PySEBS V1.0.0 Actual Evapotranspiration (ETa) Calculator

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Software and data availability

Software: PySEBS V1.0.0.

Developers: Haipeng Liu, Pinpin Ren, and Yong Chen.

Hardware required: General-purpose computer.

Software required: ArcGIS 10.1-10.6.

Program language: Python.

Software and data availability: PySEBS software and 2019 case data are freely distributed through a Github public repository (https://github.com/haipengliuCAU/PySEBS).

PySEBS V1.0.0 Actual Evapotranspiration (ET_a) Calculator User's Guide

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1. Installing the PySEBS and software requirements

The PySEBS is a software that can be used to calculate actual evapotranspiration (ET_a) on a spatial scale based on the Surface Energy Balance System model (SEBS). The software is written in Python 2.7.14 due to Python (2.7) being the latest version supported by ArcGIS 10.1-10.6. Since ET_a is calculated on a spatial scale, the software operation utilizes some of the built-in tools in ArcGIS and the proper operation of these tools depends on calling of the Arcpy package in ArcGIS. Therefore, the user needs to ensure that the ArcGIS software is installed successfully.

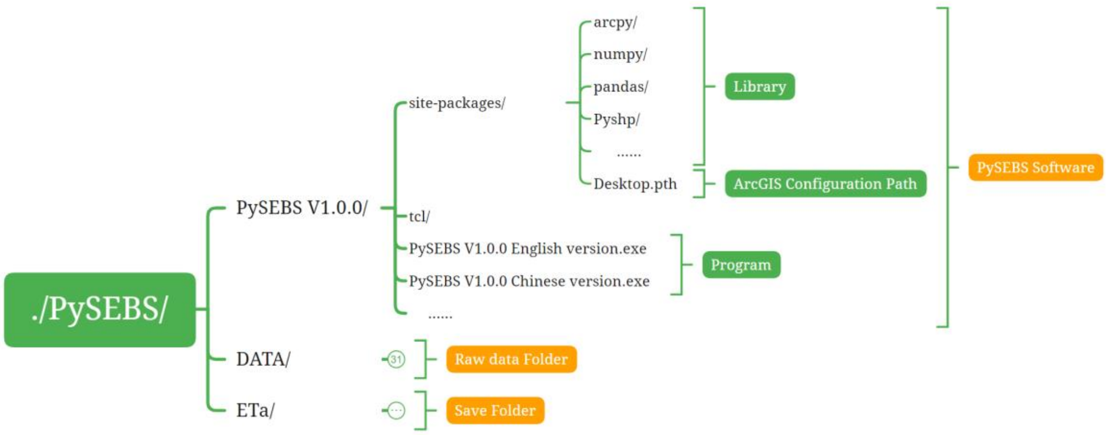


Figure S1 Schematic diagram of the PySEBS software file structure

The PySEBS software is compressed into a **PySEBS V1.0.0.zip** file. The schematic diagram of PySEBS file structure is shown in Figure S1. The schematic box labeled **./PySEBS/** represents a folder named PySEBS in the working directory, where the PySEBS 1.0.0.zip file will be stored after extraction. The PySEBS folder contains two parts: the **PySEBS V1.0.0.exe** program; and the site-packages folder containing the code libraries (arcpy package, numpy package, pandas package, Pyshp package, etc.) and the configuration **Desktop.pth** file.

To successfully run the software, the file path of the bin folder in the ArcGIS installation directory must be added to the **Desktop.pth** file so that the arcpy packages can be properly called (see Figure S2 for the procedure). The path of the bin folder in the ArcGIS installation directory is usually: **.\ArcGIS\Desktop10.6\bin**; and the location of the **Desktop.pth** file is: **.\PySEBS\site-packages.**

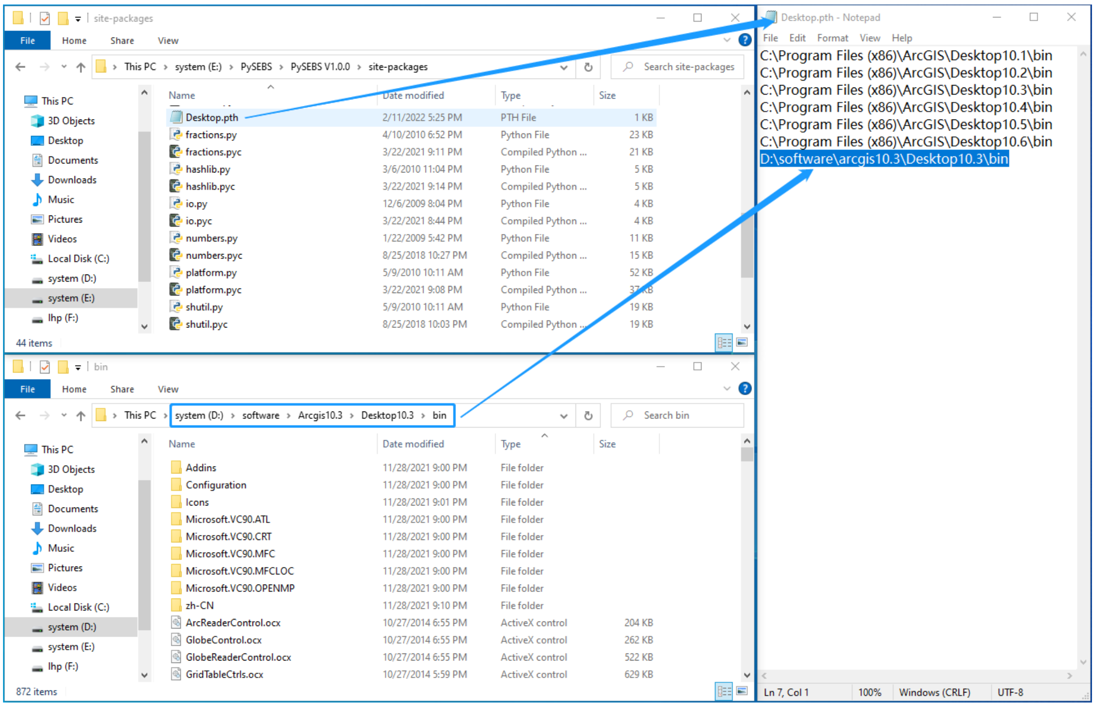


Figure S2 The path to the bin folder in the ArcGIS installation directory, and add the bin folder to the Desktop.pth file

2. Graphical User Interface Introduction

PySEBS software is a concise and straightforward scientific computing tool. It contains one main interface (Figure S3) and three sub-interfaces (Figs. 4-6). The main interface consists of three button controls: the remote sensing data processing module button, the meteorological data processing module button, and the PySEBS calculation and processing module button. Each button control accesses the corresponding module (sub-interface): Module 1 - Remote Sensing Data Processing interface, Module 2 - Meteorological Data Processing interface, and Module 3 - PySEBS Calculation Procedure interface.

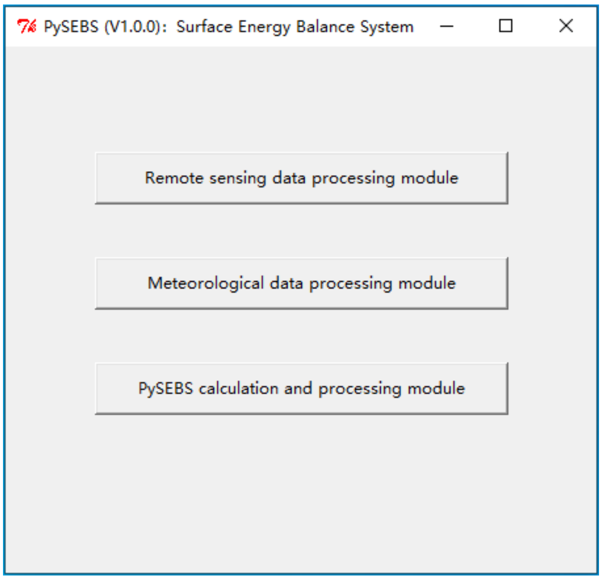


Figure S3 Main menu of PySEBS software

The main functions of Module 1 and Module 2 are to provide properly processed and formatted input data for use in Module 3. Module 3 is used to calculate ET_a on a daily/monthly/annual scale or for any period of time within a year and across years based on the input data (raster data) prepared by Modules 1 and 2. There is no processing priority between Modules 1 and 2. Moreover, there are common properties configured for all three modules, including time setting of the start and end year, file and folder pathway settings, selection of processing method, and information output.

Detailed instructions and notes for usage of each Module are provided below:

2.1 Module 1 - Remote Sensing Data Processing

Module 1 is used to process remote-sensed data and generate the daily data files in **.asc** format for input into Module 3 (Figure S4). Module 1 can only process data on an annual basis, and therefore the user must arrange the downloaded remote sensing files in specific folders by data type and by the year. For example, the path to MOD09A1 remote sensing data for the year of 2019 should be **.\PySEBS\DATA\RemoteSensingData\MOD09A1\2019**; and the path to the MOD11A2 remote sensing data for the year of 2019 should be **.\PySEBS\DATA\RemoteSensingData\MOD11A2\2019**.

The downloaded remote-sensed data needs to be pre-processed before it can used in the PySEBS program. For demonstration, remote-sensed data were obtained from the National Aeronautics and Space Administration (NASA, http://modis-land.gsfc.nasa.gov/). In this example, images h26v04 and h27v04 were downloaded and the MRT (MODIS Reprojection Tool) projection tool was applied to preprocess the data for merging, resampling, format conversion, etc., and Cygwin software was used for batch processing (Table S1 for specific parameters). The purpose of pre-processing is to convert the remote sensing data from hierarchical data format (**.hdf**) format to raster files (**.tif**). The location of the **.tif** file will be in the same folder as the **.hdf** file, and the name of the preprocessed **.tif** file must contain the date information string (7 digits) of the corresponding data; an example file name is **MOD09A1_2019001.sur_refl_b01.tif**.

