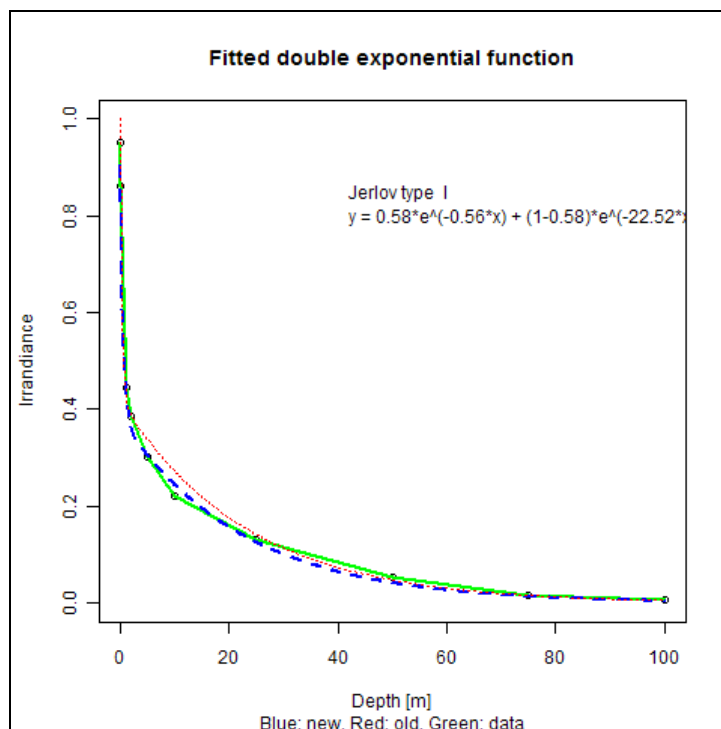


Fitting measured irradiance of Jerlov water types to double exponential functions using R

Adolf Konrad Stips



EUR 24658 EN - 2010

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JRC59066

EUR 24658 EN
ISBN 978-92-79-18924-1
ISSN 1018-5593
doi:10.2788/80912

Luxembourg: Publications Office of the European Union

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Printed in Italy

Fitting irradiance of Jerlov water types to double exponential functions using R

Abstract

The distribution of solar radiation in the upper ocean is important for physical modelling, as it is determining the warming of the upper layers by absorption. The solar irradiance measurements from Jerlov, 1976 are approximated by double exponential functions which are to be used in the hydrodynamic model. New improved estimates for the parameters a , g_1 and g_2 are presented for the classical as well as for different other coastal water types. The goodness of fit and therefore the estimated parameters could be improved by applying the R function `nls`, hence it is recommended to use the here derived parameters for application within regional modelling of the European coastal waters.

Introduction

The light absorption in the upper water layers is the most critical process which is largely determining the near surface temperatures in the ocean. Therefore this light absorption has to be taken into account in ocean modelling. As known the light absorption is depending strongly on the wave length, with smaller blue/green absorption than in the red/infrared part. For reasons of efficiency usually not the full spectrum but only the major frequency ranges are considered.

In the 60/70ties total irradiance (I) and hence absorption was considered in the models only as an exponential function of depth with only 1 attenuation coefficient (K_d). Because of the preferential absorption of the longer wave length near to the surface this approximation is rather poor in the uppermost 5 to 10m. The use of only 1 attenuation coefficient for the full spectral has proven also in modelling studies to be too simple to provide good results (Kara et al. 2005). Therefore now typically at least 2 spectral ranges (visible and near infrared) are considered, using a double exponential representation of downward irradiance.

The first authors proposing this idea were most like Paulson and Simpson 1977 who fitted the irradiance measurements for different water types as published in Jerlov 1968. Their derived fit values have been widespread used and cited, but they did not provide any details about the applied procedure for achieving this non-linear fit to a double exponential function. Jerlov 1968 has made a classification of 5 water types, namely I, IA, IB, II and III, to which Paulson and Simpson 1976 added a type I1, derived from type I, but performing the fit only in the uppermost 50m of the water column.

Further already in the new edition Jerlov 1976 new and additional irradiance measurements were published. Jerlov added the coastal water types 1, 3, 5, 7, 9 (see Appendix 1) exhibiting rather strong absorption. These facts call for an assessment of the old fits also under consideration of the new data.

Methodology

The by Jerlov 1976 published data are total irradiance measurements (including direct sun light and reflected light from the sky) in the wavelength range from about 300nm to about 2500nm.

Unfortunately no wavelength separation (spectrum) is available.

