R for Photobiology

A handbook

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DRAFT

Contents

List of abbreviations and symbols

For quantities and units used in photobiology we follow, as much as possible, the recommendations of the Commission Internationale de l'Éclairage as described by Sliney2007.

Symbol	Definition
α	absorptance (%).
Δe	water vapour pressure difference (Pa).
ϵ	emittance ($\mathrm{W\,m^{-2}}$).
λ	wavelength (nm).
θ	solar zenith angle (degrees).
ν	frequency (Hz or $\mathrm{s^{-1}}$).
ρ	reflectance (%).
σ	Stefan-Boltzmann constant.
τ	transmittance (%).
χ	water vapour content in the air ($\mathrm{g\,m^{-3}}$).
A	absorbance (absorbance units).
ANCOVA	analysis of covariance.
ANOVA	analysis of variance.
BSWF	BSWF.
c	speed of light in a vacuum.
CCD	charge coupled device, a type of light detector.
CDOM	coloured dissolved organic matter.
CFC	chlorofluorocarbons.
c.i.	confidence interval.
CIE	Commission Internationale de l'Éclairage; or erythemal action spectrum standardized by CIE.
CTC	closed-top chamber.
DAD	diode array detector, linear light detector based on photodiodes.
DBP	dibutylphthalate.
DC	direct current.
DIBP	diisobutylphthalate.
DNA(N)	UV action spectrum for 'naked' DNA.
DNA(P)	UV action spectrum for DNA in plants.
DOM	dissolved organic matter.
DU	Dobson units.
e	water vapour partial pressure (Pa).
E	(energy) irradiance ($\mathrm{W\,m^{-2}}$).
$E(\lambda)$	spectral (energy) irradiance ($\mathrm{W\,m^{-2}\,nm^{-1}}$).

E_0	fluence rate, also called scalar irradiance ($W\,m^{-2}$).
ESR	early stage researcher.
FACE	free air carbon-dioxide enhancement.
FEL	a certain type of 1000 W incandescent lamp.
FLAV	UV action spectrum for accumulation of flavonoids.
FWHM	full-width half-maximum.
GAW	Global Atmosphere Watch.
GEN	generalized plant action spectrum, also abreviated as GPAS Caldwell1971.
GEN(G)	mathematical formulation of GEN by Green1974 .
GEN(T)	mathematical formulation of GEN by Thimijan1978.
h	Planck's constant.
h'	Planck's constant per mole of photons.
H	exposure, frequently called dose by biologists ($kJ\,m^{-2}\,d^{-1}$).
H^{BE}	biologically effective (energy) exposure ($kJ\,m^{-2}\,d^{-1}$).
H_p^{BE}	biologically effective photon exposure ($mol\,m^{-2}\,d^{-1}$).
HPS	high pressure sodium, a type of discharge lamp.
HSD	honestly signifcant difference.
k_B	Boltzmann constant.
L	radiance ($W\,sr^{-1}\,m^{-2}$).
LAI	leaf area index, the ratio of projected leaf area to the ground area.
LED	light emitting diode.
LME	linear mixed effects (type of statistical model).
LSD	least significant difference.
n	number of replicates (number of experimental units per treatment).
N	total number of experimental units in an experiment.
N_A	Avogadro constant (also called Avogadro's number).
NIST	National Institute of Standards and Technology (U.S.A.).
NLME	non-linear mixed effects (statistical model).
OTC	open-top chamber.
PAR	PAR, 400–700 nm.
	measured as energy or photon irradiance.
PC	polycarbonate, a plastic.
PG	UV action spectrum for plant growth.
PHIN	UV action spectrum for photoinhibition of isolated chloroplasts.
PID	PID (control algorithm).
PMMA	polymethylmethacrylate.
PPFD	PPFD, another name for
	PAR photon irradiance (Q_{PAR}).
PTFE	polytetrafluoroethylene.
PVC	polyvinylchloride.
q	energy in one photon ('energy of light').
q'	energy in one mole of photons.
Q	photon irradiance ($mol\,m^{-2}\,s^{-1}$ or $\mu mol\,m^{-2}\,s^{-1}$).
$Q(\lambda)$	spectral photon irradiance ($mol\,m^{-2}\,s^{-1}\,nm^{-1}$ or $\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}$).
r_0	distance from sun to earth.
RAF	RAF (nondimensional).
RH	relative humidity (%).
s	energy effectiveness (relative units).