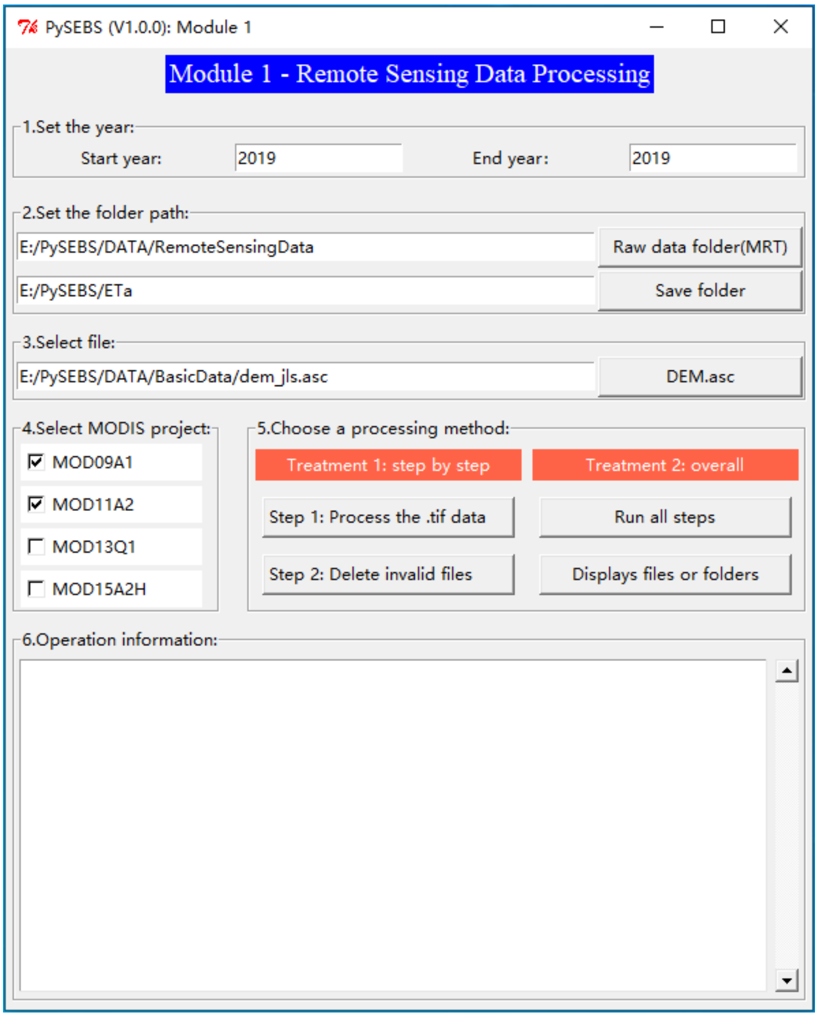


Figure S4 Module 1 - remote sensing data processing graphical user interface

Table S1 Basic information on MODIS products

Products	Surface characteristics parameters	Temporal resolution	Spatial resolution
MOD09A1	Surface albedo (Band 1-7) Solar zenith angle (Szen)	8 d	500 m
MOD11A2	Surface temperature (lst)	8 d	1000 m

The following describes the procedure for remote sensing data processing:

1. Locate all processed **.tif** files and copy them to the designated folder to preserve the integrity of the original data.

2. Clip all **.tif** files using the **DEM.asc** file of the study area to isolate the only the remote-sensed data in the study area.

3. Assign all invalid values as NoData (setnull) to prevent the influence of spurious values on the final calculation results of ET_a. The invalid values of "szen" parameter in MOD09A1 and "LST" parameter in MOD11A2 are 0; the invalid value of the band1-band7 parameter in MOD09A1 is -28672; the invalid value of "Fpar" parameter in MOD15A2H is 255; the invalid value of NDVI parameter in MOD13Q1 is -3000.

4. Convert **.tif** format files to **.asc** format.

5. Rename the files and save them as daily data in the required format.

Module 1 contains 6 label frames with the following corresponding functions:

1. The **Set the year** section defines the period of calculation, the **Start year** input box requires the users to specify the start year of the data processing; the **End year** input box requires the users to specify the end year of the data processing (Figure S4).

2. The **Raw data folder (MRT)** button in the **Set the folder path** section indicates the folder where the output data will be stored following MRT pre-processing; the **Save folder** button indicates the folder where the processed results are saved, and if this folder does not exist, the folder will be automatically created in the corresponding path.

3. The **DEM.asc** button in the **Select file** section is used to select the **DEM.asc** file of the study area, which is used to clip the remote sensing data within the study area.

4. The **Select MODIS project** section that contains checkboxes for MOD09A1, MOD11A2, MOD13Q1, and MOD15A2H options, which represent the types of remote-sensed data to be processed. During computing in this case study, the PySEBS model only used MOD09A1 and MOD11A2, so the default setting was selected for these two options. The remaining two options can be used in other studies.

5. The **Choose a processing method** section contains two data processing methods; "Treatment 1: step by step" means the data will be processed step by step, and "Treatment 2: overall" in which all steps will be processed (Figure S4). The **Step 1:**

Process the .tif data button performs a series of remote sensing data processing; The **Step 2: Delete invalid files** button deletes the transitional files generated during the processing of remote-sensed data, which is recommended due to the large amount of memory occupied by remote sensing. The **Run all steps** button proceeds to run Step 2 after the completion of Step 1. The **Display files or folders** button is a test button used to output the path of the selected files or folders, but does perform any actual computing processes.

6. The **Operation information** displays software prompt messages during the operation process, which is used to reveal the progress information.

2.2 Module 2 - Meteorological Data Processing

The function of Module 2 is to process the meteorological data and generate the daily file in **.asc** format required by Module 3 (Figure S5). The meteorological data used in this study is China's surface climate data daily value data set (V3.0), which is derived from the Chinese National Meteorological Information Center (http://data.cma.cn/site/index.html); the platform contains the daily meteorological data from 824 reference weather stations. The meteorological data in the dataset includes atmospheric pressure, air temperature, precipitation, evaporation, sunshine hours, surface temperature, wind speed and direction, and relative humidity at each station. The downloaded original meteorological data is in **.txt** format and includes all meteorological stations in each folder, which need to be preprocessed. Once the downloaded V3.0 weather datasets are placed in the same folder, Module 2 can be used to process the raw data directly. If meteorological datasets from other sources are used, they need to be organized in **.csv** format and stored in the 1RawData folder. An example of the corresponding path may be: **.\PySEBS\ETa\2MeteorologicalData\1RawData\2019.csv.**

The meteorological data will be processed as follows:

1. Pre-processing of V3.0 raw meteorological data. The raw meteorological dataset V3.0. can only be calculated on an annual basis. If the xxxx.csv (xxxx stands for the year, e.g., 2019) already exists in the folder (.\PySEBS\ETa\2MeteorologicalData\1RawData), no new file will be recreated, this

will help reduce computation time.

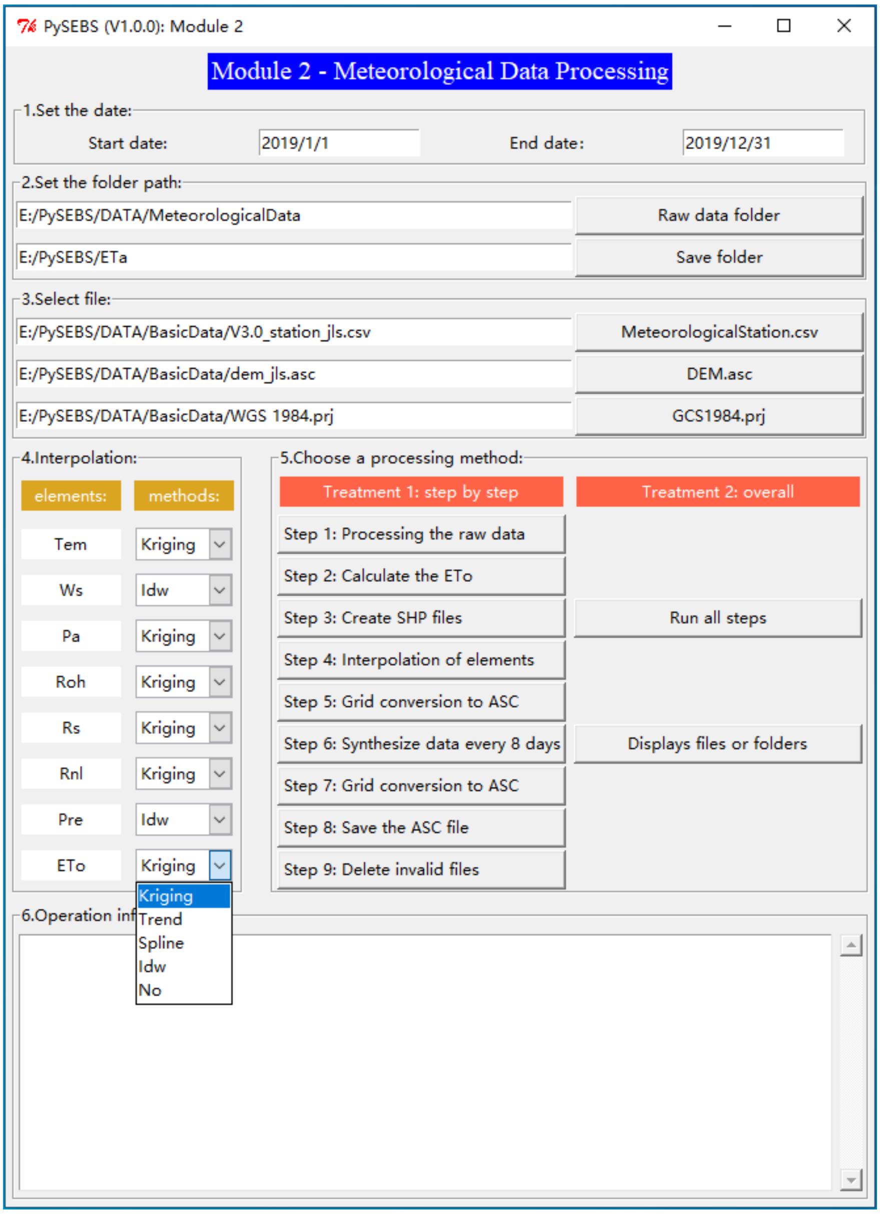


Figure S5 Module 2 - Meteorological data processing user graphical interface

2. Calculation of reference evapotranspiration (ET_o) and the parameters that require interpolation. ET_o and interpolation parameters can only be calculated on an annual basis. If the ET_o_xxxx.csv already exists in the folder (.\PySEBS\ETa\2MeteorologicalData\2SourceData), no file will be recreated.

3. Create a shapefile that includes all weather stations on a given day and define the projection to 1984.prj. The calculation can be done on a daily scale. No file will be

recreated if the shapefile already exists.

4. Interpolation is conducted for .shp files on a daily basis. If the interpolated file already exists, no file will be recreated.

5. The **GRID** format file can be converted to **.asc** format on a daily scale. If the .asc file already exists, no file will be recreated.

6. Synthesizing 8-day meteorological data. Since the temporal resolution of the remote sensing data is 8 days, the 8-day average of meteorological data will also be calculated. In this case, operations on a daily basis are allowed. If the 8-day average file already exists, no file will be recreated. Since the parameters Pre and ET_o are not involved in the operations of the PySEBS model, these two parameters do not perform processes 6 to 9.

