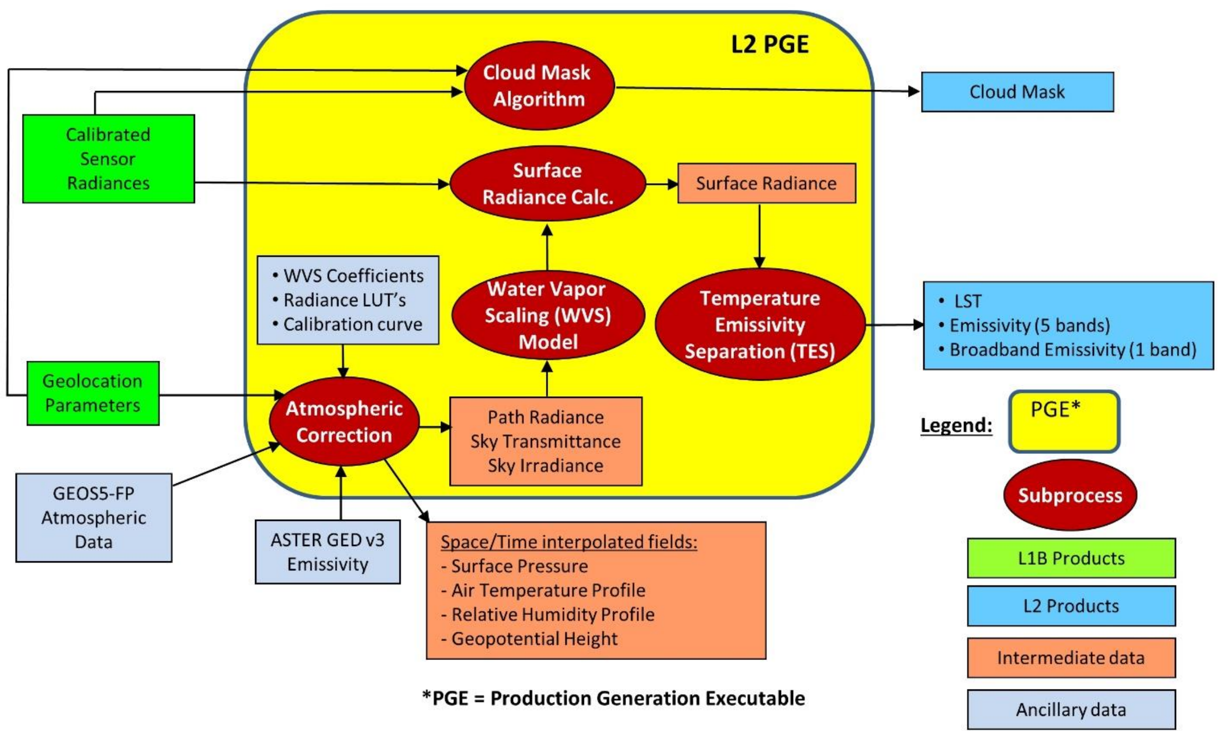

Figure 3-1. Schematic representing overall design of the L2 LST&E algorithm.

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3.2.1 Atmospheric correction

The atmospheric correction module uses the Radiative Transfer for TOVS (RTTOV) radiative transfer model with input atmospheric profile data from the GEOS5 reanalyses data provided by the NASA Global Modeling and Assimilation Office (GMAO, https://gmao.gsfc.nasa.gov/products/). One daily GEOS5 file consisting of 8 3-hourly 'snapshots' of atmospheric geophysical data are required per ECOSTRESS scene in order to temporally interpolate to the ECOSTRESS observation time. If the observation time is greater than 21 UTC, then a GEOS5 file for the following day at 00 UTC used. The code deals with this logic automatically. One radiance conversion table is required to convert output radiances from RTTOV from mWatts/cm2/steradian/micron to Watts/m2/steradian/micron before gridding the 1/3 degree longitude, ¼ degree latitude GEOS5 data onto the ECOSTRESS swath.

Once the atmospheric parameters from the RTTOV run have completed, a Water Vapor Scaling (WVS) model is used to further improve the accuracy of these outputs. The WVS model requires input precipitable water vapor (PWV) outputs from RTTOV, emissivity from the ASTER GED v3, and view angle information from ECOSTRESS L1B_GEO data. The ASTER GED v3 is first gridded onto the ECOSTRESS swath and then spectrally adjusted to match the spectral response functions of ECOSTRESS using a linear regression method with input laboratory spectra.

3.2.2 Cloud Mask

The cloud mask algorithm is embedded in the primary L2 PGE since it relies on both input L1B data and outputs from the atmospheric correction module, thereby saving computational time in having to read in L1B data twice through a different PGE, or process. The cloud mask product (ECOCLOUD) will indicate whether a given view of the earth surface is unobstructed by clouds or optically thick aerosol for each 70-m ECOSTRESS pixel. Inputs to the ECOCLOUD algorithm include calibrated, geolocated, and good quality L1B TIR radiance data, geolocation parameters (latitude, longitude, satellite view angle), and gridded PWV derived from the atmospheric correction module. The final cloud mask is output as an 8-bit mask (see Table 2-3), with per-pixel information on whether the cloud mask was determined or not; final cloud mask (1=cloud, 0=clear) set to cloud if either of three thermal tests resulted in cloud, results of three individual thermal tests (1=cloud, 0=clear), and a land/water mask (1=water, 0=land). In summary, the ECOSTRESS cloud mask will provide a binary confidence level output for each pixel. If the user so desires, any one of, or a combination of the three thermal tests can be used to determine the cloud mask, and the land/water mask is included to give the user additional information on setting thresholds for their own tests if desired. More detailed information on the thermal tests is available in the L2 Cloud ATBD.

