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Estimating the photosynthetically active radiation under clear skies by means of a new approach

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Abstract. The k -distribution method and the correlated- k approximation of Kato et al. (1999) is a computationally efficient approach originally designed for calculations of the broadband solar radiation by dividing the solar spectrum in 32 specific spectral bands from 240 to 4606 nm. This paper describes a technique for an accurate assessment of the photosynthetically active radiation (PAR) from 400 to 700 nm at ground level, under clear-sky conditions using twelve of these spectral bands. It is validated against detailed spectral calculations of the PAR made by the radiative transfer model libRadtran. For the direct and global PAR irradiance, the bias is -0.4 W m^{-2} (-0.2%) and -4 W m^{-2} (-1.3%) and the root mean square error is 1.8 W m^{-2} (0.7%) and 4.5 W m^{-2} (1.5%). For the direct and global Photosynthetic Photon Flux Density, the biases are of about $+10.3 \mu\text{mol m}^{-2} \text{ s}^{-1}$ ($+0.8\%$) and $1.9 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (-0.1%) respectively, and the root mean square error is $11.4 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (0.9%) and $4.0 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (0.3%). The correlation coefficient is greater than 0.99. This technique provides much better results than two state-of-the-art empirical methods computing the daily mean of PAR from the daily mean of broadband irradiance.

1 Introduction

Photosynthetically active radiation, abbreviated in PAR, is the solar radiation in the range [400, 700] nm that can be used by organisms via the process of photosynthesis. PAR is defined as the incident power per unit surface for this spectral interval and may be expressed in W m^{-2} . PAR is also a measure of the photosynthetic photon flux density, abbreviated in PPF and expressed in $\mu\text{mol m}^{-2} \text{ s}^{-1}$, and is defined as the number of the incident photons per unit time per unit surface. Both units are linked by the widely used approximation $1 \text{ W m}^{-2} \approx 4.57 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (McCree, 1972). PAR is a portion of the total, also known as broadband, solar irradiance. Whatever the spectral interval, the solar radiation available at ground level on a horizontal plane is called the global radiation. The global is the sum of the direct component that comes from the direction of the sun and the diffuse component that comes from the rest of the sky vault. Let note respectively G , P_G and Q_P , the global broadband irradiance, the global PAR irradiance, and the global PPF at ground level.

In situ measurements of PAR are rare in space and time. This scarcity leads researchers and practitioners to calculate PAR from the global broadband solar irradiance by empirical means. For example, Udo and Aro (1999) proposed a ratio of 2.079 between the daily mean of G and the daily mean of Q_P :

$$Q_P = 2.079G \quad (1)$$

where the constant 2.079 is in $\mu\text{mol J}^{-1}$. Jacovides et al. (2004) suggested a ratio of 1.919. These authors acknowledge that the actual ratio depends on the sky conditions and atmospheric properties.

Other approaches to PAR assessment and more generally to assessment of the solar radiation in any spectral interval are atmospheric radiative transfer models (RTM). Besides the difficulty in knowing all inputs requested by RTMs, their main disadvantage is the computational load because many spectral calculations must be performed. Several methods have been proposed to reduce the number of calculations. Among them, are the k -distribution method and the correlated- k approximation proposed by Kato et al. (1999)

Table 1. KB covering and close to PAR spectral interval, selected sub-intervals $\delta\lambda_i$, slopes and intercepts of the affine functions between the clearness indices in KB and sub-intervals $\delta\lambda_i$ obtained from libRadtran simulations.

KB	Interval $\Delta\lambda$, nm	Sub-interval $\delta\lambda$, nm (#i)	Global		Direct normal	
			Slope a_i	Intercept b_i	Slope c_i	Intercept d_i
6	363–408	385–386 (#1)	0.9987	−0.0023	1.0030	−0.0032
7	408–452	430–431 (#2)	1.0026	−0.0004	0.9995	0.0013
8	452–518	484–485 (#3)	1.0034	0.0005	0.9979	0.0000
9	518–540	528–529 (#4)	0.9998	−0.0005	1.0008	−0.0013
10	540–550	545–546 (#5)	1.0001	0.0003	1.0003	−0.0003
11	550–567	558–559 (#6)	1.0004	0.0004	0.9997	0.0012
		569–570 (#7)	0.9960	−0.0119	1.0024	−0.0100
12	567–605	586–587 (#8)	1.0123	0.0064	0.9929	0.0267
		589–590 (#9)	0.9568	−0.0109	0.9804	−0.0434
		602–603 (#10)	1.0150	0.0167	1.0051	0.0212
13	605–625	615–616 (#11)	1.0004	0.0009	0.9977	0.0033
		625–626 (#12)	1.0104	−0.0174	1.0622	−0.0551
14	625–667	644–645 (#13)	1.0072	0.0029	0.9960	0.0154
		656–657 (#14)	0.9915	0.0068	0.9698	0.0205
15	667–684	675–676 (#15)	1.0006	0.0007	0.9978	0.0036
		685–686 (#16)	1.0473	0.0212	0.9681	0.1036
16	684–704	687–688 (#17)	0.9602	−0.0130	1.0041	−0.0531
		694–695 (#18)	0.9828	−0.0153	1.0323	−0.0642
17	704–743	715–716 (#19)	1.0262	0.0121	0.9771	0.0596