7. Convert the 8-day average raster file to .asc format. It can be run on a daily basis. If the .asc file already exists, no file will be recreated.

8. Copy the .asc file to the designated folder. It can be run on a daily basis. No file will be recreated if the file already exists.

9. Delete the intermediate files generated during the operations to free up memory. When the date reaches the last day of the year, files generated in steps 4 to 7 will be deleted.

Module 2 contains 6 label frames with the following corresponding functions:

1. In the **Set the date** section, the **Start date** input box refers to the date when meteorological data processing begins; the **End date** input box refers to the date when meteorological data processing ends (Figure S5).

2. In the **Set the folder path** section, users can select a path where the raw meteorological dataset V3.0 can be saved using the **Raw data folder** button; the **Save folder** button indicates the folder where the processed meteorological results are saved, and if such folder does not exist, a new folder will be created automatically in the corresponding path to save the data.

3. In the **Select file** section, the **MeteorologicalStation.csv** button indicates the station zone number extracted from the meteorological dataset V3.0, which contains the information of the weather stations within the study area; the **DEM.asc** button allows the user to select the **DEM.asc** file of the study area, which has three purposes: 1) to define the output range of the study area during interpolation; 2) to multiply DEM.asc by 0 as an initial term of the accumulation; and 3) to be copied to the daily standard file and used as an input parameter for the PySEBS calculation. The **GCS1984.prj** button indicates the selection of the GCS1984.prj geographic coordinate system file, which is used to define the coordinate system in the interpolation process.

4. The **Interpolation** section contains two columns: the meteorological elements to be interpolated and the corresponding combobox of available interpolation methods. There are eight meteorological elements that need to be interpolated: Tem (mean air temperature, °C), Ws (wind speed at 2 m above earth's surface, m s^{-1}), Pa (atmospheric pressure at 2 m above earth's surface, kPa), Roh (specific humidity, kg kg^{-1}), Rs (daily mean shortwave radiation, MJ m^{-2} day^{-1}), Rnl (daily mean net outgoing longwave radiation, MJ m^{-2} day^{-1}), Pre (precipitation, mm), and ET_o (reference evapotranspiration, mm). All the main parameters are required in the Module 3 calculation, except for precipitation and ET_o. The corresponding interpolation methods include Kriging, Trend, Spline, and Inverse distance weight (Idw); in addition, the users may select **No** under the interpolation method, if certain parameters do not require interpolation.

Different parameters require different interpolation methods, and the default setting for each parameter in Module 2 is the most suitable interpolation method (Figure S5). The optimal interpolation method was selected based on the 10-fold cross validation results generated by different interpolation methods (Kriging, Trend, Spline, and Inverse distance weighting methods) using the meteorological data from 57 weather stations in Jilin province and its surrounding regions in 2017. The validation metrics include Mean Absolute Error (*MAE*), Mean Relative Error (*MRE*), Root Mean Square Error (*RMSE*), and Nash-Sutcliffe Efficiency (*NSE*). The optimal interpolation method for each parameter is shown in Tables 2 and 3.

Table S2 The most suitable interpolation method for each parameter

Parameter	Interpolation method	Parameter	Interpolation method
Mean air temperature (Tem)	Kriging	Wind speed (Ws)	Idw
Atmospheric pressure (Pa)	Kriging	Specific humidity (Roh)	Kriging
Daily average net outgoing longwave radiation (Rnl)	Kriging	Daily mean shortwave Radiation (Rs)	Kriging
Precipitation (Pre)	Idw	Reference evapotranspiration (ET_o)	Kriging

Table S3 Comparison of interpolation methods for each parameter

Validation metrics	Mean air temperature (Tem)				Wind speed (Ws)			
	Kriging	Trend	Spline	Idw	Kriging	Trend	Spline	Idw
MAE	0.8639	1.3015	1.1319	0.9344	0.4985	0.5372	0.7043	0.4823
MRE	-	-	-	-	-	-	-	-
RMSE	1.1925	1.7410	1.6028	1.2630	0.6815	0.7194	0.9802	0.653
NSE	0.9925	0.9841	0.9865	0.9916	0.5741	0.5253	0.1188	0.6089
Validation metrics	Atmospheric pressure (Pa)				Relative humidity (Roh)			
	Kriging	Trend	Spline	Idw	Kriging	Trend	Spline	Idw
MAE	668.46	1188.45	886.25	794.42	0.0004	0.0005	0.0005	0.0004
MRE	0.0003	0.0005	0.0007	0.0002	0.0126	0.0194	0.0078	0.0256
RMSE	982.62	1601.77	1193.10	1084.37	0.0006	0.0008	0.0008	0.0007
NSE	0.7249	0.2689	0.5944	0.6649	0.9856	0.9779	0.9768	0.9846
Validation metrics	Shortwave Radiation (Rs)				Net outgoing longwave radiation (Rnl)			
	Kriging	Trend	Spline	Idw	Kriging	Trend	Spline	Idw
MAE	15.497	20.116	19.580	15.792	5.5267	7.1679	7.0491	5.6463
MRE	22.710	28.312	28.915	22.986	7.7102	9.5248	9.8900	7.8061
RMSE	0.1134	0.1508	0.1386	0.1169	0.1121	0.1502	0.1381	0.1156
NSE	0.9822	0.9734	0.9718	0.9817	0.9815	0.9728	0.9701	0.9811
Validation	Precipitation (Pre)				Reference evapotranspiration (ET_o)			

metrics	Kriging	Trend	Spline	Idw	Kriging	Trend	Spline	Idw
MAE	-	1.5790	1.6705	1.2271	0.2680	0.3619	0.3428	0.2751
MRE	-	5.0624	6.1559	4.5141	0.0381	0.0622	0.0272	0.0425
RMSE	-	-	-	-	0.4007	0.5199	0.5229	0.4092
NSE	-	0.3334	-0.2875	0.4878	0.9531	0.9211	0.9201	0.9511

5. The **Choose a processing method** section includes 2 data processing treatments: **Treatment 1: step by step** indicates the data can be processed step by step; **Steps 1-9** represent a series of processing steps for meteorological data, which are described previously. **Treatment 2: overall** means to process data at once; **Run all steps** means to run **Steps 1-9** in order. **Display files or folders** is a test button to output the path of selected files and folders, which is not involved in the calculation. If the users select "Treatment 1", the next step cannot be proceeded until the previous step is finished. However, some procedures are very time-consuming, such as interpolation. By contrast, "Treatment 2" performs more efficiently in data processing.

6. **Operation information** section shows system information during the software operation to indicate progress information.

2.3 Module 3 - PySEBS Calculation Procedure

Module 3 uses the daily input data (in .asc format) generated by Module 1 and Module 2 to calculate ET_a on a daily/monthly/annual basis or for a specified period of time (Figure S6). The PySEBS model requires 15 necessary parameters. Module 1 provides 8 essential parameters, including 7 parameters from MOD09A1 (Band1, Band2, Band3, Band4, Band5, Band7, and Szen) and 1 parameter from MOD11A2 (Lst). Module 2 provides 7 essential parameters, including the DEM parameter and 6 meteorological related parameters (Tem, Ws, Pa, Roh, Rs, and Rnl). Moreover, there are 2 non-essential parameters, Pre and ET_o, which are not involved in the PySEBS calculation process.

Module 3 includes 5 label frames, with the following corresponding functions:

1. In the **Set the date** section, users can specify the starting and ending dates of the data processing.

2. In the **Select folder path and file** section, the **Save folder** button allows the users to select the path, where the PySEBS input files (folder 3PySEBSInputData) and output files (folder 4PySEBSOutputData) will be stored; if the folder for output data does not exist, a new folder will be created in the corresponding path. The **DEM.asc** button means to select the DEM.asc file for the study area, which can be used as the initial term of the accumulation after multiplying the DEM.asc by 0.

