

SCOPE

Version 1.70 User Manual

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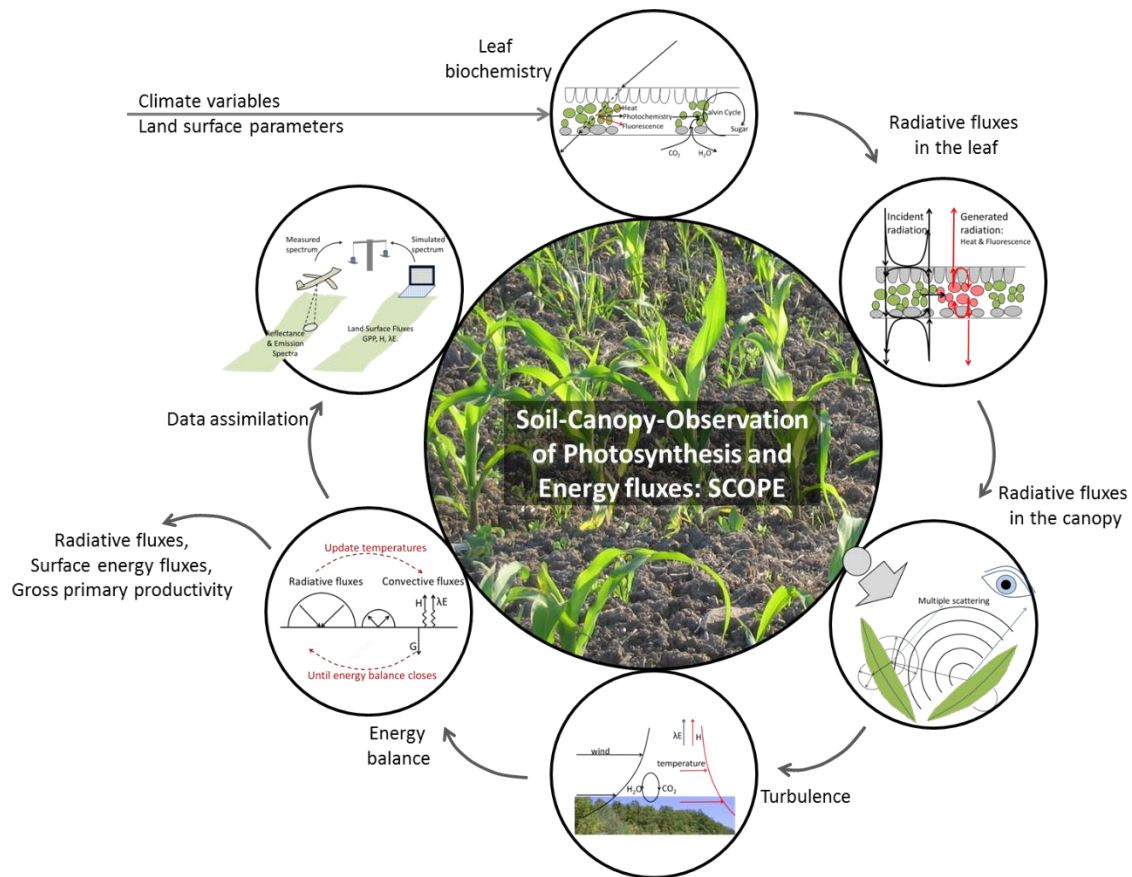


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1 Brief history of the model

The SCOPE model has been developed between 2006 and 2009 by Wout Verhof, Joris Timmermans, Christiaan van der Tol, Anne Verhoef and Bob Su. The idea of the model was to develop a simulator for hyperspectral VNIR observations, the surface energy budget and photosynthesis. Chlorophyll fluorescence has been part of the model. It was originally the idea to develop a 3-D radiative transfer scheme, but this idea was (temporally) abandoned, and 1-D remained a 1-D vertical model. This had the advantage that the well-known SAIL model could be used as a basis, which is easily invertible, does not require many parameters, is computationally efficient and sufficient in many cases.

The key elements of the model have been the extension to the thermal domain (Joris Timmermans) and the radiative transfer of fluorescence (Wout Verhoef), the simulation of sensible, latent and ground heat flux, stomatal opening and photosynthesis (Christiaan van der Tol) and an aerodynamic resistance scheme (Anne Verhoef). Model inversion tools are not also available, see for example Van der Tol et al., (2016). There have been several updates since the published version of the model (version 1.21) in 2009. Other people have contributed to the model development as well, including Ari Kornfeld, Joe Berry, Federico Magnani (mainly the biochemical part, but also other parts), and many users provided useful feedback and suggestions (see Acknowledgement).

Information about the model

Questions about the model can be addressed to Christiaan van der Tol (c.vandertol@utwente.nl) and Wout Verhoef (w.verhoef@utwente.nl).

Model description: Van der Tol, C., Verhoef, W., Timmermans, J., Verhoef, A. and Su, Z. (2009) An integrated model of soil - canopy spectral radiances, photosynthesis, fluorescence, temperature and energy balance. In: Biogeosciences 6 (2009)12, pp. 3109-3129

Biochemical routine: Van der Tol, C., Berry, J. A., Campbell, P. K. E., & Rascher, U. (2014). Models of fluorescence and photosynthesis for interpreting measurements of solar-induced chlorophyll fluorescence. Journal of Geophysical Research: Biogeosciences.

Leaf radiative transfer scheme: Vilfan, N., van der Tol, C., Muller, O., Rascher, U., & Verhoef, W. (2016). Fluspect-B: A model for leaf fluorescence, reflectance and transmittance spectra. Remote Sensing of Environment, 186, 596-615.