For fitting the total irradiance data the statistical open source software R is used, which allows principally also for reproducible research. The R (<http://www.r-project.org/>) function `nls` (Nonlinear Least Squares) determines the nonlinear weighted least-squares estimates of the parameters of a nonlinear model, using a Gauss-Newton algorithm as standard. The standard algorithm has had problems with fitting the coastal water types (strong bending) and could not estimate the parameters for them. Therefore finally for all water types the algorithm “*plinear*” was used, which applies a Golub-Pereyra algorithm for partially linear least-squares models (Bates and Chambers, 1992). This algorithm did not show any stability problems and resulted in improved parameter estimates, demonstrated by the reduced residual error.

For comparison purposes some fits using the IDL (interactive data description language) function `curvefit` were also performed.

Additionally to the water types classified by Jerlov 1976, I had introduced a water type IAB, which is a linear combination of the types IA and IB and represents a mixed type of Mediterranean water.

The function for estimating the parameters is of the form:

$$I/I_0 = a \exp(z/g_1) + (1-a) \exp(z/g_2)$$

with relative irradiance I/I_0 , depth z and the fit parameters a for the relative importance of the different spectral ranges, g_1 for the long wave absorption and g_2 for the short wave absorption (measured in meter).

In an optimization procedure using the *nls* function the parameters a , g_1 , g_2 are estimated, by minimizing the least square error.

Table1 Water types used in this report with some typical regional examples

Type	Examples
I	Open Pacific
II	Artificial – fit to upper 50m of type I data
IA	Eastern Mediterranean, Indian ocean
IB	Western Mediterranean, Open Atlantic
IAB	Artificial – (IA+IB) Mixed Mediterranean
II	Coastal waters, Azores
III	Coastal waters, North Sea
1	Skagerrak
3	Baltic
5	Black Sea
7	

Results

The results from estimating the parameters a , g_1 and g_2 using the non-linear least squares fit are presented in 2 tables (2 and 3) and are also graphically presented in the respective figures. In table 2 the detailed estimates from the fit, their respective standard error the corresponding t-value from the students t test and the resulting significance level (probability $>|t|$) are given. In table 3 the old Paulsen and Simpson 1977 fits are compared to the new fit results from the *nls* R-function. Two old fits using the IDL curvefit function are also given, marked by(*).

In the figures the experimental data are presented together with the old fit and the respective fit derived here.

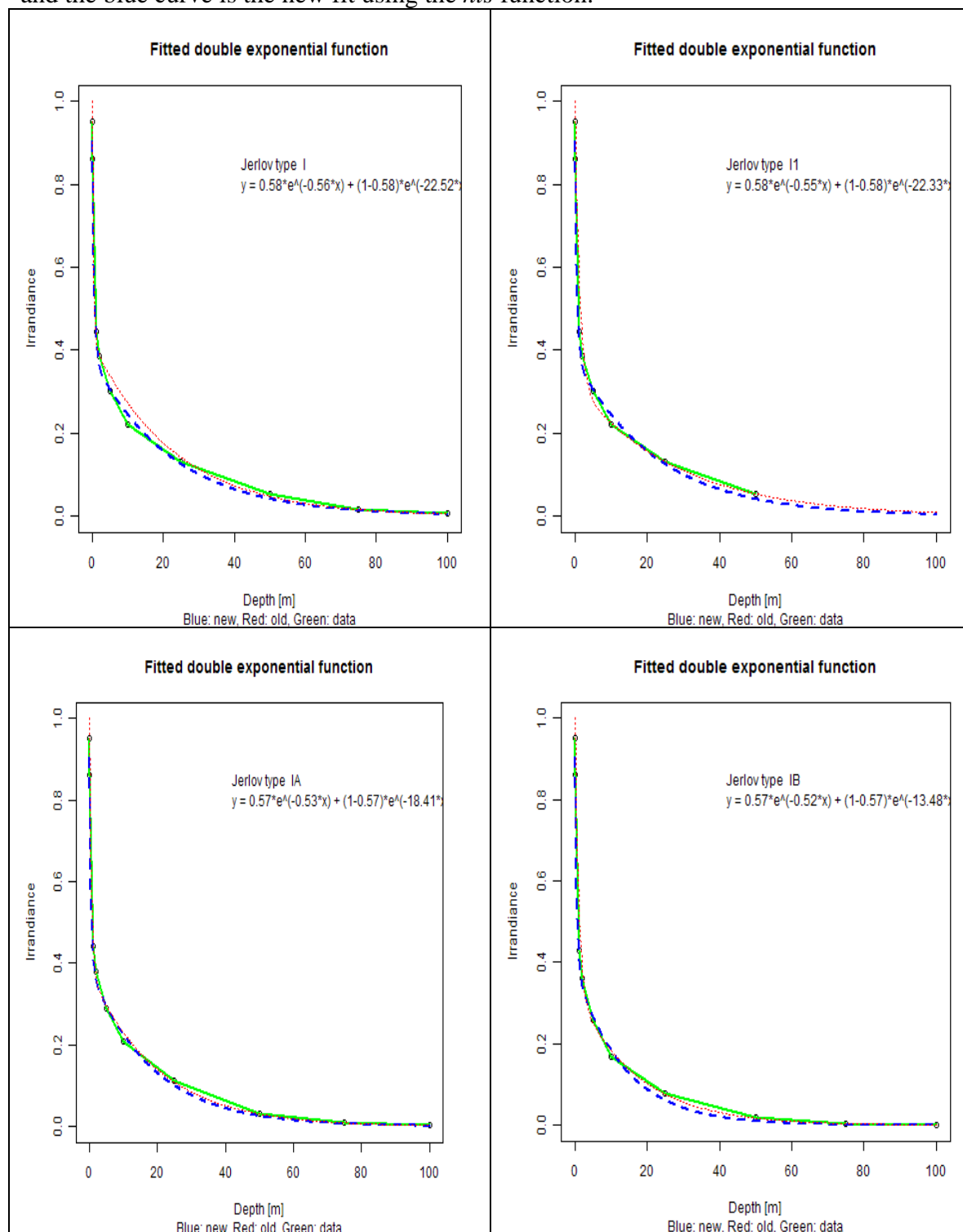
Table 2 Detailed results of the fits, including 4 values with the estimated parameter first, then its standard error, the t-value for the student distribution and the significance level ($\Pr(>|t|)$).