3.2.3 Water Vapor Scaling (WVS) model

In order to minimize atmospheric correction errors and improve the accuracy in retrieved temperature and emissivity, a Water Vapor Scaling (WVS) model is implemented to improve the accuracy of the water vapor atmospheric profiles on a band-by-band basis for each observation using an Extended Multi-Channel/Water Vapor Dependent (EMC/WVD) algorithm. The EMC/WVD equation models the at-surface brightness temperature, given the at-sensor brightness temperature, along with an estimate of the total water vapor amount, sensor view angle, and emissivity. A four-dimensional look-up table (LUT) is used to correctly assign the regression coefficients in the EMC/WVD equation for the five TIR bands given the three independent variables (water vapor, view angle, emissivity range). The EMC/WVD LUT is then used on a pixel-by-pixel basis for adjusting the atmospheric parameters used to estimate the

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surface radiance. Emissivity information from the ASTER Global Emissivity Dataset (v3) is first gridded to the ECOSTRESS swath, spectrally adjusted, and then used to compute the minimum band emissivity at each pixel for assigning the appropriate WVS coefficients. Then the EMC/WVD coefficients are mapped to all ECOSTRESS pixels in a given swath through bi-cubic interpolation of the coefficients derived from the four factors: day/night case, view angle, minimum band emissivity, and precipitable water vapor. Bi-cubic interpolation assures smooth transitions in the EMC/WVD coefficients across the pixels.

3.2.4 Surface radiance

Before the TES algorithm can be applied to separate the temperature and emissivity components from the observed radiance, the surface radiance is computed by atmospherically correcting the observed L1 calibrated radiances (L1B_RAD) using atmospheric parameters output from the atmospheric correction module. These include the transmittance, path radiance, and downwelling sky irradiance for each band that have been geolocated to the ECOSTRESS swath. Details on the physics of this procedure are detailed in the L2 LST&E ATBD.

3.2.5 TES algorithm

Inputs to the TES algorithm include the surface radiance (at-sensor radiance corrected for transmittance and path radiance), downwelling sky irradiance term, MMD calibration coefficients, and LUT's for converting radiance into temperature and vice versa. Before the surface radiance is estimated, the accuracy of the atmospheric parameters are improved using a WVS model as described in 3.2.3. The TES outputs include LST, and emissivity for the 5 ECOSTRESS bands. The error estimates and broadband emissivity (EmisWB) are computed once TES is complete. Details of the NEM, ratio, and MMD modules within the TES algorithm are described in the L2 ATBD, including computation of the error estimates and EmisWB.

4.0 OTHER CONSIDERATIONS

4.1 Error handling

Error handling is managed using operating system exit codes. Each foreseeable disruption to data processing is assigned a unique exit code that is returned to the Process Control System (PCS).

4.2 Dependencies on existing software

The C language was chosen to implement the LST&E code to maximize the efficiency of processing large arrays. The main dependency linked to by the LST&E PGE is the Hierarchical Data Format (HDF) library, which is required for writing the ECOSTRESS product to file.

4.3 Assumptions and limitations

This software will process both day and nighttime ECOSTRESS scenes. It assumes calibrated and geolocated input radiances for each band with missing scan lines in bands 1 and 5 filled using the spatial neural net algorithm.

4.4 Quality assessment and recording

Indicators of quality are described exclusively in the quality control (QC) group in Table 2-2 generated during production. In addition to data quality, the QC data provides information on

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algorithm metrics for each pixel (e.g. convergence statistics). The QC SDS unsigned 16-bit data are stored as bit flags in the SDS. This QC information can be extracted by reading the bits in the 16-bit unsigned integer. The purpose of the QC SDS is to give the user information on algorithm results for each pixel that can be viewed in a spatial context. The QC information tells if algorithm results were nominal, abnormal, or if other defined conditions were encountered for a pixel. The QC information should be used to help determine the usefulness of the LST and Emissivity data for a users' needs.

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Appendix A: Abbreviations and Acronyms

ALEXI	Atmospheric-Land Exchange Inversion
ASD	Algorithm Specifications Document
ATBD	Algorithm Theoretical Basis Document
BESS	Breathing Earth Systems Simulator
DAAC	Distributed Active Archive Center
DisALEXI	ALEXI Disaggregation algorithm
ECOSTRESS	ECOsystem Spaceborne Thermal Radiometer on Space Station
ESI	Evaporative Stress Index
ET	Evapotranspiration
FLiES	Forest Light Environmental Simulator
GDS	Ground Data System
HDF	Hierarchical Data Format
Hz	Hertz
ICD	Interface Control Document
ISS	International Space Station
JPL	Jet Propulsion Laboratory
Km	kilometer
L0 – L4	Level 0 through Level 4
LP	Land Processes
LST	Land Surface Temperature
LSTE	Land Surface Temperature and Emissivity
m	meter
MODIS	Moderate Resolution Imaging Spectroradiometer
NASA	National Aeronautics and Space Administration
NCEP	National Centers for Environmental Protection
netCDF	Network Common Data Format
PCS	Process Control System
PGE	Product Generation Executable
PSD	Product Specifications Document
LST&E	Priestly-Taylor-JPL
QA	Quality Assurance
SDOS	Science Data Operations System
SDS	Science Data System
TBD	To Be Determined
TBR	To Be Reconciled
TBS	To Be Specified
USDA	United State Department of Agriculture
USGS	United States Geological Society
UTC	Coordinated Universal Time
WUE	Water Use Efficiency
XML	Extensible Markup Language

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