$s(\lambda)$	spectral energy effectiveness (relative units).
s^{p}	quantum effectiveness (relative units).
$s^{\mathrm{p}}(\lambda)$	spectral quantum effectiveness (relative units).
s.d.	standard deviation.
SDK	software development kit.
s.e.	standard error of the mean.
SR	spectroradiometer.
t	time.
T	temperature.
TUV	tropospheric UV.
U	electric potential difference or voltage (e.g. sensor output in V).
UV	ultraviolet radiation (λ = 100–400 nm).
UV-A	ultraviolet-A radiation (λ = 315–400 nm).
UV-B	ultraviolet-B radiation (λ = 280–315 nm).
UV-C	ultraviolet-C radiation (λ = 100–280 nm).
UV^{BE}	biologically effective UV radiation.
UTC	coordinated universal time, replaces GMT in technical use.
VIS	radiation visible to the human eye ($\approx$ 400–700 nm).
WMO	World Meteorological Organization.
VPD	water vapour pressure deficit (Pa).
WOUDC	World Ozone and Ultraviolet Radiation Data Centre.

Part I

Getting ready

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Introduction

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In this chapter we explain the physical basis of optics and photo-chemisatry.

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Unweighted irradiance

Abstract

In this chapter we explain how to calculate unweighted energy and photon irradiances from spectral irradiance.

6.1   Task: (energy) irradiance from spectral irradiance

The task to be completed is to calculate the (energy) irradiance (E) in $\mathrm{W\,m^{-2}}$ from spectral (energy) irradiance ($Q(\lambda)$) in $\mathrm{W\,m^{-2}\,nm^{-1}}$ and the corresponding wavelengths (λ) in nm.

$$Q_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda)\,\mathrm{d}\,\lambda \tag{6.1}$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) energy irradiance, for which the most accepted limits are $\lambda_1 = 400$nm and $\lambda_1 = 700$nm. In this example we will use example data for sunlight to calculate $E_{400\,\mathrm{nm} < \lambda < 700\,\mathrm{nm}}$:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad,
                                 new_waveband(400, 700)))

## range.400.700
##       196.7
```

Function PAR() is predefined in package photobiologyVIS as a convenience function, so the code above can be replaced by:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad, PAR()))

##    PAR
## 196.7
```

If no waveband is supplied as argument, then the whole range of wavelengths in the spectral data is used for the integration, and the 'name' attribute is generated accordingly:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad))

## range.293.800
##        268.9
```

If a waveband that does not fully overlap with the data is supplied as argument, then spectral irradiance for wavelengths outside the range is assumed to be zero:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad,
                                 new_waveband(700,1000)))

## range.700.1000
##          44.1
```

If a waveband that does not overlap with the data is supplied as argument, then spectral irradiance for wavelengths outside the range is assumed to be zero:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad,
                                 new_waveband(100,200)))