Model inversion: van der Tol, C., Rossini, M., Cogliati, S., Verhoef, W., Colombo, R., Rascher, U., & Mohammed, G. (2016). A model and measurement comparison of diurnal cycles of sun-induced chlorophyll fluorescence of crops. Remote Sensing of Environment, 186, 663-677.

2 Software requirements

The model SCOPE_v1.70 is written in Matlab R2015b running on a Windows operating system. We took care not to use functions that are available in all recent Matlab versions, but we cannot give any warranty that it works under other operating systems and other Matlab versions.

3 Summary of improvements since first release

Since the first publication of the model, a number of changes have been made to the model (Table 1). The most significant of these were: the leaf optical model Fluspect replaced PROSPECT (in version 1.33), the leaf-level biochemical model for fluorescence was changed (version 1.34), the way of programming was changed by organizing variables in structures (version 1.40), and a new alternative physically based leaf fluorescence biochemical model was introduced by Federico Magnani (version 1.51). The changes are cumulative: they were made to the preceding version. Since version 1.60, the scattered fluorescence flux has been added, and the programming of the function RTMf was optimized to reduce computation time by a factor 9 (by Ari Kornfeld). SCOPE with fluorescence switched on is $4 \times$ as fast as version 1.54 was. In version 1.61, small bugs have been corrected.

Version 1.70 is a major update, and the following changes have been made:

- The FLUSPECT model is now consistent with the PROSPECT-D model (Feret et al., 2017, RSE 193, 204–215).
- The FLUSPECT model includes dynamic Xanthophyll reflectance due to the de-epoxydation state (the ‘PRI effect’)
- A new radiative transfer model, RTMz, has been added which simulates the TOC reflectance changes as a result of the de-epoxydation state changes induced by light, water or temperature stress.
- The fluorescence emission spectra have been tuned to FluoWat leaf clip measurements. Important note: The optimized spectrum does not differentiate the two photosystems, but simulates the fluorescence spectrum as a whole. It was not possible to differentiate the two with FluoWat leaf clip measurements. However, it is still possible to use the original Franck et al. spectra and work with PSI and PSII fluorescence as in the earlier versions of SCOPE. This is done with the option ‘calc_PSI = 1’.
- The biochemical routine has been updated, and now the internal CO₂ concentration in the leaf is calculated iteratively (Ari Kornfeld)
- The soil spectrum can be provided in two ways: either by providing the spectrum directly as input (as in previous versions of SCOPE) by pointing to the file and a column in this file, or it can be simulated with the BSM model. In that case the user should enter parameter values of the BSM model in the input, these include: soil brightness and soil moisture, and two parameters (‘lat’ and ‘lon’) that determine the shape of the spectrum. Note that these parameters are not related to the

geographical location! The parameters can also be retrieved from measured spectra with a separate retrieval code of RTMo+ RTMf + BSM.

- The option to load the leaf inclination distribution from a file (besides the option to use the LIDFa and LIDFb parameters to simulate the distribution)
- A separate SCOPE script for MAC/ Linux users does no longer exist. Instead, the user has the option to select the names of the input files in a file 'set_parameter_filenames.m'. Either a spreadsheet or text files can be chosen as input. The code has also been tested on a Linux platform.
- The total emitted fluorescence irradiance by all photosystems (i.e. before reabsorption within the leaf and canopy), the total emitted fluorescence irradiance by all leaves accumulated (i.e. before reabsorption by soil and canopy), and the fluorescence originating from sunlit and shaded leaves and the (multiple) scattered flux have been added as separate output files.
- The bottom of canopy irradiance flux (the flux on the soil) has been added to the output as a spectrum.
- Several outputs have been added to the 'fluxes' and 'radiation' files, including the incident PAR and the incident radiation.
- Two bugs in the RTMt_Planck have been fixed.

Some specific notes about the leaf level fluorescence and photosynthesis model in versions 1.51 and higher:

The model "Von Caemmerer-MD12" (`biochemical_MD12.m`) (in short: MD12 model) was implemented by Federico Magnani as an alternative to the `biochemical.m` model. The MD12 model is based on the Farquhar et al. (1980) and von Caemmerer (2000) models. MD12 contains to parameters that are not in the empirical model: qLs for photodamage and kNPQs for sustained photoprotection. These parameters are specified in the input data spreadsheet. An un-stressed value of 1 and 0 is currently used, although more specific values could be derived from field measurements (as in SMEAR) and read from a LUT. Both the full and the simplified versions of the Von Caemmerer model for C4 species have been coded, but the simplified version is currently commented out in the code. The simplified version appears to be almost correct under most (but not all) circumstances, and could be used if the full model is too computationally demanding.

Table 1. Overview of modifications made to the SCOPE model.