Type	A	G1	G2	Comment
I	0.5788761 0.03966578 14.593844 6.495347e-06	-0.5577946 0.14921058 -3.738305 9.641729e-03	-22.5154789 4.45784794 -5.050751 2.331901e-03	
II	0.5777610 0.04963704 11.639716 3.113925e-04	-0.5548220 0.18464427 - 3.004815 3.975283e-02	-22.3289493 5.66381564 - 3.942386 1.692583e-02	
IA	0.5706303 0.04266608 13.374329 1.081542e-05	-0.5295439 0.15272877 - 3.467218 1.334907e-02	-18.4075176 3.74657331 - 4.913161 2.675157e-03	
IB	0.5735061 0.05225242 10.975686 3.398349e-05	-0.5163736 0.16621765 - 3.106611 2.093913e-02	-13.4778149 3.11209154 - 4.330790 4.924441e-03	
II	0.5458170 0.05822277 9.374630 8.360390e-05	-0.4400475 0.17975956 - 2.447978 4.992765e-02	-9.5351780 2.08762964 - 4.567466 3.820681e-03	
III	0.5435685 0.11879350 4.575743 3.787475e-03	-0.3762882 0.32442875 - 1.159849 2.901740e-01	-5.5677833 1.99846300 - 2.786033 3.174323e-02	
IAB	0.5753810 0.04686654 12.277011 1.779199e-05	-0.5298768 0.15798000 - 3.354075 1.534174e-02	-16.0044912 3.49433245 - 4.580128 3.770014e-03	
1	0.5687449 0.10824978 5.254005 6.280055e-03	-0.4198229 0.25090734 - 1.673219 1.695992e-01	-5.1258117 1.62829027 - 3.147972 3.458140e-02	!g1
3	0.5671134 0.14968970 3.788593 1.929226e-02	-0.3677754 0.30459111 - 1.207440 2.937751e-01	-3.5352418 1.35014356 - 2.618419 5.889699e-02	! g1, g2
5	0.5741874 0.30904193 1.857960 1.601538e-01	-0.3316218 0.49201601 - 0.674006 5.485932e-01	-2.3385039 1.52858690 - 1.529847 2.235405e-01	! g1, g2
7	0.545848839 0.0176908532 30.85486 7.479285e-05	-0.00468592 0.0003127158 - 14.98460 6.450827e-04	-1.50794299 0.0671979274 - 22.44032 1.937704e-04	