## range.100.200
##             0
```

6.2   Task: photon irradiance from spectral irradiance

The task to be completed is to calculate the photon irradiance (Q) in $\mathrm{mol\,m^{-2}\,s^{-1}}$ from spectral (energy) irradiance ($E(\lambda)$) in $\mathrm{W\,m^{-2}\,nm^{-1}}$ and the corresponding wavelengths (λ) in nm.

The energy of a quantum of radiation in a vacuum, q, depends on the wavelength, λ, or frequency[1], ν,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \qquad (6.2)$$

with the Planck constant $h = 6.626 \times 10^{-34}$ Js and speed of light in vacuum $c = 2.998 \times 10^8$ $\mathrm{m\,s^{-1}}$. When dealing with numbers of photons, the equation (6.2) can be extended by using Avogadro's number $N_A = 6.022 \times 10^{23}$ $\mathrm{mol^{-1}}$. Thus, the energy of one mole of photons, q', is

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \qquad (6.3)$$

with $h' = h \cdot N_A = 3.990 \times 10^{-10}$ $\mathrm{Js\,mol^{-1}}$. Example 1: red light at 600 nm has about 200 $\mathrm{kJ\,mol^{-1}}$, therefore, 1 µmol photons has 0.2 J. Example 2: UV-B

---

[1]Wavelength and frequency are related to each other by the speed of light, according to $\nu = c/\lambda$ where c is speed of light in vacuum. Consequently there are two equivalent formulations for equation 6.2.

radiation at 300 nm has about 400 $kJ\,mol^{-1}$, therefore, 1 μmol photons has 0.4 J. Equations 6.2 and 6.3 are valid for all kinds of electromagnetic waves.

Combining equations 6.1 and 6.3 we obtain:

$$Q_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda)\, \frac{h' \cdot c}{\lambda} \mathrm{d}\,\lambda \tag{6.4}$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) photon irradiance. In this example we will use example data for sunlight.

```
with(sun.data,
     photon_irradiance(w.length, s.e.irrad, PAR()))

##        PAR
## 0.0008938
```

If we want to have Q_{PAR} (PPFD) expressed in the usual units of $\mu mol\,m^{-2}\,s^{-1}$, we need to multiply the result above by 10^6:

```
with(sun.data,
     photon_irradiance(w.length, s.e.irrad, PAR())) * 1e6

##    PAR
## 893.8
```

PAR() is predefined in package photobiologyVIS as a convenience function, see section 6.1 for an example with arbitrary values for λ_1 and λ_2.

6.3   Task: calculate energy and photon irradiances from spectral photon irradiance

In the case of the calculation of energy irradiance from spectral photon irradiance the calculation is:

$$I_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} Q_\lambda\, \frac{\lambda}{h' \cdot c} \mathrm{d}\,\lambda \tag{6.5}$$

And the code[2]:

```
with(sun.data, energy_irradiance(w.length, s.q.irrad, PAR()),
     unit.in = "photon")

##        PAR
## 0.0008938
```

The calculation of photon irradiance from spectral photon irradiance, is a simple integration, analogous to that in equation 6.1, and the code is:

```
with(sun.data, photon_irradiance(w.length, s.q.irrad, PAR()),
     unit.in = "photon")

##        PAR
## 4.158e-09
```

---

[2]The dataframe sun.data contains both spectral energy irradiance vales in 'column' s.e.irrad and spectral photon irradiance in 'column' s.q.irrad

6.4 Task: irradiances for more than one waveband

It is possible to calculate the irradiances for several wavebands with a single function call by supplying a `list` of `wavebands` as argument:

```
with(sun.data, photon_irradiance(w.length, s.e.irrad, list(Red(),
    Green(), Blue()))) * 1e+06

##    Red.ISO Green.ISO  Blue.ISO
##      452.2     220.2     149.0

Q.RGB <- with(sun.data, photon_irradiance(w.length, s.e.irrad,
    list(Red(), Green(), Blue()))) * 1e+06
signif(Q.RGB, 3)

##    Red.ISO Green.ISO  Blue.ISO
##        452       220       149

Q.RGB[1]

## Red.ISO
##    452.2

Q.RGB["Green.ISO"]

## Green.ISO
##     220.2
```

A named list can be used to override the use as names for the output of the waveband names:

```
with(sun.data, photon_irradiance(w.length, s.e.irrad, list(R = Red(),
    G = Green(), B = Blue()))) * 1e+06

##      R     G     B
## 452.2 220.2 149.0
```

Even when using a single waveband:

```
with(sun.data,
    photon_irradiance(w.length, s.e.irrad,
                      list(UVB=UVB()))) * 1e6