Version number	Note
Version 1.21 (2009)	The SCOPE model as published in Biogeosciences (2009)
Version 1.32 (2012)	The leaf level optical model FLUSPECT was introduced, which produces leaf reflectance, transmittance and fluorescence spectra. Rather than using given fixed fluorescence matrices as inputs, SCOPE now uses FLUSPECT to calculate the excitation to fluorescence conversion matrices.
Version 1.34 (2012)	Update of FLUSPECT with separate fluorescence spectra for PSI and PSII . Replacing the TVR09 model for fluorescence with an empirical model. Hemispherically integrated fluorescence is added as an output. The photosynthesis model is made consistent with Collatz et al (1991 and 1992), also used in CLM and SiB models, includes C3 and C4 vegetation , and empirically calibrated fluorescence model according to Lee et al. (2013) . The possibility to create Look-Up Tables has been introduced, as well as more options for running only parts of the model.
Version 1.40 (2013)	Major changes in the structure of the model. Coupling with MODTRAN -derived output files. The irradiance spectral input data are now calculated from MODTRAN atmospheric files. The input is specified in a spreadsheet. Variables are organized in structures which makes it easier to plug in new modules . <i>This version has a bug in the unit of the CO2 concentration. Version 1.40 is no longer available.</i>
Version 1.51 (2013)	Addition of an alternative leaf level photosynthesis and fluorescence model according to Von Caemmerer (2000) and Magnani et al (2013) . Correction of the bug in version 1.40.
Version 1.52 (2013)	Additional fluorescence output, change in the input data of optipar, and some modification of biochemical_MD12.m. Saves also the path of the code (including SCOPE version) to the output. Bug fixed in Fluspect (a scattering coefficient). Correction for PSI fluorescence moved from RTMf to biochemical.m.
Version 1.53 (2014)	Correction of a bug in Fluspect, which caused the fluorescence spectra to be $2 \times$ too low in version 1.52.
Version 1.54 (2014)	Fluspect replaced by Fluspect_bcar, an updated version of Fluspect with the absorption by carotenoids included, similar to PROSPECT 5

Continued...

Version 1.60 (2015)	<p>Major revision of RTMf: computation speed improved (Ari Kornfeld), scattered fluorescence flux added to the directional flux (Christiaan van der Tol).</p> <p>Improved calculation speed of RTMt_sb (AK)</p> <p>Revision of Ball-Berry model in biochemical.m: now iterative calculation of C_i and stomatal conductance (AK)</p> <p>Minor improvements in the energy balance (soil heat flux computation, suggested by Georg Wolfahrt).</p> <p>Input spreadsheet in 'SCOPE' has changed from "input_data.xls" to "input_data.xlsx". Way of reading the sheets 'filenames' and 'options' has changed (AK and CvdT). 'SCOPE' should now also work for MAC and LINUX, but to be sure, SCOPE_mac_linux.m has been maintained.</p> <p>Default value of parameter 'fqe' in input spectrum has been tuned to FluoWat measurements</p>
Version 1.61 (2015)	<p>Bug in the saving of total evaporation data corrected (bug in versions 1.40 to 1.60). Bug in the loading of time series of roughness length for momentum (z_0) and zero plane displacement height (d) calculated from LAI and canopy height was corrected.</p>
Version 1.62 (2016)	<p>Photosynthesis is a function of aPAR absorbed by Chlorophyll (only) rather than total leaf aPAR as in earlier versions.</p>
Version 1.70 (2017)	<p>OPTIPAR of PROSPECT-D model used, complemented with Xanthophyll spectra for the Violaxanthin to Zeaxanthin conversion.</p> <p>The FLUSPECT model includes dynamic Xanthophyll reflectance due to the de-epoxydation state (the 'PRI effect') and Anthocyanins</p> <p>A new radiative transfer model, RTMz, simulates the TOC reflectance as a function of the de-epoxydation state induced by light, water or temperature stress.</p> <p>The fluorescence emission spectra have been tuned to FluoWat leaf clip measurements. The option to use the fluorescence spectra of V1.62 and older remains.</p> <p>The biochemical routine has been updated, and now the internal CO_2 concentration in the leaf is calculated iteratively (Ari Kornfeld)</p>

The BSM model for soil reflectance added as an option.

SCOPE and SCOPE_mac_linux merged into a single script.

The option to load the leaf inclination distribution from a file (besides the option to use the LIDFa and LIDFb parameters to simulate the distribution)

New outputs: The total emitted fluorescence irradiance by all photosystems (i.e. before reabsorption within the leaf and canopy), the total emitted fluorescence irradiance by all leaves accumulated (i.e. before reabsorption by soil and canopy), and the fluorescence originating from sunlit and shaded leaves and the (multiple) scattered flux have been added as separate output files. The bottom of canopy irradiance flux (the flux on the soil) has been added to the output as a spectrum. Several outputs have been added to the 'fluxes' and 'radiation' files, including the incident PAR and the incident radiation.

Two bugs in the RTMt_Planck have been fixed.

4 Model architecture

After reading in the main input file (a spreadsheet with tabs or alternatively, three text files), the supporting data are loaded. These consist of soil and leaf optical coefficients, and (optional) meteorological time series. The model performs a number of simulations. Each simulation starts with the leaf optical model FLUSPECT and the radiative transfer model RTMo for scaling from leaf to canopy. Next, the energy balance can be calculated. The energy balance routine calculates the turbulent heat fluxes, photosynthesis, and the leaf and soil temperatures (for each leaf orientation, leaf layer, and for the sunlit and shaded fraction separately). The temperatures are solved by iteration until the energy balance closure error is small enough. The optional calculations that may follow include the radiative transfer of fluorescence, the thermal emission spectra (2.5- 50 μm), and the calculation of a complete BRDF using simulations of many observation angles.