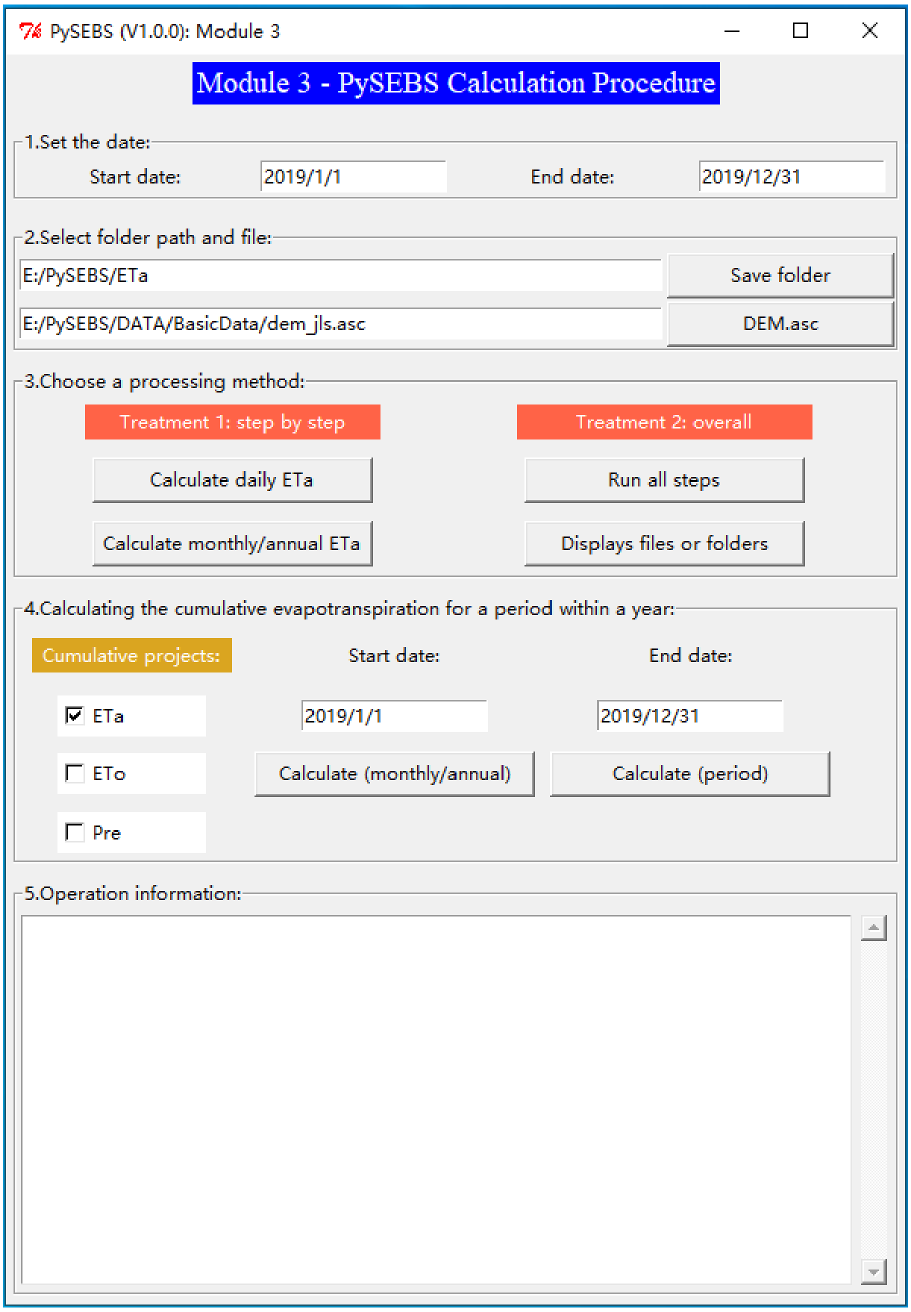


Figure S6 Module 3 - PySEBS calculation and processing user graphical interface

3. The **Choose a processing method** section includes 2 data processing methods: **Treatment 1: Step by step** means to process the data in separate steps; **Treatment 2: overall** means to run all steps automatically. **Calculate daily ET_a** button indicates to calculate daily ET_a; the **Calculate monthly/annual ET_a** button indicates to calculate monthly/annual ET_a; the **Run all steps** button indicates to calculate the daily, monthly, and annual ET_a at the same time; the **Display files or folders** is a test button, which is used to output the path of the selected files or folders and is not involved in the software calculation process.

4. In the **Calculating the cumulative evapotranspiration for a period within a year** section, the **Cumulation projects** contain three checkboxes (ET_a, ET_o, and Pre) representing the selection of the project to be accumulated; the users may specify the dates for the calculation period in the **Start date** and **End date** input boxes; the **Calculate (monthly/annual)** button indicates to calculate the monthly, and annual project at the same time; the **Calculate (period)** button indicates to calculate the cumulative project for a period of time within a year.

5. In the **Operation information** section, the system information can be shown to reveal the progress information.

3. PySEBS software theoretical foundation

The SEBS model as proposed by Su (2002) is a single-layer model based on the surface energy balance principle (Su, 2002), which consists of four components: 1) The determination of the land surface physical parameters based on the remotely sensed spectral reflectance and radiance; 2) The estimation of the roughness length for heat transfer; 3) The calculation of sensible heat flux; and 4) The calculation of latent heat flux. Compared with other single-layer models based on the energy balance principle, the PySEBS model has the advantage that the data in each gird is calculated independently, so that even if some grids have missing data on a certain day due to the influence of rain and clouds, the calculation in other grids will not be affected; this can maximize the utilization of the remote sensing data. The calculation process of the surface energy balance system and the implementation steps of PySEBS software are shown in Figure 7.

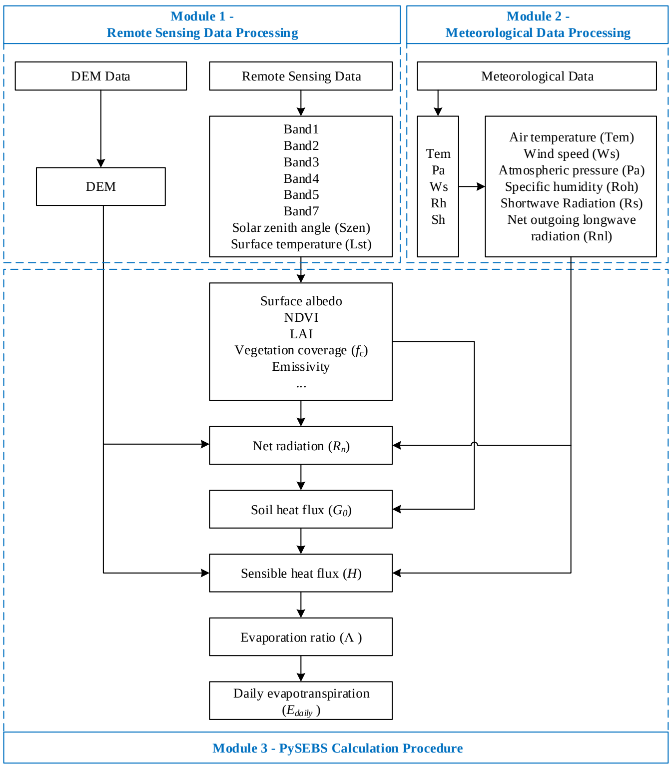


Figure S7 The calculation process of surface energy balance system and the steps of PySEBS software implementation.

The net earth's surface radiation is the basis of various energy exchanges and can be divided into three parts: 1) The soil heat flux that warms the soil; 2) The sensible heat flux that warms the atmosphere; and 3) The latent heat flux of evapotranspiration (the latent heat of soil evaporation and crop transpiration). The equation for surface energy balance can be expressed as:

$$R_n = G_0 + H + \lambda E \tag{1}$$

where R_n is the net radiation (W m^{-2}), G_0 is the soil heat flux (W m^{-2}), H is the sensible heat flux (W m^{-2}), and λE is the latent heat flux (W m^{-2}), in which λ is the latent heat of evaporation (J kg^{-3}) and E is the actual evopotranspiration (mm d^{-1}). After calculating each parameter of the surface energy balance separately, the actual daily ET_a can be obtained according to the constant evaporation ratio within one day.

3.1 Calculations of net radiation R_n

$$R_n = (1-\alpha) \cdot R_{swd} + \varepsilon \cdot R_{lwd} - \varepsilon \cdot \sigma \cdot T_0^4 \tag{2}$$

where α is surface albedo, a ratio of radiation reflected by the surface to global radiation (a sum of direct solar radiation and scattered radiation); R_{swd} and R_{lwd} (W m^{-2}) represent downward solar radiation and downward long-wave radiation, respectively; ε is surface emissivity and can be classified into ε_{land} (surface emissivity of land) and ε_{water} (surface emissivity of water) according to different underlying surfaces; σ is the Stephan Boltzmann constant equal to 5.67×10^{-8} (W m^{-2} K^{-2}); and T_0 is the surface temperature (K).

The equations for calculating each component are as follows:

$$\alpha = 0.160 \cdot r_1 + 0.291 \cdot r_2 + 0.243 \cdot r_3 + 0.116 \cdot r_4 + 0.112 \cdot r_5 + 0.018 \cdot r_7 - 0.0015 \tag{3}$$

$$R_{swd} = I_{sc} \cdot d_r \cdot cos\theta_z \cdot \tau \tag{4}$$

$$R_{lwd} = \varepsilon_a \cdot \sigma \cdot T_a^4 \tag{5}$$

$$\varepsilon = \begin{cases} \varepsilon_{land} & ,\alpha \geq 0.035 \\ \varepsilon_{water} & ,\alpha < 0.035 \end{cases} \tag{6}$$

$$\varepsilon_{land} = \begin{cases} 0.9825 - 0.051 \cdot Bred & ,NDVI < 0.2 \\ 0.971 + 0.018 \cdot f_c & ,0.2 \leq NDVI \leq 0.5 \\ 0.990 & ,NDVI > 0.5 \end{cases} \tag{7}$$

$$\varepsilon_{water} = 0.995 \tag{8}$$

$$\tau_{sw} = 0.75 + 2 \times 10^{-5} \cdot DEM \tag{9}$$

$$\varepsilon_a = 9.2 \cdot 10^{-6} \cdot T_a^2 \tag{10}$$

$$d_r = 1 + 0.033 \cdot \cos(2\pi \cdot dn / 365) \tag{11}$$

$$f_c = (NDVI - NDVI_{\min})^2 / (NDVI_{\max} - NDVI_{\min})^2 \tag{12}$$

$$NDVI = (Bnir - Bred) / (Bnir + Bred) \tag{13}$$

where r_1, r_2, r_3, r_4, r_5, and r_7 are wave bands 1-7 of MOD09A1; I_{sc} is a solar constant, I_{sc} = 1367 (W m^{-2}); d_r is orbital eccentricity correction coefficient of the earth; θ_z is solar zenith angle derived from MOD9A1; τ_{sw} is atmospheric transmissivity; ε_{land} and ε_{water} represent emissivity for land and emissivity for water, respectively; $Bred$ is the infrared band i.e., r_1; f_c is vegetation coverage inversed through remote sensing data; DEM is the elevation (m); ε_a is atmospheric transmissivity; T_a is air temperature (K) at the reference elevation; dn refers to the day of year; $NDVI$ is a normalized vegetation coverage index; $NDVI_{min}$ and $NDVI_{max}$ are the minimum and maximum values of vegetation coverage index, where $NDVI_{min}$ = 0.2 and $NDVI_{max}$ = 0.5; DEM is the elevation (m); and $Bnir$ is the near-infrared band i.e., r_2.

3.2 Calculations of soil heat flux G_0

$$G_0 = R_n \cdot [\Gamma_c + (1 - f_c) \cdot (\Gamma_s - \Gamma_c)] \tag{14}$$

where Γ_c is the ratio of soil heat flux to net radiation in the condition of total vegetation cover, (Γ_c = 0.05), and Γ_s is a ratio of soil heat flux to net radiation in the condition of bare soil (Γ_s = 0.315).

3.3 Calculations of sensible heat flux H

The theoretical calculation of the sensible heat flux is given by:

$$H = \rho C_p \frac{\theta_0 - \theta_a}{r_a} \tag{15}$$

$$r_a = \frac{1}{k u_*}\left[\ln\left(\frac{z - d_0}{z_{0h}}\right) - \Psi_h\left(\frac{z - d_0}{L}\right) + \Psi_h\left(\frac{z_{0h}}{L}\right)\right] \tag{16}$$

where ρ for air density (kg m^{-3}); C_p for constant-pressure specific heat (J kg^{-1} K^{-1}); θ_0 for latent surface temperature (K); θ_a for latent air temperature (K) at an elevation of z; r_a for external resistance; k for Karman constant (k=0.4); u_* for friction velocity (m s^{-1}); z for reference measured elevation (m), generally between 2 and 10 m; d_0 for zero plane displacement height (m); z_{0h} for scalar roughness height for heat transfer (m); Ψ_h for stability correction coefficients of heat exchange MOS; and L for Obukhov length (m).