##    UVB
## 1.527
```

6.5 Task: use simple wavebands

Please, consult the packages' documentation for a list of predefined functions for creating wavebands. Here we will present just a few examples of their use. We usually associate wavebands with colours, however, in many cases there are different definitions in use. For this reason, the functions provided accept an argument that can be used to select the definition to use. In general, the default, is to use the ISO standard whenever it is applicable. The case of the various definitions in use for the UV-B waveband are described on page 19

We can use a predefined function to create a new `waveband` object, which as any other R object can be assigned to a variable:

```
uvb <- UVB()
uvb

## UVB.ISO
## low (nm) 280
## high (nm) 315
```

As seen above, there is a specialized `print` function for `wavebands`. Functions available are `min`, `max`, `range`, `center_wl`, `labels`, and `color`.█

```
red <- Red()
red

## Red.ISO
## low (nm) 610
## high (nm) 760

min(red)

## [1] 610

max(red)

## [1] 760

range(red)

## [1] 610 760

midpoint(red)

## [1] 685

labels(red)

## $label
## [1] "Red.ISO"

color(red)

## Red.ISO CMF  Red.ISO CC
##   "#900000"    "#FF0000"
```

Here we demonstrate the use of an argument to choose a certain definition:

```
UVB()

## UVB.ISO
## low (nm) 280
## high (nm) 315

UVB("ISO")

## UVB.ISO
## low (nm) 280
## high (nm) 315
```

```r
UVB("CIE")

## UVB.CIE
## low (nm) 280
## high (nm) 315

UVB("medical")

## UVB.medical
## low (nm) 290
## high (nm) 320

UVB("none")

## UVB.none
## low (nm) 280
## high (nm) 320
```

Here we demonstrate the importance of complying with standards, and how much the photon irradiance calculated can depend on the definition used.

```r
with(sun.data,
     photon_irradiance(w.length, s.e.irrad, UVB("ISO"))) * 1e6

## UVB.ISO
##   1.527

with(sun.data,
     photon_irradiance(w.length, s.e.irrad, UVB("none"))) * 1e6

## UVB.none
##    3.282
```

6.6   Task: define simple wavebands

Here we briefly introduce `new_waveband`, and only in chapter **??** we describe its use in full detail, including the use of spectral weighting functions (SWFs).

Defining a new `waveband` based on extreme wavelengths expressed in nm.

```r
wb1 <- new_waveband(500,600)
wb1

## range.500.600
## low (nm) 500
## high (nm) 600

with(sun.data,
     photon_irradiance(w.length, s.e.irrad, wb1)) * 1e6

## range.500.600
##          314.1

wb2 <- new_waveband(500,600, wb.name="my.colour")
wb2
```

```
## my.colour
## low (nm) 500
## high (nm) 600

with(sun.data,
     photon_irradiance(w.length, s.e.irrad, wb2)) * 1e6

## my.colour
##      314.1
```

6.7 Task: photon ratios

In photobiology sometimes we are interested in calculation the photon ratio between two wavebands. It makes more sense to calculate such ratios if both numerator and denominator wavebands have the same 'width' or if the numerator waveband is fully nested in the denominator waveband. However, frequently used ratios like the UV-B to PAR photon ratio do not comply with this. For this reason, our functions do not enforce any such restrictions.

For example a ratio frequently used in plant photobiology is the read to far-red photon ratio (R:FR photon ratio or ζ). If we follow the wavelength ranges in the definition given by **Morgan1981a** using photon irradiance[3]:

$$\zeta = \frac{Q_{655nm<\lambda<665nm}}{Q_{725nm<\lambda<735nm}} \qquad (6.6)$$

To calculate this for our example sunlight spectrum we can use the following code:

```
with(sun.data,
     photon_ratio(w.length, s.e.irrad, Red("Smith"), Far_red("Smith")))

## [1] 1.251
```

or using the predefined convenience function R_FR_ratio:

```
with(sun.data,
     R_FR_ratio(w.length, s.e.irrad))

## [1] 1.251
```

Using defaults for waveband definitions:

```
with(sun.data,
     energy_ratio(w.length, s.e.irrad, UVB(), PAR()))