Pseudocode:

```
Load input files: filenames, options and input data
Loop over number of simulations
    Simulate leaf spectra (Fluspect)
    Simulate radiative transfer of incident light (RTMo)
    If option 'calculate energy balance' is on
        Repeat
            Simulate radiative transfer of emitted thermal radiation (RMTt)
            Simulate non-radiative energy balance fluxes (heatfluxes)
        Until the energy balance closes
    end
    If option 'calculate fluorescence' is on
        Simulate radiative transfer of emitted fluorescence
    end
    If option 'calculate Xanthophyll reflectance' is on
        Simulate radiative transfer of incident light due to change in reflectance per leaf (RTMz)
    end
    If option 'calculate Directional' is on
        Repeat the calculations above for many observation zenith and azimuth angles
    end
    Store the output
end
Optional: make plots of the output
Optional: compare the output to a reference simulation
```

Table 2 lists the directory structure of the model. The two main directories are ‘Data’, containing data in files (input and optional validation data), and ‘SCOPE_vx’, containing the model code, model output and model documentation. The data directory has again two folders: a compulsory input data folder, and a folder for optional validation or supporting data. The input data has folders specific for projects (for example meteorological data for a site) organized in folders starting with ‘Dataset ...’. One example is provided: ‘Dataset for_verification’. In addition, there are folders with data specific for SCOPE, such as soil reflectance, leaf optical properties, and FLUSECT parameters.

The folder ‘SCOPE_v1.70’ has the code, the model output, and documentation (readme). The spreadsheet and text files with the basic model input (parameters and links to input data file) are located here too. When the model is executed, then the output will automatically appear in a new directory under output, with the name of the simulation run and the date in the directory name. The spreadsheet with parameters is saved along with the model output.

Table 2: Directory structure of the model. The data are saved at the same level as the model.

Level 1	Level 2	Level 3	Level 4	Description
Data	Input	Dataset [<i>project or site name</i>]		ASCII files with meteorological data for a project
		Directional		Table with observation angles to be included in the BRDF calculation
		Fluspect_parameters		Optical characteristics of plant pigment and fluorescence spectra of PSI and PSII
		Radiation data		MODTRAN atmospheric files
	Measured	Soil_spectrum		Selection of soil reflectance spectra
		Dataset for_verification		Location where data for verification are stored.
SCOPE_v1.61	Code_matlab			The main input spread sheet is located here
	Output	VerificationData		The MATLAB code of the model
		[<i>Project_yyyy-mm-dd-hhmm</i>]		Output of a standard SCOPE run
			Directional	Automatically generated folder with model output of a project.
			Figures	BRDF output
	Readme		Parameters	Empty folder where figures can be placed
				The input_data.xlsx file used for this run
				Documentation of the model

5 Getting started

SCOPE consists of several scripts and functions (hereafter called modules), which can be used separately or as parts of the integrated SCOPE model. When the modules are used separately, then it is important to provide input in the structures specified below. When the integrated model is called, then the input is automatically loaded from the spreadsheet and from the files specified therein. Basic knowledge of the use of Matlab is required to operate the model.

The application of the model involves the following steps:

1. **To unpack the zip file**

Unpack the model, and leave the directory structure intact.

2. **Run the model once**

Running the model once, before modifying the parameters and input, will check whether the software works under your system. The model runs with an example data set, and the output is automatically compared to output that it should produce. If there is any difference in the results, messages will show up. The model is executed by opening Matlab, navigating to the directory where the matlab code is ('cd ... **SCOPE_v1.70/code_matlab**'), and running 'SCOPE'. Running the model may take a while because almost all options are switched on. If the output of the model is not as expected, then messages will appear. There will also be graphs appearing showing the freshly produced output together with the expected output. If all is ok then no graphs or warnings are produced.

3. **Evaluate and complete the spreadsheet 'input_data.xlsx' or the input files 'filenames', 'inputdata' and 'setoptions'**

The required input is specified in the spreadsheet file 'input_data.xlsx'. Open this file. It has three sheets:

- Readme: here information about the simulation can be entered
- Options: specify the simulation options here
- Filenames: specify the name of the simulation, the soil and leaf optical property files, and the file names of meteorological input time series.

- **InputData:** specify all the parameters and input variables. Meteorological data specified here will be overwritten by values in the input files if these files have been specified (filenames) and the series option is switched on (options).

If you prefer not to use the spreadsheet, you can provide the input as a text file, and the options and file names as '.m' file (which can be edited with any text editor like notepad). Examples are given. You can set the option whether to use the spreadsheet or text input in the file 'set_parameter_filenames.m', by commenting out (with '%') the option that is not wanted. The filenames can be specified here.

4. **Simulation option 'Individual runs'**

The last simulation option is important: to run the model for a few cases only, choose the option: simulation = 0. In that case the model runs for the input specified in the InputData sheet. It is possible to specify more than one value for one input variable, by filling in values in the next column. The model will run as many simulations as there are columns in the input data spreadsheet, say n runs. For run i it will select the data from column i for all variables that have n values. For all other variables, it will select the first value only. For example:

Cab	10	20	30
Cdm	0.012		
N	1.5	2	

It will do three runs, the first time with Cab = 10, Cdm = 0.012, and N = 1.5; the second time with Cab = 20, Cdm = 0.012, and N = 1.5; and a third time with Cab = 30, Cdm = 0.012 and N = 1.5. The value of N = 2 is ignored and the run cycle ends.

The output is the same as for the time series (see below), except that two additional files are produced: 'pars_and_input.dat' and 'pars_and_input_short.dat'. Both files always have a header. The first file lists the values of all parameters and input variables (that are part of the structure 'v') that were used in the simulations, one row for each simulation. The second file lists only the parameters that were varied. Suppose that, for example, if 3 parameters were given 10 different values, while the other parameters were given only 1 single value for each simulation. In that case the pars_and_input_short.dat output file contains three columns with the parameter values corresponding to each simulation.