The following equation group can be built simultaneously to solve the friction velocity and Obukhov length through repeated iterations:

$$u = \frac{u_*}{k}\left[\ln\left(\frac{z - d_0}{z_{0m}}\right) - \Psi_m\left(\frac{z - d_0}{L}\right) + \Psi_m\left(\frac{z_{0m}}{L}\right)\right] \tag{17}$$

$$\theta_0 - \theta_a = \frac{H}{k u_* \rho C_p}\left[\ln\left(\frac{z - d_0}{z_{0h}}\right) - \Psi_h\left(\frac{z - d_0}{L}\right) + \Psi_h\left(\frac{z_{0h}}{L}\right)\right] \tag{18}$$

$$L = -\frac{\rho C_p u_*^3 \theta_v}{kgH} \tag{19}$$

where u stands for wind velocity at the reference elevation (m s^{-1}); z_{0m} for roughness height for momentum transfer (m); Ψ_m for stability correction coefficients of momentum exchange MOS; θ_v for latent near-surface virtual temperature (K); and g for gravitational acceleration, where g = 9.81 (m s^{-2}).

Calculation of vegetation height h:

$$h = h_{min} + \frac{\left(h_{max} - h_{min}\right)\cdot\left(NDVI - NDVI_{soil}\right)}{\left(NDVI_{veg} - NDVI_{soil}\right)} \tag{20}$$

where h refers to vegetation height (m); h_{min} represents the minimum height (m) of vegetation, and h_{min} = 0.0012; h_{max} is the maximum height (m) of vegetation, and h_{max} = 2.5; $NDVI_{veg}$ stands for *NDVI* in a condition of total vegetation cover and $NDVI_{veg}$ = 0.8; Regarding pixels of completely bare soil, $NDVI_{soil}$ = 0.0.

Calculation of zero plane displacement height d_0:

$$d_0 = d_{2h} \cdot h \tag{21}$$

$$d_{2h} = 1 - \frac{1 - \exp\left(-2 \cdot n_h\right)}{2 \cdot n_h} \tag{22}$$

$$n_h = \frac{C_d \cdot LAI}{2 \cdot u_{*2uh}^2} \tag{23}$$

$$u_{*2uh} = c_1 - c_2 \cdot \exp\left(-c_3 \cdot C_d \cdot LAI\right) \tag{24}$$

$$LAI = \left(\frac{NDVI \cdot \left(1 + NDVI\right)}{1 - NDVI}\right)^{1/2} \tag{25}$$

where d_{2h}, n_h, and u_{*2uh} are all intermediate parameters; while c_1 = 0.320, c_2 = 0.264, and c_3 = 15.1; C_d is a leaf drag coefficient equal to 0.2; and LAI is the leaf area index.

Calculation of roughness height for momentum transfer z_{0m}:

$$z_{0m} = z_{02h} \cdot h \tag{26}$$

$$z_{02h} = \left(1 - d_{2h}\right) \cdot \exp\left(-k \cdot u_{*2uh}^{-1}\right) \tag{27}$$

where z_{02h} is intermediate parameter.

Calculation of scalar roughness height for heat transfer z_{0h}:

$$z_{0h} = z_{0m} / \exp\left(kB^{-1}\right) \tag{28}$$

$$kB^{-1} = \frac{kC_d}{4C_t \dfrac{u_*}{u(h)}\left(1 - e^{-n_{ec}/2}\right)} f_c^2 + 2 f_c f_s \frac{k \cdot u_* / u(h) \cdot z_{0m} / h}{C_t^*} + kB_s^{-1} f_s^2 \tag{29}$$

The first term of kB^{-1} represents total vegetation cover:

$$\frac{u_*}{u(h)} = d_1 - d_2 \cdot \exp\left(-d_3 \cdot C_d \cdot LAI\right) \tag{30}$$

$$n_{ec} = \frac{C_d \cdot LAI}{2u_*^2 / u(h)^2} \tag{31}$$

The second term of kB^{-1} represents partial vegetation cover:

$$f_s = 1 - f_c \tag{32}$$

$$C_t^* = \Pr^{-2/3} \mathrm{Re}^{-1/2} \tag{33}$$

$$\mathrm{Re} = h \cdot u_* / \nu \tag{34}$$

$$u(h) = \frac{u \cdot \ln(2.446)}{\ln\left(\frac{z - d_0}{z_{0m}}\right)} \tag{35}$$

$$\nu = 1.327 \cdot 10^{-5} (p_0 / p)(T_a / T_{a0})^{1.81} \tag{36}$$

The third term of kB^{-1} represents total bare soil cover:

$$kB_s^{-1} = 2.46(\mathrm{Re}_*)^{1/4} - \ln(7.4) \tag{37}$$

$$\mathrm{Re}_* = h_s \cdot u_*^{soil} / \nu \tag{38}$$

$$u_*^{soil} = \frac{u \cdot k}{\ln\left(\frac{z}{h_s}\right)} \tag{39}$$

where B^{-1} stands for a dimensionless heat transfer coefficient, a reverse Stanton number; C_t stands for a heat transfer coefficient of leaves and $C_t = 0.01$; $u(h)$ represents horizontal wind speed (m s^{-1}) at the top of the canopy; f_c represents vegetation coverage inversed by remote sensing data; C_t^* represents a heat transfer coefficient of soil; Besides, $d_1 = 0.38$ and $d_3 = 15.1$; Pr stands for a Prandtl number and $\mathrm{Pr} = 0.71$; Re is the Reynolds number of roughness under partial vegetation cover; ν stands for aerodynamic viscosity coefficient; p_0 is standard atmospheric pressure and $p_0 =$ 101.325 (kPa); p refers to atmospheric pressure at the reference elevation (kPa); T_a is air temperature at the reference elevation (K); T_{a0} stands for standard temperature and $T_{a0} = 273.15$ (K); Re_* stands for Reynolds number of roughness; h_s stands for soil roughness and $h_s = 0.009$ (m); and u_*^{soil} is the frictional wind speed under full bare soil cover (m s^{-1}).

Calculation of the correction functions $\Psi_m(y)$ and $\Psi_h(y)$ of the Monin-Obukhov similarity (MOS) stability:

$$\Psi_m(y)=\begin{cases}-\left[a_s\cdot y+b_s\cdot\left(y-\frac{c_s}{d_s}\right)\cdot\exp\left(-d_s\cdot y\right)+\frac{b_s\cdot c_s}{d_s}\right] & ,y>0\\ \ln(a-y)-3\cdot b\cdot(-y)^{1/3}+\frac{b\cdot a^{1/3}}{2}\cdot\ln\left[\frac{(1+x)^2}{\left(1-x+x^2\right)}\right] & ,-b^{-3}\le y\le 0\\ +3^{1/2}\cdot b\cdot a^{1/3}\cdot\tan^{-1}\left[\frac{(2x-1)}{3^{1/2}}\right]+\Psi_0 & \\ \Psi_m\left(b^{-3}\right) & ,y\le -b^{-3}\end{cases}$$

(40)

$$\Psi_h(y)=\begin{cases}-\left[\left(1+\frac{2a_s}{3}y\right)^{1.5}+b_s\cdot\left(y-\frac{c_s}{d_s}\right)\cdot\exp(-d_s\cdot y)+\left(\frac{b_s\cdot c_s}{d_s}-1\right)\right] & ,y>0\\ \left[\frac{(1-d)}{n}\right]\cdot\ln\left[\frac{\left(c+y^n\right)}{c}\right] & ,y\le 0\end{cases}$$

(41)

$$x=(y/a)^{1/3} \tag{42}$$

$$\Psi_0=-\ln a+3^{1/2}\cdot b\cdot a^{1/3}\cdot\pi/6 \tag{43}$$

where x and Ψ_0 refers to integration constants; a =0.33, b =0.41, c =0.33, d =0.057, n =0.78, a_s =1, b_s =0.667, c_s =5, and d_s =1.

Other parameters:

$$\rho=1.293\cdot\frac{p}{p_0}\cdot\frac{273.15}{T_a} \tag{44}$$

$$C_p=S\cdot C_{pw}+(1-S)\cdot C_{pd} \tag{45}$$

$$S = \frac{0.622 \cdot e_a}{p - (1 - 0.622) \cdot e_a} \tag{46}$$

$$e_a = e_s \cdot \frac{RH_{mean}}{100} \tag{47}$$

$$e_s = \frac{e^o(T_{max}) + e^o(T_{min})}{2} \tag{48}$$

$$e^o(T_{max}) = 0.618 \cdot \exp\left(\frac{17.27 \cdot (T_{max} - 273.15)}{(T_{max} - 273.15) + 237.3}\right) \tag{49}$$

$$e^o(T_{min}) = 0.618 \cdot \exp\left(\frac{17.27 \cdot (T_{min} - 273.15)}{(T_{min} - 273.15) + 237.3}\right) \tag{50}$$

$$\theta_0 = T_0 \cdot \left(\frac{p_0}{p_s}\right)^{0.286} \tag{51}$$

$$\theta_a = T_a \cdot \left(\frac{p_0}{p}\right)^{0.286} \tag{52}$$

$$\theta_v = T_a \cdot \left(\frac{p_0}{p}\right)^{0.286} \cdot (1 + 0.61 \cdot S) \tag{53}$$

$$p_s = 101.3 \cdot \left(\frac{293 - 0.0065 \cdot DEM}{293}\right)^{5.26} \tag{54}$$

where ρ is the density of air (kg m^{-3}); S refers to specific humidity (kg kg^{-1}); C_{pw} refers to special heat of vapor and C_{pw}=1846.0 (J kg^{-1} K^{-1}); C_{pd} refers to special heat of dry air and C_{pd}=1005.0 (J kg^{-1} K^{-1}); e_a and e_s are the actual and saturated water vapor pressure (kPa), respectively; RH_{mean} is the daily average relative humidity (%); T_{max} and T_{min} are the daily maximum and minimum air temperature (K) at the reference altitude, respectively; T_0 is the surface temperature (K); p_s is the surface air pressure (kPa); and DEM is the elevation (m).

3.4 Calculations of evaporation ratio Λ

The evaporation ratio is a specific value of energy utilized by actual evapotranspiration to the available energy. It can be calculated by using the following equations:

$$\Lambda = \frac{\lambda E}{H + \lambda E} = \frac{\lambda E}{R_n - G_0} = \frac{\Lambda_r \cdot \lambda E_{wet}}{R_n - G_0} \tag{55}$$

$$\Lambda_r = \frac{\lambda E}{\lambda E_{wet}} = 1 - \frac{\lambda E_{wet} - \lambda E}{\lambda E_{wet}} = 1 - \frac{H - H_{wet}}{H_{dry} - H_{wet}} \tag{56}$$

where Λ_r is the relative evaporation ratio; λE_{wet} is the latent heat flux (W m^{-2}) in a condition of humidity limit; H_{wet} is the sensible heat flux (W m^{-2}) in a condition of humidity limit; and H_{dry} is the sensible heat flux (W m^{-2}) in a condition of dry limit.