whose approach is implemented in several RTMs. This approach was originally designed as a very efficient way to speed up computations of G and its direct component by using 32 specific spectral intervals across the solar spectrum from 240 to 4606 nm. Hereafter, these spectral intervals are abbreviated in KB. This article deals with the assessment of the PAR – irradiance and PPFD – using the irradiance of each KB covering the PAR spectral range in clear sky conditions.

2 Problem statement

The global PAR irradiance P_G is mathematically defined as:

$$P_G = \int_{400}^{700} G_\lambda d\lambda \quad (2)$$

where G_λ is the global spectral irradiance, λ the wavelength and the integration is made between 400 and 700 nm. The global PPFD Q_P is similarly defined as:

$$Q_P = \frac{1}{hc} \int_{400}^{700} G_\lambda \lambda d\lambda \quad (3)$$

where h is the Planck's constant and c the velocity of light.

The direct normal irradiance is the irradiance received on a plane always facing the sun rays with a normal incidence. Let note respectively B , P_B , and Q_{PB} , the direct normal broadband irradiance, the direct normal PAR irradiance, and the direct normal PPFD:

$$P_B = \int_{400}^{700} B_\lambda d\lambda \quad (4)$$

$$Q_{PB} = \frac{1}{hc} \int_{400}^{700} B_\lambda \lambda d\lambda \quad (5)$$

where B_λ is the direct normal spectral irradiance.

The integral may be replaced by a Riemann sum using very narrow spectral intervals or bands, hereafter abbreviated NB. Here, we chose $\delta\lambda = 1$ nm, assuming that the optical properties of the atmosphere do not change over 1 nm. If λ_i denotes now the center wavelength of each NB of width $\delta\lambda$, it comes:

$$P_G = \sum_{i=1}^{300} G_{\delta\lambda i} \quad (6)$$

$$Q_P = \frac{1}{hc} \sum_{i=1}^{300} G_{\delta\lambda i} \lambda_i \quad (7)$$

Similar equations hold for P_B and Q_{PB} .

The PAR spectral band [400, 700] nm is covered by 11 KB, from #6 [363, 408] nm to #16 [684, 704] nm (Table 1). Wandji Nyamsi et al. (2014) demonstrated that as a whole the approach of Kato et al. (1999) offer accurate estimates of the spectral irradiance in most of the 32 KB when compared to detailed spectral calculations in clear sky and cloudy conditions, and especially for the KB #6 to 16. It follows that the

PAR may be computed by a Riemann sum based on 11 KB instead of 300 NBs. KB #6 and #16 are partly outside the PAR range. One solution is a weighted sum based on the overlap between KB_j and the PAR interval. The weight w_j of KB_j may be defined as follows:

$$w_j = 1, \text{ if } j \text{ is not } 6 \text{ or } 16$$

$$w_6 = (408 - 400)/(408 - 363) = 0.1778$$

$$w_{16} = (700 - 684)/(704 - 684) = 0.80$$

and

$$P_G = \sum_{j=6}^{16} G_{KB_j} w_j \tag{8}$$

$$Q_P = \frac{1}{hc} \sum_{j=6}^{16} G_{KB_j} w_j \lambda_{KB_j} \tag{9}$$

where G_{KB_j} is the global irradiance for KB_j and λ_{KB_j} the center wavelength of KB_j . Similar equations hold for P_B and Q_{PB} . However, Wandji Nyamsi et al. (2014) reported a relative root mean square error less than 2% between detailed spectral calculations and the approach by Kato et al. (1999) for each KB, from #6 to #16. Though small this error may be decreased for the PAR by the technique proposed in this article.