5. Simulation option Time series

For the time series run, set `simulation = 1`. SCOPE now uses the meteorological input as saved in the ascii files specified in the sheet: 'filenames'. SCOPE runs as many times as there are values in the ascii files. For all input that is not in files, it uses the first value specified in the 'InputData' sheet. A value for an input variable in the spreadsheet is **overwritten** by the value in the time series file of that variable, if this file is provided.

Note: In version 1.70, it is possible to leave a few meteorological input data files blank. In that case, this variable will be the (constant) value in the input data spreadsheet or the general input data text file.

6. Simulation option Lookup Table

For the LUT option, specify 'simulation = 2'. This option is similar to the 'individual runs', except that the model runs over all possible combinations of parameters. For example:

Cab 10 20 30

Cdm 0.012

N 1.5 2

It will do six runs, the first time with Cab = 10, Cdm = 0.012, and N = 1.5; the second time with Cab = 20, Cdm = 0.012, and N = 1.5; a third time with Cab = 30, Cdm = 0.012, and N = 1.5; then fourth with Cab = 10, Cdm = 0.012 and N = 2.0, etc, cycling through values for Cab again.

7. To execute the model

The model can be executed by calling 'SCOPE' in the command window of Matlab. Alternatively, separate modules can be called, provided that the required input is given. The modules have a help text describing how to do this, which can be called by typing 'help modulename', for example: 'help ebal'. It is however more difficult, because the structures need to be provided.

The output of each simulation is automatically saved in an output directory, together with files documenting the parameters used for this simulation, and the spreadsheet in directory 'Parameters'.

It is also possible to use the executable SCOPE.exe. In that case you will first need to install the Matlab Runtime Compiler for Matlab 2015b, which can be found on the Mathworks web site.

8. To plot the output

An example of a module which creates graphs is provided with the model (`plots.m`). This function browses through the latest output directory, and plots all data present there in graphs. The titles of the graphs are the headings found in the output files.

6 Data structures

In SCOPE versions since 1.50, the data is organized in structures (Table 2). The elements of the structures are the variables used in the model.

Table 2. Data structures internally used in SCOPE

Name	Description
Angles	Solar and observation zenith and azimuth angles
Biochem_in	Input of the biochemical routine 'biochemical.m' for photosynthesis and fluoerescence
Biochem_out	Output of the biochemical routine 'biochemical.m' for photosynthesis and fluoerescence
Canopy	Canopy parameters, such as leaf area index and leaf inclination distribution function
Constants	Physical constants
Fluxes	Fluxes calculated by the model (turbulent heat exchange, radiation, CO ₂)
iter	Numerical parameters, such as the number of iterations needed to reach energy balance closure
Leafbio	Leaf biochemical parameters
Leafopt	Leaf optical properties
Meteo	Meteorological variables
Options	Simulation options, such as time series or look-up tables, fluorescence.
Optipar	Leaf optical parameters
Profiles	Vertical profiles of temperatures and fluxes
Rad	Radiation fluxes: both input (MODTRAN) and output
Resist_in	Aerodynamic resistance parameters
Resist_out	Aerodynamic resistance state variables
Soil	Soil properties (such as soil moisture, emissivity and the reflectance spectrum)
Spectral	Wavelength ranges of MODTRAN, SCOPE, PAR, fluorescence
Temps	Leaf, soil and air temperatures
V	All input variables
Xyt	Geographical location and time of the project

7 Output data

The module `output_data.m` saves the output of SCOPE in an output directory. In SCOPE, `output_data` is called after each calculation.

The data are stored in the following directory:

`SiteName_YYYY-mm-dd-hh-mm`

In which *YYYY* refers to the Julian year, *mm* to the month, *dd* the day, *hh* the hour and *mm* the minutes of the time when the simulation was started.

Table 5.15 shows the output files which are always created. Table 4.14 shows output files which are optionally created.

Table 5.15. Output files and their content. The columns in the output files refer to the variables in the table.

Filename	Variable	Description	Unit	Dim
fluxes.dat	Timestep	time step counter		[nt]
	Counter	number of iterations in energy balance		[nt]
	Year	year		[nt]
	T	decimal DOY		[nt]
	Rntot	Total net radiation	W m ⁻²	[nt]
	IEtot	Total latent heat flux	W m ⁻²	[nt]
	Htot	Total sensible heat flux	W m ⁻²	[nt]
	Rnctot	Net radiation of canopy	W m ⁻²	[nt]
	IEctot	Latent heat flux of canopy	W m ⁻²	[nt]
	Hctot	Sensible heat flux of canopy	W m ⁻²	[nt]
	Actot	Net photosynthesis of canopy	μmol m ⁻² s ⁻¹	[nt]
	Rnstot	Net radiation of soil	W m ⁻²	[nt]
	IEstot	Latent heat flux of soil	W m ⁻²	[nt]

	Hstot	Sensible heat flux of soil	W m^{-2}	[nt]
	Gtot	Soil heat flux	W m^{-2}	[nt]
	Resp	Respiration rate	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[nt]
	aPAR_Cab	absorbed PAR by Chlorophyll AB	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[nt]
	aPAR	Total absorbed PAR by leaves	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[nt]
	fPAR	fraction of absorbed PAR (by the canopy, excl soil)		[nt]
	aPAR_energyunits	Total absorbed PAR by leaves	W m^{-2}	[nt]
	PAR	Incident PAR	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[nt]
	Fluortot*	Hemispherically and spectrally integrated ChF at the top	W m^{-2}	[nt]
	Fluoryield*	Fluortot / aPAR_energyunits	W W^{-1}	[nt]
<hr/>				
surftemp.dat	timestep	time step counter		[nt]
	Year	year		[nt]
	T	decimal DOY		[nt]
	Ta	Air temperature above the canopy	$^{\circ}\text{C}$	[nt]
	Tss(1)	Surface temperature of shaded soil	$^{\circ}\text{C}$	[nt]
	Tss(2)	Surface temperature of sunlit soil	$^{\circ}\text{C}$	[nt]
	Tcave	Average canopy temperature	$^{\circ}\text{C}$	[nt]
	Tsave	Average soil temperature	$^{\circ}\text{C}$	[nt]
<hr/>				
aerodyn.dat	Raa	total aerodynamic resistance above canopy	s m^{-1}	[nt]
	Rawc	aerodynamic resistance below canopy for canopy	s m^{-1}	[nt]
	Raws	aerodynamic resistance below canopy for soil	s m^{-1}	[nt]
	ustar	friction velocity	m s^{-1}	[nt]
<hr/>				
radiation.dat	Timestep	time step counter		[nt]