Regarding λE_{wet} and H_{dry} in a dry limit, and λE_{wet} and H_{wet} in a humidity limit, they are expressed in the equations below:

$$\lambda E_{dry} = R_n - G_0 - H_{dry} \equiv 0 \text{ , or } H_{dry} = R_n - G_0 \tag{57}$$

$$\lambda E_{wet} = R_n - G_0 - H_{wet} \text{ , or } H_{wet} = R_n - G_0 - \lambda E_{wet} \tag{58}$$

$$H_{wet} = \left(\left(R_n - G_0 \right) - \frac{\rho_{wet} C_p}{r_{ew}} \cdot \frac{e_s - e}{\gamma} \right) / \left(1 + \frac{\Delta}{\gamma} \right) \tag{59}$$

$$r_{ew} = \frac{1}{k u_*} \left[\ln\left(\frac{z - d_0}{z_{0h}} \right) - \Psi_h \left(\frac{z - d_0}{L_w} \right) + \Psi_h \left(\frac{z_{0h}}{L_w} \right) \right] \tag{60}$$

$$L_w = -\frac{\rho_{wet} u_*^3}{kg \cdot 0.61 \cdot \left(R_n - G_0 \right) / \lambda} \tag{61}$$

$$\rho_{dry} = \frac{(p - e_a) \cdot 1000}{R_d \cdot T_a} \tag{62}$$

$$\rho_{wet} = \frac{(p - 0.378 \cdot e_a) \cdot 1000}{R_d \cdot T_a} \tag{63}$$

$$e_a = p \cdot S \cdot \frac{R_v}{R_d} \tag{64}$$

$$e_s = 0.611 \cdot \exp\left(\frac{17.502 \cdot (T_0 - 273.15)}{(T_0 - 273.15) + 240.97} \right) \tag{65}$$

$$\gamma = \frac{C_p \cdot p}{\left[2.501 - 0.00234 \cdot (T_a - 273.15)\right] \cdot 10^6 \cdot 0.622} \tag{66}$$

$$\lambda = \left[2.501 - 2.361 \cdot 10^{-3} \cdot (T_a - 273.15)\right] \cdot 10^6 \tag{67}$$

$$\Delta = \frac{4098 \cdot \left[0.6108 \cdot \exp\left(\frac{17.27 \cdot (T_a - 273.15)}{(T_a - 273.15) + 237.3} \right) \right]}{\left((T_a - 273.15) + 237.3 \right)^2} \tag{68}$$

where ρ_{wet} is the density of wet air (kg m^{-3}); ρ_{dry} is the density of dry air (kg m^{-3}); C_p for constant-pressure specific heat (J kg^{-1} K^{-1}); r_{ew} for external resistance at the wet limit; e_a and e_s are the actual and saturated water vapor pressure (kPa), respectively, $e_s - e_a$ is the saturation water vapor pressure difference (kPa); γ is a constant of psychrometer (Pa K^{-1}); Δ is the changing rate of vapor pressure versus temperature; L_w is the Obukhov length at the wet limit (m); u_* for friction velocity (m s^{-1}); k for Karman constant (k =0.4); g is the gravitational acceleration, where g = 9.81 (m s^{-2}); λ is the latent heat of vaporization of water (J kg^{-1}); p refers to atmospheric pressure at the reference elevation (kPa); R_d is a gas constant of dry air and R_d=287.04 (J kg^{-1} K^{-1}); T_0 is the surface temperature (K); T_a is air temperature at the reference elevation (K); S refers to specific humidity (kg kg^{-1}); and R_v is a gas constant of vapor and equals to 461.5 (J kg^{-1} K^{-1}).

3.5 Calculations of daily evapotranspiration E_{daily}

The previously calculated net surface radiation, soil heat flux, and sensible heat flux are based on the instantaneous values at the moment of satellite transit. In contrast, in the PySEBS model, the daily evapotranspiration is calculated from the evaporation ratio with the daily average net radiation and daily average soil heat flux. The evapotranspiration ratio remains stable throughout the day (Shuttleworth, 1989; Sugita and Brutsaert, 1991; Crago, 1996; Li,2014), and assuming that the evapotranspiration ratio is constant throughout the day, the daily evapotranspiration is calculated by the following equation:

$$E_{daily} = 8.64 \cdot 10^7 \cdot \overset{24}{\underset{0}{\Lambda}} \cdot \frac{\overline{R_n} - \overline{G_0}}{\lambda \rho_w} \tag{69}$$

$$\overline{R_n} = (1-\alpha) K_{24}^{\downarrow} + \varepsilon L_{24} \tag{70}$$

$$\overline{G_0} \approx 0 \tag{71}$$

In the above equation, E_{daily} stands for the actual daily evapotranspiration (mm day^{-1}); 8.64×10^7 stands for a unit conversion coefficient; $\overset{24}{\underset{0}{\Lambda}}$ stands for daily mean evaporation ratio that can be substituted by the evaporation ratio Λ figured out by the PySEBS model; $\overline{R_n}$ stands for daily mean net radiation flux (W m^{-2}); and $\overline{G_0}$ stands for daily mean soil heat flux (W m^{-2}), considering that the amount of heat absorbed and released by soil is approximately equal during the day, the daily mean soil heat flux is set to 0. Additionally, λ refers to the latent heat of vaporization of water and λ=2.45 · 10^6 (J kg^{-1}); ρ_w refers to the density of water and ρ_w=1000 (kg m^{-3}); α is the surface albedo (see Equation 3); $K_{24}^{\downarrow}$ refers to incident global radiation (W m^{-2}), which is obtained through the unit conversion of the incident solar radiation (MJ m^{-2} day^{-1}) expressed in the Penman-Monteith equation; ε is surface emissivity(see Equation 6, 7, 8); and L_{24} refers to daily net outgoing long-wave radiation (W m^{-2}), which is obtained through the unit conversion of the net long-wave radiation (MJ m^{-2} day^{-1}) expressed in the Penman-Monteith equation.

The daily incident shortwave radiation $K_{24}^{\downarrow}$ at the surface is calculated as follows:

$$K_{24}^{\downarrow} = \frac{R_s \cdot 10^6}{24 \cdot 3600} \tag{72}$$

$$R_s = R_a \cdot \tau \tag{73}$$

$$\tau = a_{s0} + b_{s0} \frac{n}{N} \tag{74}$$

$$R_a = \frac{24 \cdot 60}{\pi} \cdot G_{sc} \cdot d_r \cdot \left[\omega_s \cdot \sin(\varphi) \cdot \sin(\delta) + \cos(\varphi) \cdot \cos(\delta) \cdot \sin(\omega_s) \right] \tag{75}$$

$$d_r = 1 + 0.033 \cdot \cos\left(\frac{2\pi}{365} \cdot J \right) \tag{76}$$

$$\omega_s = \arccos\left[-\tan(\varphi) \cdot \tan(\delta) \right] \tag{77}$$

$$\varphi = \frac{latitude}{180} \cdot \pi \tag{78}$$

$$\delta = 0.409 \cdot \sin\left(\frac{2\pi}{365} \cdot J - 1.39 \right) \tag{79}$$

$$N = \frac{24}{\pi} \cdot \omega_s \tag{80}$$

where R_s represents the incident solar radiation (MJ m^{-2} day^{-1}); R_a stands for extraterrestrial radiation (MJ m^{-2} day^{-1}); and τ stands for atmospheric transmissivity. In addition, the constants a_s and b_s equal to 0.25 and 0.5, respectively. n and N are the actual and theoretical sunshine hours, respectively. G_{sc} is a solar constant and equals 0.0820 (MJ m^{-2} min^{-1}). d_r is a reciprocal value of the relative distance between the Sun and the Earth. Moreover, ω_s refers to acronical angle (rad), φ

refers to latitude (rad), δ refers to solar declination (rad), J refers to the day of year, and $latitude$ is the geographical latitude (°).

The daily net longwave radiation L_{24} at the surface is calculated as follows:

$$L_{24} = \frac{R_{nl} \cdot 10^6}{24 \cdot 3600} \tag{81}$$

$$R_{nl} = -\sigma \cdot \left(\frac{T_{max}{}^4 + T_{min}{}^4}{2} \right) \cdot \left(0.34 - 0.14 \cdot \sqrt{e_a} \right) \cdot \left(1.35 \cdot \frac{R_s}{R_{so}} - 0.35 \right) \tag{82}$$

$$e_a = \frac{RH_{mean}}{100} \cdot \left[\frac{e^o\left(T_{max}\right) + e^o\left(T_{min}\right)}{2} \right] \tag{83}$$

$$R_{so} = \left(0.75 + 2 \cdot 10^{-5} \cdot DEM \right) \cdot R_a \tag{84}$$

$$e^o\left(T\right) = 0.6108 \cdot \exp\left(\frac{17.27 \cdot \left(T - 273.15\right)}{\left(T - 273.15\right) + 237.3} \right) \tag{85}$$

where R_{nl} represents net outgoing longwave radiation (MJ m^{-2} day^{-1}); σ is the Stefan Boltzmann constant equal to 4.903×10^{-9}(MJ m^{-2} K^{-4} day^{-1}); T_{max} and T_{min} are the daily maximum and minimum air temperature (K) at the reference altitude, respectively; e_a is the actual water vapor pressure (kPa); R_{so} is the clear-sky radiation (MJ m^{-2} day^{-1}); R_s / R_{so} is relative shortwave radiation (limited to ≤ 1.0); RH_{mean} is the daily average relative humidity (%); $e^o\left(T_{max}\right)$ and $e^o\left(T_{min}\right)$ are the saturated water vapor pressure (kPa) at the daily maximum and minimum temperatures, respectively; DEM is the altitude of the station (m); and $e^o\left(T\right)$ is the arithmetic relationship between saturated water vapor pressure and temperature.