3 Description of the technique

Actually, the bandwidth in several KB is larger than 30 nm and may be considered large for estimating PAR in an accurate manner. The concept underlying the proposed technique is to determine several narrower spectral bands NB whose transmissivities are correlated to those of the KB and then use these transmissivities in a linear interpolation process to compute the PAR. This technique is elaborated and validated by the means of the RTM libRadtran (Mayer and Kylling, 2005).

The clearness index KT_i and the direct clearness index KT_{Bi} – also called atmospheric transmissivity and direct atmospheric transmissivity – are defined as follows:

$$KT_i = \frac{G_{\delta\lambda i}}{E_{o_i} \cos(\theta_s)} \tag{10}$$

$$KT_{Bi} = \frac{B_{\delta\lambda i}}{E_{o_i}} \tag{11}$$

where θ_s is the solar zenithal angle; E_{o_i} is the irradiance at the top of atmosphere on a plane normal to the sun rays for the i th NB. Several solar spectra E_{o_i} have been published. That of Gueymard (2004) is available in libRadtran and has been used here. By introducing the clearness index in Eqs. (6) and (7), it comes:

Table 2. Ranges and distributions of values taken by the solar zenith angle, the ground albedo and the 7 variables describing the clear atmosphere.

Variable	Value
– Solar zenith angle θ_s	– Uniform between 0 and 89 (degree)
– Ground albedo ρ_g	– Uniform between 0 and 0.9
– Total column content of ozone	– Ozone content is: $300 \times \beta + 200$, in Dobson unit. Beta distribution, with A parameter = 2, and B parameter = 2, to compute β
– Total column content of water vapor	– Uniform between 0 and 70 (kg m^{-2})
– Elevation of the ground above mean sea level	– Equiprobable in the set: {0, 1, 2, 3} (km)
– Atmospheric profiles (Air Force Geophysics Laboratory standards)	– Equiprobable in the set: {"Midlatitude Summer", "Midlatitude Winter", "Subarctic Summer", "Subarctic Winter", "Tropical", "US Standard"}
– Aerosol optical depth at 550 nm	– Gamma distribution, with shape parameter = 2, and scale parameter = 0.13
– Angström coefficient	– Normal distribution, with mean = 1.3 and standard-deviation = 0.5
– Aerosol type	– Equiprobable in the set: {"urban", "rural", "maritime", "tropospheric", "desert", "continental", "Antarctic"}

$$P_G = \cos(\theta_s) \sum_{i=1}^{300} E_{o_i} KT_i \tag{12}$$

$$Q_P = \frac{\cos(\theta_s)}{hc} \sum_{i=1}^{300} E_{o_i} KT_i \lambda_i \tag{13}$$

Similar equations hold for P_B and Q_{PB} . A set of 60 000 clear sky atmospheric states is built by the mean of Monte-Carlo technique that will be input to libRadtran. Table 2 reports the nine input variables selected with seven of them describing the clear sky atmosphere: θ_s , ground albedo, total column content of water vapor and ozone, the vertical profile of temperature, pressure, density, and volume mixing ratio for gases as a function of altitude, the aerosol optical depth at 550 nm, Angström coefficient, and aerosol type, and the elevation of the ground above sea level. The random selection of inputs takes into account the modelled marginal distribution established from observation proposed by Lefevre et al. (2013) and Oumbe et al. (2011). More precisely, the uniform distribution is chosen as a model for marginal probability for all parameters except aerosol optical thickness, Angstrom coefficient, and total column content of ozone. The chi-square law for aerosol optical thickness, the normal law for the Angstrom coefficient, and the beta law for total column content of ozone have been selected. The selection of these parametric probability density functions and their corresponding parameters have been empirically determined from the analyses of the observations made in the AERONET network for aerosol properties and from meteorological satellite-based ozone products (Lefevre et al., 2013).

Several plots were made superimposing KT_{KB} and KT_i obtained every nm for the interval [363, 743] nm. A visual inspection of the differences between KT_{KB} and KT_i helps in establishing a set of selected NB, taking into account that the number of these sub-intervals should be as small as possible but still retaining a high accuracy when using a linear interpolation between the sub-intervals to compute the PAR, as explained later. Table 1 reports the 12 KB and the 19 sub-intervals NB. The KB #17 is necessary to obtain NBs enclosing the PAR interval. All KBs contain one NB, except KB #12, 14 and 16, where 4, 3 and 3 NBs were found respectively. These bands exhibit strong variations of KT_i that cannot be accounted for with a single NB.