	Year	year		[nt]
	T	decimal DOY		[nt]
	ShortIn (Rin)	Incoming shortwave radiation (copy from input)	W m^{-2}	[nt]
	LongIn (Rli)	Incoming longwave radiation (copy from input)	W m^{-2}	[nt]
	ShortOut (Louto)	hemisph. outgoing radiation, shortwave (<2.5 μm)	W m^{-2}	[nt]
	LongOut (Loutt)	hemisph. outgoing radiation, long wave (>2.5 μm)	W m^{-2}	[nt]
	TotalOut (Lout)	total hemispherical outgoing radiation	W m^{-2}	[nt]
gap.dat	Ps Po Pso	Sunlit, viewed and sulit-viewed fraction, per layer		[nt,nl]
spectrum_hemis_optical.dat	Lout_	hemispherical outgoing radiation	$\text{W m}^{-2} \mu\text{m}^{-1}$	[nt,nwl]
spectrum_obsdir_optical.dat	Lo_	outgoing radiance in observation direction	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt,nwl]
spectrum_obsdir_BlackBody.LotBB_		Outgoing BlackBody thermal radiance in observation direction	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	
dat				
irradiance_spectra.dat	Rin*(fEsun+fEsky)	spectrum of incoming radiation used in the simulation	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt,nwl]
reflectance.dat	Lo_*pi/ Rin*(fEsun+fEsky)	Apparent reflectance in observation direction. For the entire spectrum, but outside the visible (wl>2.5 μm), NaN are placed		[nt,nwl]
wl.dat	wl	wavelengths	Mm	[nwl]

Table 4.16. Optional output files: for vertical profiles

File	Variable	Description	Unit	Dim
leatemp	Tc1ld', Tc0', Tc1d'	sunlit leaf temperature, shaded leaf temperature average leaf temperature	$^{\circ}\text{C}$	[nt, 3 x nl]
layer_h	Hc1d', Hstot	sensible heat flux of leaf layers and soil	W m^{-2}	[nt, nl+1]
layer_le	IEc1d', lEstot	latent heat flux of leaf layers and soil	W m^{-2}	[nt, nl+1]
layer_a	A1d' Resp	photosynthesis of leaf layers and soil respiration	W m^{-2}	[nt, nl+1]
layer_pn	Pn1d' 0	aPAR of leaf layers (and dummy for soil)		[nt, nl+1]
Layer_NPQ	Profiles.qE	Non-photochemical quenching per leaf layer		[nt, nl+1]
layer_rn	Rn1d' Rnstot	net radiation of leaf layers and soil	W m^{-2}	[nt, nl+1]

Table 4.17. Other optional output files

File	Variable	Description	Unit	Dim
fluorescence	LoF_	fluorescence between 0.64 and 0.85 μm (1 nm res)	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]
fluorescencePSI	LoF1_	fluorescence PSI betw 0.64 - 0.85 μm (1 nm res)	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]
FluorescencePSII	LoF2_	fluorescence PSII betw 0.64 - 0.85 μm (1 nm res)	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]
Fluorescence_hemis	Fhem	Hemispherically integrated fluorescence	$\text{W m}^{-2} \mu\text{m}^{-1}$	[nt, nwl]
Fluorescence_sunlit	LoF_sunlit	Fluorescence coming directly from sunlit leaves	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]

Fluorescence_shaded	LoF_shaded	Fluorescence coming directly from shaded leaves	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]
Fluorescence_scattered	LoF_scattered	Fluorescence reaching the sensor after (multiple) scattering	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]
Fluorescence_emitted_by_all_leaves	Fem_	Emitted fluorescence irradiance by all leaves together	$\text{W m}^{-2} \mu\text{m}^{-1}$	[nt, nwl]
Fluorescence_emitted_by_all_photosystems	Femtot	Similar to above, but excluding the reabsorption within the leaf where fluorescence is formed	$\text{W m}^{-2} \mu\text{m}^{-1}$	[nt, nwl]
spectrum_hemis_thermal.dat	Eoutt_	hemispherical outgoing thermal radiation	$\text{W m}^{-2} \mu\text{m}^{-1}$	[nt, nwl]
spectrum_obsdir_thermal.dat	Lot_	outgoing thermal radiance in observation direction	$\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$	[nt, nwl]
layer_fluorecence.dat	Profiles.fluorescence	upward fluorescence per layer	W m^{-2}	[nt,nl+1]
layer_fluorescenceEm.dat	Profiles.fluorescenceEm	fluorescence emission per layer	W m^{-2}	[nt,nl+1]
BOC_irradiance.dat	Emin, Emin+Esun*Ps	Irradiance at the bottom of the canopy for the shaded fraction (first 2162 columns) and average BOC irradiance (sunlit+shaded fraction).	$\text{W m}^{-2} \mu\text{m}^{-1}$	[nt,2xnwl]

8 Description of individual modules

The following modules for the core of the model:

Highest hierarchal level:

SCOPE (script) is the master script.