3.6 Source of formula

Table S4 Formula and source information

Formula	Source
1, 2, 5, 10, 14, 17-19, 28, 29, 31-34, 36,	Su, 2002

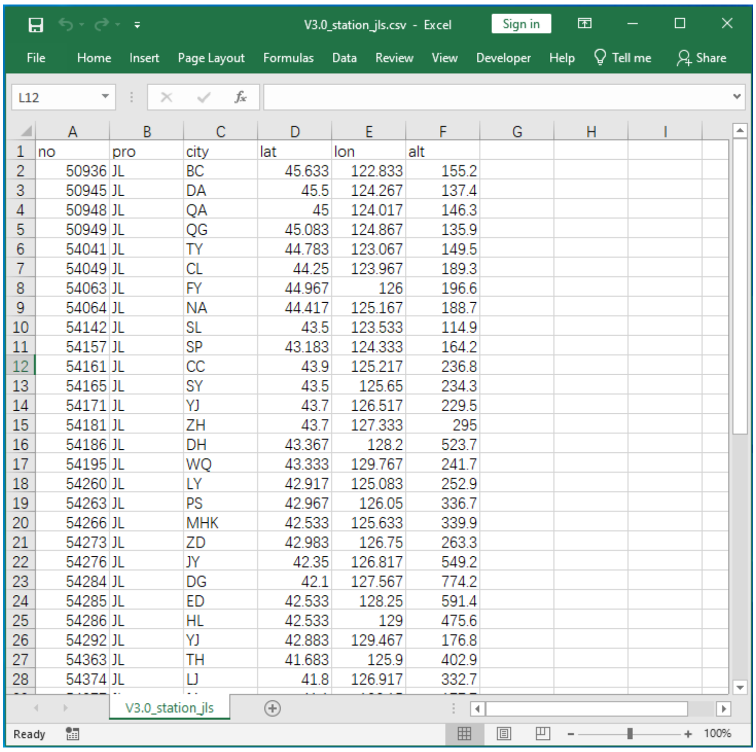
37, 55-61, 69-71	
3	Liang, 2001
3, 6-8, 12, 13, 20-27, 30	ILWIS software; Han et al., 2008
4	Yang, 2017
4, 9	Wu, 2010
11, 38, 39, 46-50, 54, 66, 68, 71-85	FAO56, 1998
15, 16, 35, 38, 39	Li, 2012
20, 30, 35, 38, 39, 67	Hao, 2018
37, 44, 45, 51-53, 62-65	Jobson, 1982
40-43	Su, 2002; Hogstrom, 1988; Kader and Yaglom, 1990; Beljaars and Holtslag, 1991; VandenHurk and Holtslag, 1997; Brutsaert, 1999

Note: ILWIS software website (https://52north.org/software/software-projects/ilwis)

4. Initial input data

Input data required by Modules 1, 2, and 3 can be divided into three parts: the first part is the basic data, which includes the information file (V3.0_station_jls.csv) of weather stations for the V3.0 meteorological dataset within the study area (Figure S7 for the file structure), the study area DEM file (dem_jls.asc), and the geographic coordinate system file (WGS 1984.prj); the second part is the remote sensing data, which includes MOD09A1 and MOD11A2; the third part is the meteorological data, which includes the raw data of V3.0 meteorological dataset. Meteorological data from other sources can also be used, the data needs to be prepared by the users following the format of 2019.csv and located in the corresponding folder.

The input data or files described above are all saved in the designated folders. Each module is connected to the file or the folder so that the data can serve as the input of the module. Specifically, the basic data is connected in a form of files; remote-sensed data and meteorological data are connected in a form of subdirectory.



no	pro	city	lat	lon	alt
50936	JL	BC	45.633	122.833	155.2
50945	JL	DA	45.5	124.267	137.4
50948	JL	QA	45	124.017	146.3
50949	JL	QG	45.083	124.867	135.9
54041	JL	TY	44.783	123.067	149.5
54049	JL	CL	44.25	123.967	189.3
54063	JL	FY	44.967	126	196.6
54064	JL	NA	44.417	125.167	188.7
54142	JL	SL	43.5	123.533	114.9
54157	JL	SP	43.183	124.333	164.2
54161	JL	CC	43.9	125.217	236.8
54165	JL	SY	43.5	125.65	234.3
54171	JL	YJ	43.7	126.517	229.5
54181	JL	ZH	43.7	127.333	295
54186	JL	DH	43.367	128.2	523.7
54195	JL	WQ	43.333	129.767	241.7
54260	JL	LY	42.917	125.083	252.9
54263	JL	PS	42.967	126.05	336.7
54266	JL	MHK	42.533	125.633	339.9
54273	JL	ZD	42.983	126.75	263.3
54276	JL	JY	42.35	126.817	549.2
54284	JL	DG	42.1	127.567	774.2
54285	JL	ED	42.533	128.25	591.4
54286	JL	HL	42.533	129	475.6
54292	JL	YJ	42.883	129.467	176.8
54363	JL	TH	41.683	125.9	402.9
54374	JL	LJ	41.8	126.917	332.7

Figure S8 V3.0_station_jls.csv file structure diagram

Note: **no** represents station number, **pro** represents province, **city** represents city, **lat** represents latitude, **lon** represents longitude, and **alt** represents altitude.

The structure diagram of the path to the initial input data has shown in Figure S8, and **./PySEBS/** indicates that a folder named PySEBS is created in the project directory. The path to the basic data is **./PySEBS/DATA/BasicData/**. The path to the remote sensing data is **./PySEBS/DATA/RemoteSensingData/MOD09A1/2019/** and **./PySEBS/DATA/RemoteSensingData/MOD11A2/2019/**. The meteorological data is saved in a path of **./PySEBS/DATA/MeteorologicalData/**.

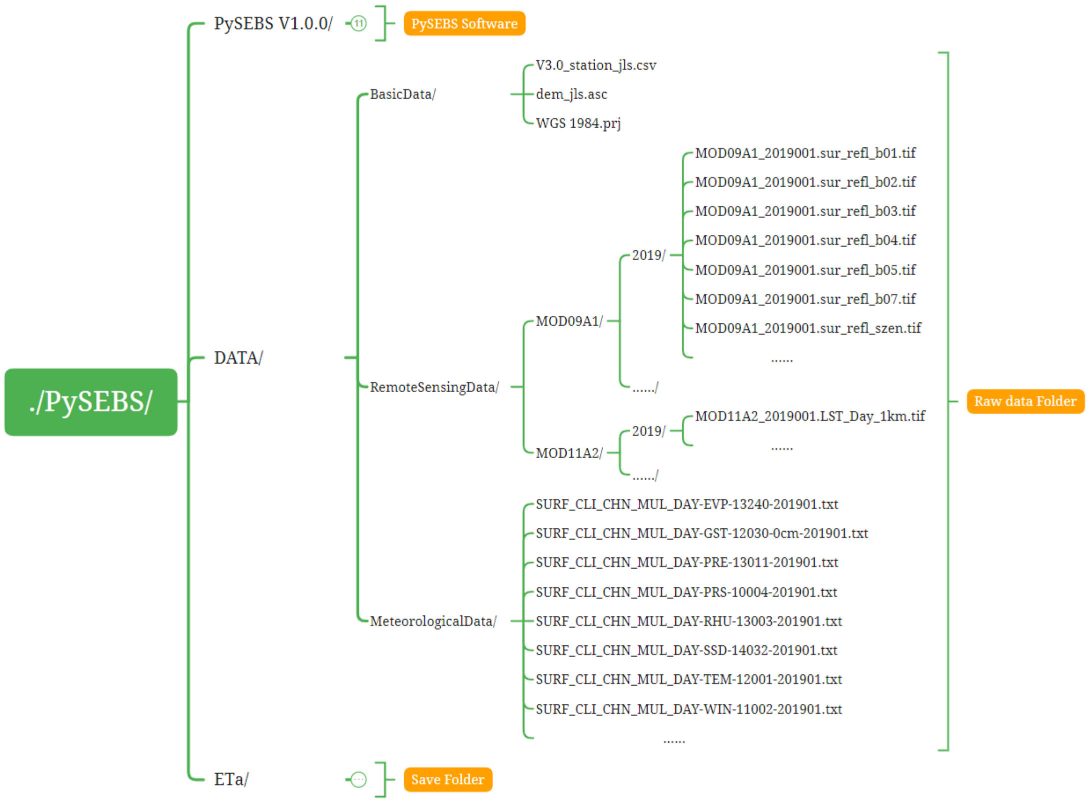


Figure S9 Structure of the path to the initial input data

5. Output results

The **./PySEBS/ET$_a$/** file path is a user-defined folder to save the output results, which will be created automatically if such a folder does not exist in the project directory. The folder **1RemoteSensingData/** is used to save the intermediate files generated during the remote sensing data processing in Module 1. The folder **2MeteorologicalData/** is used to save the intermediate files generated during the meteorological data processing in Module 2. The folder **3PySEBSInputData/** is used to save the final processing results of remote sensing and meteorological data. In addition, the folder **3PySEBSInputData/** also serves as the path of input files for Module 3. The **4PySEBSOutputData/** folder will store the daily ET_a results, and the **5sum_ET$_a$/** folder will store the monthly and annual ET_a results calculated by Module 3 (Figure S9). The **6sum_ET$_0$/** folder and the **7sum_Pre/** folder are used to store cumulative reference evapotranspiration and precipitation, respectively.

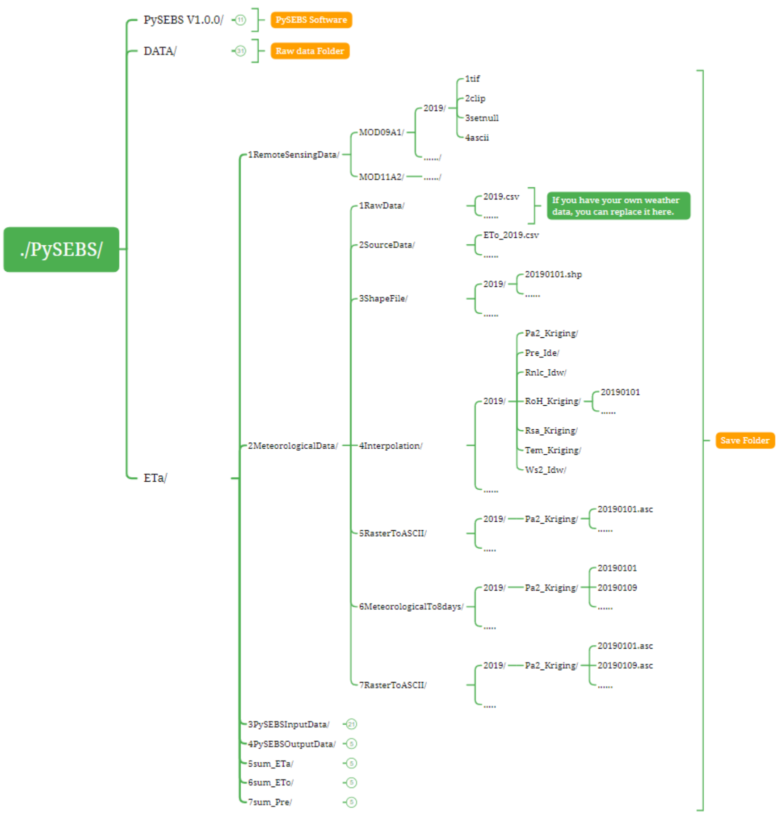


Figure S10 Schematic diagram of the structure of folder **1RemoteSensingData/** and folder **2MeteorologicalData/**