In each selected NB, an affine function is determined by least-square fitting technique:

$$KT_i = a_i KT_{KB_j} + b_i \quad (14)$$

$$KT_{Bi} = c_i KT_{BKB_j} + d_i. \quad (15)$$

Table 1 also reports the slope and intercept for the global and direct clearness indices for each selected NB. This set of affine functions is established once for all. For any atmospheric state, given the twelve values of KT_{KB_j} and KT_{BKB_j} , the nineteen KT_i and KT_{Bi} are computed for each corresponding NB using the affine functions. Then, KT and KT_B are computed for each nm between 400 and 700 nm using a linear interpolation with KT_i and KT_{Bi} as nodes. Finally, Eqs. (12)–(13) provide P_G and Q_P . A similar process yields the direct normal PAR: P_B and Q_{PB} .

4 Numerical validation

A comparison of the results of the proposed technique against the results from the detailed spectral calculations made by libRadtran considered as a reference is performed to assess the performances of the proposed technique for P_G , Q_P , P_B and Q_{PB} . Then, these performances are compared to those obtained for Q_P by the methods proposed by Jacovides et al. (2004), Udo and Aro (1999) and the weighted sum (Eq. 9). Another sample of 15 000 atmospheric states has been constructed and used for validation.

4.1 Performance of the proposed technique

Deviations: estimates minus reference, are computed for each state of the validation sample for P_G , Q_P , P_B and Q_{PB} . They are synthesized by the bias, the root mean square error (RMSE) and the correlation coefficient. The relative bias and RMSE are computed relative to the mean value of the reference. Figure 1 exhibits these statistical parameters for the global and direct normal PAR irradiance and PPFd. For the direct component, the bias for PAR irradiance, respectively PPFd, is -0.4 W m^{-2} , i.e. -0.2% in relative value, and $+10.3 \mu\text{mol m}^{-2} \text{ s}^{-1}$, i.e. $+0.8\%$ in relative value. The RMSE is respectively 1.8 W m^{-2} (0.7%) and

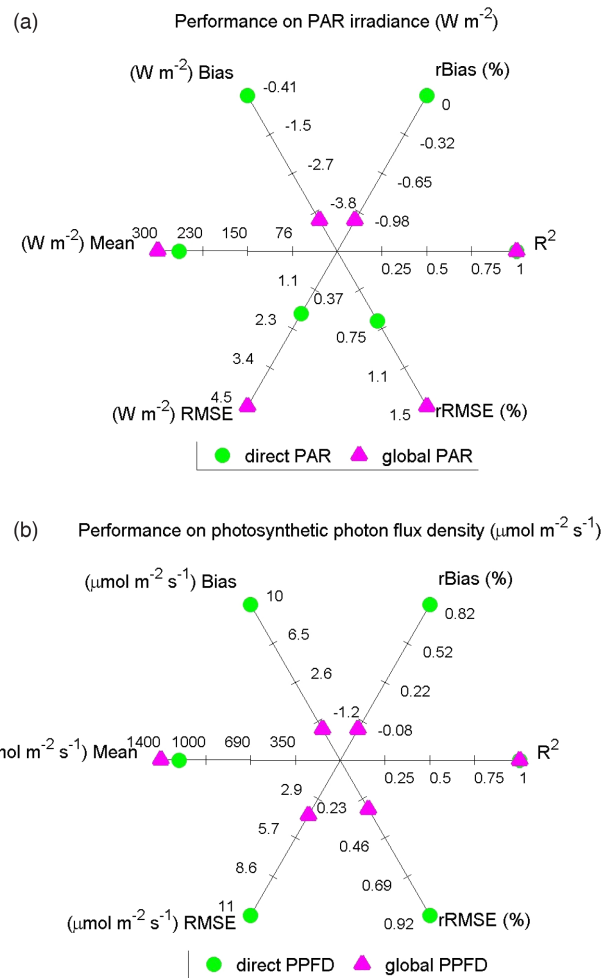


Figure 1. Synthesis of the performance of the proposed technique.

$11.4 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (0.9%). For the global, the bias for PAR irradiance, respectively PPFd, is -4.0 W m^{-2} , i.e. -1.3% in relative value, and $1.9 \mu\text{mol m}^{-2} \text{ s}^{-1}$, i.e. -0.1% in relative value. The RMSE is respectively 4.5 W m^{-2} (1.5%) and $4.0 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (0.3%). The coefficient of determination R^2 is greater than 0.99. These figures prove the good level of performance of the proposed technique.