RTMf, **RTMo**, **RTMt_planck**, **RTMz**, and **RTMt_sb** (functions) are called by **SCOPE** or **Ebal**. They are five radiative transfer models based on the SAIL model, but with numerical solutions where necessary, and analytical solutions where possible. **RTMo** solves the radiative transfer of **incident** radiation, that **RTMf** of **fluorescence emission** (each leaf angle class may have a different emission), **RTMt_sb** is similar to **RTMf**, but for **thermal emission**, and **RTMt_planck** is similar to **RTMt_sb**, but for **high spectral resolution in the thermal range**, and **RTMz** modifies the output of **RTMo** to allow for different reflectance and transmittance of each leaf in the 530-600 nm range.

BSM (function) simulates a soil reflectance spectrum.

Ebal (function) solves the energy balance of leaves and soil. The fluxes of net radiation and sensible, latent and soil heat flux are calculated.

Fluspect (function) calculates the leaf reflectance and transmittance spectra, and the fluorescence excitation to emission matrices of leaves.

Heatfluxes (function) is called by **Ebal** and calculates sensible and latent heat flux as a function of a gradient and resistance (K-theory in micro-meteorology).

Resistances (function) called by **Ebal**. It calculates the aerodynamic resistances within the canopy as a function of wind speed, stability and canopy structure.

Biochemical and **Biochemical_MD12** (functions) are two alternative modules that each calculate leaf photosynthesis and fluorescence relative to the dark adapted level (the spectral distribution of fluorescence is calculated with **RTMf** and **Fluspect**).

Calc_brdf (function) is an optional module called by **SCOPE** that runs the radiative transfer modules over a large number of observation angles to produce a complete BRDF (computationally demanding module).

The following modules contain physical or empirical equations used in the model:

Brightness_T (function) inverts Stefan-Boltzman's law.

Calc_rssrbs (function) calculates the soil surface resistance and soil boundary resistance empirically after Wallace and Verhoef (1997).

Calczenithangle (function) calculates the solar zenith angle from the geographical location, day of the year and hour of the day.

Define_constants (function) defines physical constants such as molecular masses, used in the SCOPE model.

Planck (function). Planck's law.

Satvap (function) calculates the saturated vapour pressure (es) and slope of the es-T curve as a function of temperature T.

Soil_Inertia0 and **Soil_Inertia1** (function) calculates the thermal inertial as a function of soil texture (0) or empirically as a function of soil moisture content (1).

Soil_respiration (function). Dummy module where soil respiration could be implemented.

Vangenuchten (function). Calculates soil moisture from hydraulic pressure, or vice versa. This function is not yet used in SCOPE.

Zo_and_d (function) calculates roughness length for momentum and zero plane displacement from vegetation height and LAI.

The following modules are supporting modules that prepare files, read data, etcetera:

Aggreg (function) aggregates MODTRAN data over SCOPE bands by averaging (over rectangular band passes).

Assignvarnames (script) assigns names to a large structure of input variables.

Calculate_vert_profiles (script) integrates the model output over layers and places the output per layer in the structure 'profiles'.

Count (function) is used in the Lookup-table option. Brilliant function by Wout Verhoef that browses through the list of variables over all combinations.

Create_output_files (script) creates files where the output can be stored, and (optional) writes headers of these files.

Define_bands (function) sets the spectral intervals of the SCOPE model, and writes them to a structure called 'spectral'.

Initialize_output_structures (function) that initializes the structures where the output will be placed. Initially these contain only NaN's.

Leafangles (function) calculates the leaf inclination distribution from the parameters LIDFa and LIDFb.

Load_timeseries (function) loads the data from the files specified in the input data directory.

Meanleaf (function) calculates the layer average and the canopy average of leaf properties that are defined per layer, per leaf angle and per leaf azimuth (36).

Output_data (script) writes output variables to files. The output is added to existing files. This script is executed after each simulation or time step.

Output_verification (script) checks if the output of the latest run with SCOPE_v1.61 matches with a 'standard' output located in a directory called 'verificationdata'. If it does not, then warnings will appear in the Matlab command window.

Plots.m (script) plots all the output of the model. It is an automatic procedure; no polishing of the plots was carried out.

Select_input (function) selects for each time step or for each simulation (of the Lookup-Table) the values for each variable.

Sint (function) carries out Simpson integration.

The following modules are not used by SCOPE, but they are useful for visualization of the results

Plot_directional_figure4 (script) plots hemispherical plots of the output, similar to the paper in Biogeosciences. The script needs some editing (reference to the correct output directory to plot) to work.

Resizefigure (function) is used by `Plot_directional_figure4` to scale the size of the plots. This script has been made by Dr. Michiel van der Molen many years ago.

9 The directory 'data'

The model is supplied with an example data set, collected during the EAGLE field campaign. This chapter explains how to work with the data, the directory structure and file types, etc. It is possible to add new datasets.

After unzipping the files, the directory 'data' can be found at the same hierarchical level as 'SCOPE_v1.61'.

9.1 Directory 'dataset *'

'Dataset for_verification' contains time series of meteorological data. In this case, half-hourly data are provided. It is possible to work with any time interval, but due to the thermal inertia of the soil, the calculation of soil temperature may not be accurate when the time interval is longer than three hours.

It is recommended to name your own dataset 'dataset sitename or projectname'.