As mentioned earlier, if meteorological data derived from other sources need to be used, the data must be prepared in a required format (Figure S10) and stored in the file path **2Meteorologicaldata/1RawData/** to replace the V3.0 meteorological data (Table S5). The files in the file path **2MeteorologicalData/2SourceData/** (e.g., ET_o_2019.csv) used the data in the **2Meteorologicaldata/1RawData/** folder as input and calculated the ET_o and its process variables; the purpose of these files is to provide the six required meteorological parameters for **Module 3**. The calculation of ET_o is also a strength of this software, if the users need to use ET_o and other parameters in the calculation process, the information can be found in the folder of **2MeteorologicalData/2SourceData/** (Table S6).

no	pro	city	lat	lon	alt	year	month	day	Tmax	Tmin	Tem	Ws	Pa	Rh	Sh	Pre
50877	HLJ	YL	46.3	129.58	100.1	2019	1	1	-11.8	-17.9	-15.1	5.98	101.58	50	0.9	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	2	-9.8	-18.8	-14.3	3.07	101.7	62	7	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	3	-8	-15.6	-12.5	3.81	101.85	60	7.1	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	4	-7.4	-16.2	-11.7	3.44	101.04	70	4.8	0.4
50877	HLJ	YL	46.3	129.58	100.1	2019	1	5	-11.1	-16.1	-14.2	3.74	101.27	60	7	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	6	-10.3	-18.5	-14.8	3.44	101.64	58	7.1	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	7	-10.6	-19.6	-15.1	2.17	101.21	56	4.9	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	8	-10.7	-19.3	-14.9	3.81	101.14	57	6.7	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	9	-6.2	-16.1	-11.1	4.86	100.68	45	7.1	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	10	-3.3	-14.3	-8.9	3.22	100.54	53	7.3	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	11	-4.3	-19.6	-12.9	1.35	101.3	64	7.3	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	12	-3.4	-20.3	-14.3	0.45	101.16	67	7.1	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	13	-10.9	-19.1	-14.9	0.9	101.31	74	0	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	14	-7.7	-16.7	-11.5	1.27	101.14	75	0	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	15	-8.5	-17.5	-12.2	2.77	100.78	62	3.8	1.9
50877	HLJ	YL	46.3	129.58	100.1	2019	1	16	-10.6	-18.1	-15	4.11	100.3	51	4.6	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	17	-15.7	-23.6	-20.3	4.86	100.88	39	7.8	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	18	-12.2	-21.5	-17.3	3.22	101.38	45	7.9	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	19	-7.1	-23.8	-15.7	1.94	100.81	52	7.4	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	20	-11.3	-18.2	-15	2.77	100.33	62	3.1	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	21	-8.3	-22.7	-15.3	1.2	100.16	59	8	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	22	-4	-17.4	-9	2.77	99.8	56	0.9	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	23	-6.7	-13.8	-11.3	3.37	100.44	58	3.7	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	24	-7.5	-18.7	-12.7	2.54	101.19	55	7.9	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	25	-7	-15.2	-11.7	1.57	101.3	64	7.2	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	26	-6.1	-16.6	-11.6	2.54	101.32	62	8.2	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	27	-1.3	-10.4	-6.9	4.11	100.24	46	6.1	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	28	-6.8	-14	-10.6	4.11	100.22	61	7	0
50877	HLJ	YL	46.3	129.58	100.1	2019	1	29	-3.1	-16.8	-11.2	1.27	100.93	61	5	0

Figure S11 The example format of the meteorological data in replacement for the V3.0 data in **1RawData/**

The six parameters required by the Module 3, all except Tem, Ws, and Pa need to be calculated based on the parameters in the **1RawData/** folder, with the following dependencies:

$$RoH = f\left(Pa, Rh, T\,min, T\,max\right) \tag{86}$$

$$Rs = f\left(lat, year, month, day, Sh\right) \tag{87}$$

$$Rnl = f\left(lat, year, month, day, Sh, Rh, T\,min, T\,max\right) \tag{88}$$

Table S5 Description of meteorological data parameters of the files in folder **1RawData/** (e.g., 2019.csv)

Parameters	Explanation	Unit	Necessity
no	Station number	-	yes
pro	Province	-	no
city	city	-	no
lat	Destination site longitude	°	yes
lon	Destination site latitude	°	no
alt	Destination site altitude	°	yes
year	Year	year	yes
month	Month	month	yes
day	Day	day	yes
Tmax	Maximum air temperature	℃	yes
Tmin	Minimum air temperature	℃	yes
Tem	Daily average air temperature	℃	yes
Pa	Daily average wind speed at 2 m	Pa	yes
Ws	Daily average air pressure	m/s	yes
Rh	Daily average relative humidity	%	yes
Sh	Sunshine hours	hour	yes
Pre	Precipitation	mm	no

Note: Necessity means whether the parameter is a required parameter in the calculation of ET_o.

Table S6 Description of the parameters of the file in folder **2SourceData/** (e.g., ET_o_2019.csv)

Parameters	Explanation	Unit	Necessity
no	Station number	-	no
pro	Province	-	no
city	city	-	no

lat	Destination site longitude	°	yes
lon	Destination site latitude	°	yes
alt	Destination site altitude	°	no
year	Year	year	no
month	Month	month	no
day	Day	day	no
Tmax	Maximum air temperature	℃	no
Tmin	Minimum air temperature	℃	no
Tem	Daily average air temperature	℃	yes
Ws	Daily average wind speed at 2 m	m/s	yes
Pa	Daily average air pressure	kPa	yes
Rh	Daily average relative humidity	%	no
Sh	Sunshine hours	hour	no
Pre	Precipitation	mm	no
RoH	Specific humidity	$kg\ kg^{-1}$	yes
e0Tmax	Max saturation vapor pressure	kPa	no
e0Tmin	Min saturation vapor pressure	kPa	no
e0Tem	Mean saturation vapor pressure	kPa	no
ea	Actual vapor pressure	kPa	no
phi	Latitude with rad φ	rad	no
J	Jay day	day	no
delta0	Solar declination δ	rad	no
ws0	Sunset hour angle	rad	no
dr	Inverse relative distance earth_sun	-	no
N	Day light hours N	hour	no
r	Psychrometric constant γ	$kPa\ ℃^{-1}$	no
Delta	Slope of Saturation vapor pressure curve Δ	$kPa\ ℃^{-1}$	no
Ra	Daily extraterrestrial radiation	$MJ\ m^{-2}\ day^{-1}$	no
Rs0	Daily average clearsky solar radiation	$MJ\ m^{-2}\ day^{-1}$	no
Rs	Daily average solar radiation	$MJ\ m^{-2}\ day^{-1}$	yes
Rns	Daily average net solar radiation	$MJ\ m^{-2}\ day^{-1}$	no
Rnl	Daily average net outgoing longwave radiation	$MJ\ m^{-2}\ day^{-1}$	yes
Rn	Daily average net radiation	$MJ\ m^{-2}\ day^{-1}$	no

G	Daily average soil heat flux density	MJ m^{-2} day^{-1}	no
ETo	Reference evapotranspiration	mm d^{-1}	no

The **3PySEBSInputData/** folder stores the final processing results calculated from Module 1 and Module 2 and the input files from Module 3. The files are stored in the form of one folder per day and contain 15 .asc files that are required for the PySEBS model calculation and 1 optional precipitation file (pre.asc). The required parameters include 1 DEM file (dem.asc), 7 MOD09A1 files (band1.asc, band2.asc, band3.asc, band4.asc, band5.asc, band7.asc, and szen.asc), 1 MOD11A2 file (lst.asc), and 6 meteorological parameter files (tem.asc, ws.asc, pa.asc, roh.asc, rs.asc, and rnl.asc) (Figure S11).

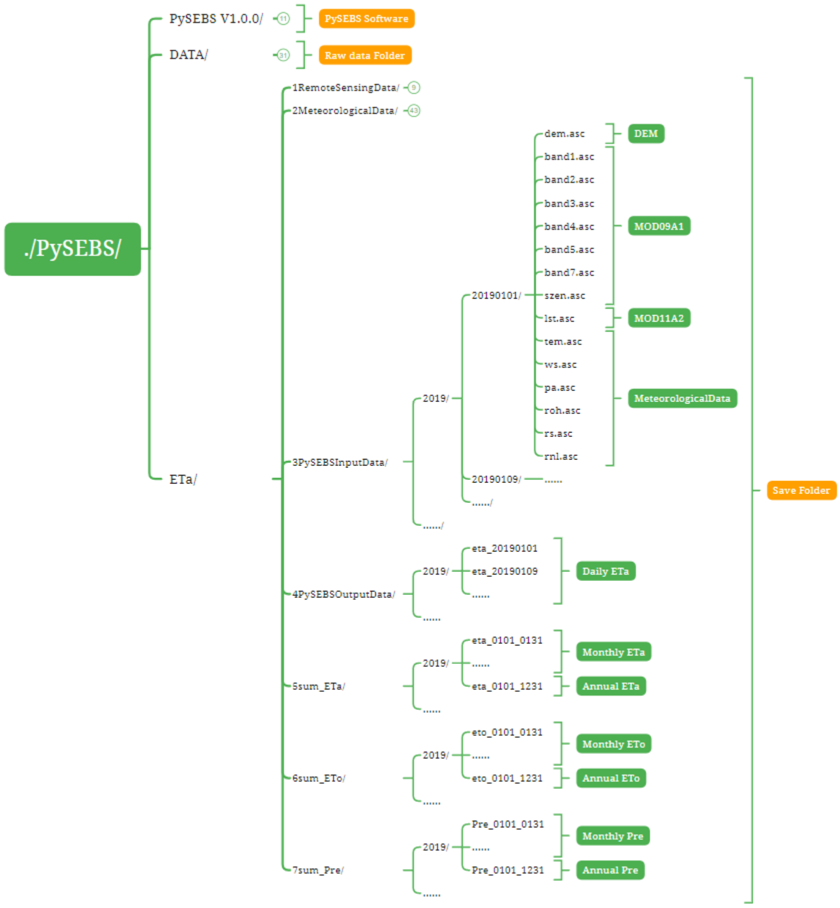


Figure S12 Schematic diagram of the structure of folders 3PySEBSInputData/, 4PySEBSOutputData/, and 5sum_ET_a/, 6sum_ET_o/, and 7sum_Pre/

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