## [1] 0.00299
```

---

[3]In the original text photon fluence rate is used but it not clear whether photon irradiance was meant instead.

6.8 Task: energy ratios

An energy ratio, equivalent to ζ can be calculated as follows:

```
with(sun.data,
     energy_ratio(w.length, s.e.irrad, Red("Smith"), Far_red("Smith")))

## [1] 1.384
```

For this infrequently used ratio, no pre-defined function is provided.

6.9 Task: calculate average number of photons per unit energy

When comparing photo-chemical and photo-biological responses under different light sources it is of interest to calculate the photons per energy in $\mathrm{mol\,W^{-1}}$. In this case only one waveband definition is used to calculate the quotient:

$$\bar{q}' = \frac{Q_{\lambda_1 < \lambda < \lambda_2}}{E_{\lambda_1 < \lambda < \lambda_2}} \tag{6.7}$$

```
with(sun.data,
     photons_energy_ratio(w.length, s.e.irrad, PAR()))

## [1] 4.544e-06
```

For obtaining the same quotient in $\mathrm{\mu mol\,W^{-1}}$ we just need to multiply by 10^6. We can use such a multiplier to convert $E\,[\,\mathrm{W\,m^{-2}}\,]$ into $Q\,[\,\mathrm{\mu mol\,m^{-2}\,s^{-1}}\,]$, or as a divisor to convert $Q\,[\,\mathrm{\mu mol\,m^{-2}\,s^{-1}}\,]$ into $E\,[\,\mathrm{W\,m^{-2}}\,]$, *for a given light source and waveband*:

```
with(sun.data, photons_energy_ratio(w.length, s.e.irrad, PAR())) *
    1e+06

## [1] 4.544
```

6.10 Task: calculate the contribution of different regions of a spectrum to energy irradiance

It can be of interest to split the total (energy) irradiance into adjacent regions delimited by arbitrary wavelengths. We can use the function `split_energy_irradiance` to obtain to energy of each of the regions delimited by the values in nm supplied in a numeric vector:

```
with(sun.data, split_energy_irradiance(w.length, s.e.irrad, c(400,
    500, 600, 700)))

## range.400.500 range.500.600 range.600.700
##         69.63         68.53         58.54
```

Here we demonstrate that the sum of the four 'split' irradiances add to the total for the range of wavelengths covered:

```
with(sun.data, sum(split_energy_irradiance(w.length, s.e.irrad,
    c(400, 500, 600, 700))))

## [1] 196.7

with(sun.data, energy_irradiance(w.length, s.e.irrad, PAR()))

##    PAR
## 196.7
```

It also possible to obtain the 'split' as a vector of fractions adding up to one,

```
with(sun.data, split_energy_irradiance(w.length, s.e.irrad, c(400,
    500, 600, 700), scale = "relative"))

## range.400.500 range.500.600 range.600.700
##        0.3540        0.3484        0.2976
```

or as percentages:

```
with(sun.data, split_energy_irradiance(w.length, s.e.irrad, c(400,
    500, 600, 700), scale = "percent"))

## range.400.500 range.500.600 range.600.700
##        35.40         34.84         29.76
```

A vector of two wavelengths is valid input, although not very useful for percentages:

```
with(sun.data, split_energy_irradiance(w.length, s.e.irrad, c(400,
    700), scale = "percent"))

## range.400.700
##           100
```

Although for `scale="absolute"`, the default, it can be used as a quick way of calculating an irradiance for a range of wavelengths without having to define a `waveband`:

```
with(sun.data, split_energy_irradiance(w.length, s.e.irrad, c(400,
    700)))

## range.400.700
##         196.7
```

6.11 Task: calculate the contribution of different regions of a spectrum to photon irradiance

The function `split_photon_irradiance` takes the same arguments as the equivalent function for photon irradiance, consequently only one code example is provided here (see section 6.10 for more details):

```r
with(sun.data, split_photon_irradiance(w.length, s.e.irrad, c(400,
    500, 600, 700), scale = "percent"))
```

```
## range.400.500 range.500.600 range.600.700
##         29.41         35.14         35.45
```

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Weighted and effective irradiance

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