The directory contains the following compulsory files (all in ASCII format):

- A time vector ('t_.dat'): a vertical array of time values, in decimal days of the year [1:366.99]. For example, 10 January 2009, 12:00 would be: 10.5. All other files (see below) should correspond to this time vector (and thus have the same size).
- A year vector ('year_.dat'): the year corresponding to the time vector. For example, 10 January 2009, 12:00 would be: 2009
- TOC incoming shortwave radiation ('Rin_.dat'): a broadband (0.3 to 2.5 μm) measurement of incoming shortwave radiation (W m^{-2}), perpendicular to the surface.
- TOC incoming long wave radiation ('Rli_.dat'): a broadband (2.5 to 50 μm) measurement of incoming long wave radiation (W m^{-2}), perpendicular to the surface.
- Air pressure ('p_.dat'): air pressure (hPa or mbar)
- Air temperature measured above the canopy ('Ta_'): air temperature above the canopy in $^{\circ}\text{C}$.
- Vapour pressure measured above the canopy ('e_.dat'): vapour pressure above the canopy (hPa or mbar).
- Wind speed ('u_.dat'): wind speed measured above the canopy (m s^{-1})

The following additional files (not compulsory) can be added:

- Carbon dioxide concentration measured above the canopy (mg m^{-3})

And the following tables (not compulsory):

- Leaf area index ('LAI_.dat')
- Measurement height ('z_.dat') (m)
- Vegetation height ('h_.dat') (m)
- Maximum carboxylation capacity (Table_Vcmax_.dat')
- Chlorophyll content file (Table_Cab_.dat')

If a table is not present, then the corresponding a priori value specified in the file `input_data.xlsx` file is used instead. It is only useful to create the tables LAI_dat etc. if the leaf area index, measurement height, vegetation height etc. change with time during the measurement period.

A table has a slightly different format than the other input files. A table has two columns: the first column contains the decimal DOY, the second column contains the value of the variable. The reason why tables have a different format is that the variables in the table are usually not measured at the same time interval as the meteorological input. For example, the LAI may be measured only once per month.

An example of a table can be found in 'dataset for_verification'.

The measurement height is only relevant for wind speed, vapour pressure and the carbon dioxide concentration. It is currently not possible to specify separate measurement heights for each of these variables.

The carbon dioxide concentration must be provided in mg m^{-3} . This is a commonly used unit in most data sets. SCOPE automatically converts this to ppm and to umol m^{-3} internally. If the carbon dioxide concentration file is not provided, SCOPE assumes a constant concentration corresponding to 380 ppm.

Note: it is important that all files except for the tables have equal length, and that all measurements correspond to the time vector. A Julian calendar is used. The time zone should be provided (the difference between the local time in the file and UTC or GMT). Input files should be comma separated, space separated or tab separated ASCII files. They should not contain empty lines or comment lines.

In case SCOPE is run in individual mode, then the meteorological input files are not used. In that case, all meteorological data are taken from the spreadsheet.

9.2 Directory ‘directional’

The input in the directory ‘directional’ is only used for multi-angle simulations (if the option ‘directional’ is switched on in `parameters`). In this directory one can provide the observer’s zenith and azimuth angles. The files in this directory have two columns: the first column is the observer’s zenith angle, the second the observer’s azimuth (relative to that of the sun, counterclockwise), both in degrees. If the option ‘directional’ is switched on, SCOPE will calculate the radiance spectrum in all directions given in the input file.

9.3 The directory ‘Fluspect_parameters’

In this directory, absorption spectra of different leaf components are provided, according to PROSPECT 3.1, as well as Fluspect input: standard spectra for PSI and PSII.

9.4 The directory ‘radiationdata’

RTM₀ calculates spectra based on MODTRAN5 outputs. One .atm (atmospheric) file is provided in the data, 12 more are provided separately in a different .zip folder (in order to minimize the size of the SCOPE package, these are not provided standard). Note that in the input data (files as well as the spreadsheet), the broadband input radiation may be provided. SCOPE linearly scales the input spectra of the optical and the thermal domain in such a way, that the spectrally integrated input shortwave and long wave radiation matches with the measured values. A limitation of this approach is that the same *shape* of the input spectrum is used independent on the atmospheric conditions. If this scaling is not wanted, then leave ‘Rin’ and ‘Rli’ empty in the spreadsheet.

NOTE: In earlier versions of the model (1.34 and older), two input spectra of solar and sky radiation were provided (rad.txt and rad2.txt) in this directory. The data were calculated with MODTRAN4. The ASCII file in this directory consisted of three columns containing the following. The first column contained the wavelength in nm, the second column the solar radiation in $W m^{-2} \mu m^{-1}$, and the third column the sky radiation in $W m^{-2} \mu m^{-1}$. These data are now obsolete (since version 1.40).

9.5 The directory 'soil_spectrum'

In this directory, the soil spectrum is provided. The ASCII file in this directory consists of two columns containing the following: The first column contains the wavelength in μm , the following columns reflectance spectra. Note that it is also possible to simulate a soil reflectance spectrum with the BSM model. In that case the values for the BSM model parameters are taken from the input data, and the archived spectra in this folder are not used.

9.6 The directory 'leafangles'

In this folder, example leaf inclination distribution data are provided. It is possible to use these distributions instead of the leafinclination model of Verhoef (1998) with the two parameters LIDFa and LIDFb. In that case, provide a filename in the input data tab 'filenames' or the file filenames.m.

9.7 Validation data

The validation data are stored in directory 'measured'. It is up to the user to organize this directory.