4.2 Comparison with other methods

Figure 2 exhibits the statistical indicators for Q_P obtained by the methods of Jacovides et al. (2004), Udo and Aro (1999), weighted sum and the proposed technique. The method of Jacovides et al. underestimates the PAR by -7.4% ; the relative RMSE is 9.6%. The method of Udo and Aro shows better results with a relative bias of 0.3% and a relative RMSE of 4.7%. The weighted sum exhibits very low relative bias: -0.2% , and relative RMSE: 0.3%. The proposed technique shows also a very good agreement with a relative bias of

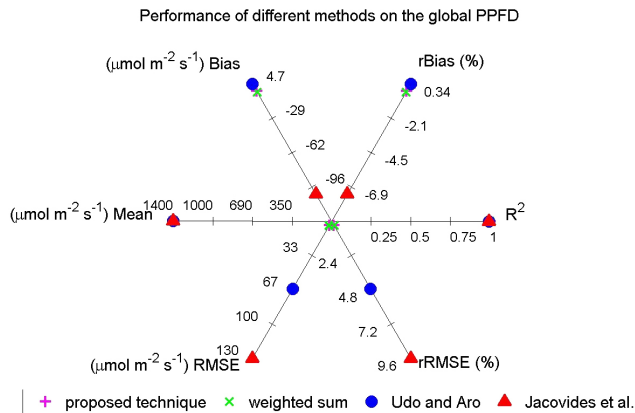


Figure 2. Performance of different methods: Jacovides et al. (2004); Udo and Aro (1999), weighted sum and the proposed technique.

−0.1 % and relative RMSE of 0.3 % and offers the same results than the weighted sum.

There are two causes for this similarity. The first cause is that all KB contain one $\delta\lambda_i$, except KB #12, 14 and 16. For these bands, variations of KT_i with λ_i are very small. If it were the case for all KB, from #6 to #17, the proposed technique and the weighted sum would agree and provide similar results. But small discrepancies happen between both techniques due to the bands KB #12, 14 and 16, which are subdivided by respectively 4, 3 and 3 $\delta\lambda_i$. However, the contribution of these bands to the PAR outside the atmosphere is only 25 % approximately. As a consequence, these small discrepancies have a small influence on the final result. Both the weighted sum and the proposed technique exhibit better performances than the empirical method because both take into account the actual atmospheric effects by the means of the Kato et al. approach.

5 Conclusions

The k -distribution method and the correlated- k approximation of Kato et al. (1999) is a computationally efficient approach originally designed for calculations of the broadband solar radiation at ground level by dividing the solar spectrum in 32 specific spectral bands from 240 to 4606 nm. This paper describes a technique for an accurate assessment of the PAR under clear-sky conditions using the irradiance estimated in twelve of these spectral bands. The validation against numerical simulation exhibits very good performances. For the direct and global PAR irradiance, the bias is -0.4 W m^{-2} (−0.2 %) and -4 W m^{-2} (−1.3 %) and the RMSE is 1.8 W m^{-2} (0.7 %) and 4.5 W m^{-2} (1.5 %). For the direct and global PPFD, the bias of is $+10.3 \mu\text{mol m}^{-2} \text{s}^{-1}$ (+0.8 %) and $1.9 \mu\text{mol m}^{-2} \text{s}^{-1}$ (−0.1 %) and the RMSE is $11.4 \mu\text{mol m}^{-2} \text{s}^{-1}$ (0.9 %) and $4.0 \mu\text{mol m}^{-2} \text{s}^{-1}$ (0.3 %). The correlation coefficient is greater than 0.99. It is also

shown that the proposed technique provides better results than two state-of-the-art empirical methods estimating the global PPFD from the global irradiance (Jacovides et al., 2004; Udo and Aro, 1999).

The proposed technique is very useful for the operational estimation of PAR when computational load and great accuracy in PAR are major issues. In addition, this technique may be extended to be able to accurately estimate other spectral quantities taking into account spectral absorption of photosynthetic pigments found in plants and algae such as chlorophyll, carotenoids. The authors are aware of the heuristic way used for selecting the specific NBs for each KB in their work. Other ways are possible. For example, one may think of using the variance between KT_{KB} and all KT_i within a given KB to determine automatically the need for more than one sub-interval. The greater the number of sub-intervals, the higher the accuracy in PAR computation at the expense of a greater number of affine functions.

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