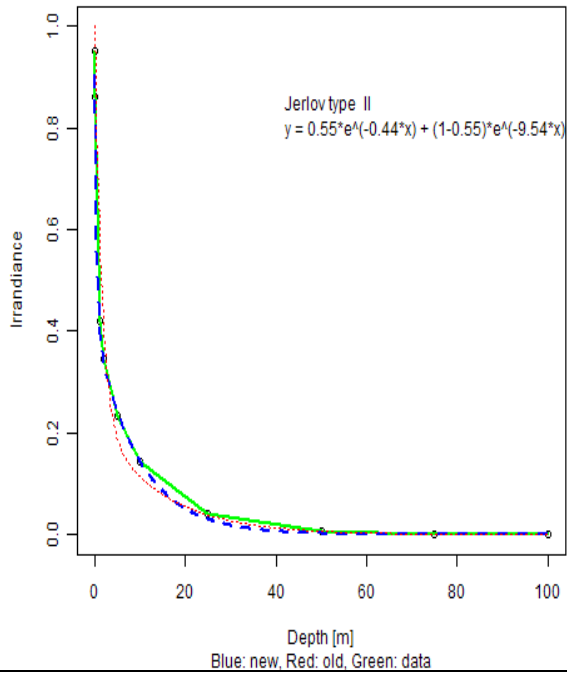
Table 3 Comparison of the existing parameter estimates (Simpson and Paulson 1977, IDL *curvefit*) “Old” and their residuals to the new parameters estimates and their residuals using *nls* “New”. IDL *curvefit* results are marked by (*) under “Old”.

Type	Old	Residuals Old	New	Residuals New	Comment
I	0.58 -0.35 -23	0.02561	0.58 -0.56 -22.52	0.00519	
II	0.68 -1.2 -28	0.04959	0.58 -0.55 -22.33	0.00518	
IA	0.62 -0.6 -20	0.02392	0.57 -0.53 -18.41	0.00488	
IB	0.67 -1 -17	0.03928	0.57 -0.52 -13.48	0.00490	
II	0.77 -1.5 -14	0.06381	0.55 -0.44 -9.54	0.00429	
III	0.78 -1.4 -7.9	0.05896	0.54 -0.38 -5.57	0.00994	
IAB	0.61 -0.47 -15.7 (*)	0.02271	0.58 -0.53 -16.00	0.00490	
1			0.57 -0.42 -5.13	0.00401	
3	0.57 -0.34 -5.5 (*)	0.03907	0.57 -0.37 -3.54	0.00395	
5			0.57 -0.33 -2.34	0.00391	
7			0.55 0 -1.51	0.00004	

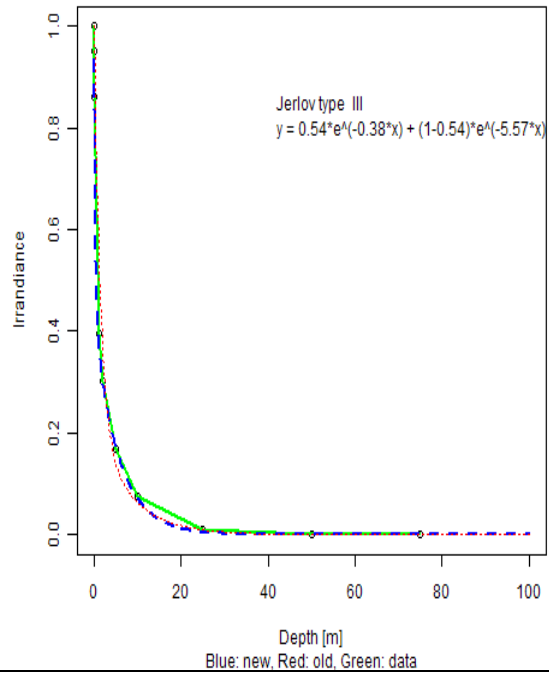
Figure 1 Graphical presentation of the estimated parameters for the different cases. The green curve are the experimental data from Jerlov 1976, the red curve is the old fit (Simpson and Paulson, 1977) and the blue curve is the new fit using the *nls* function.



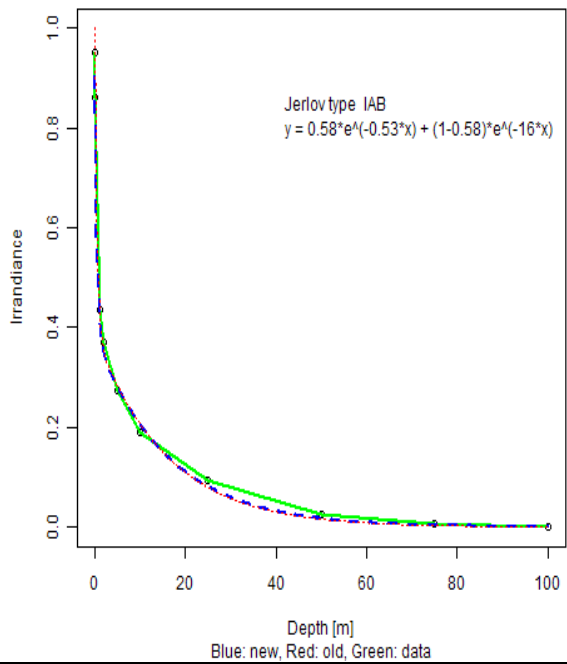
Fitted double exponential function



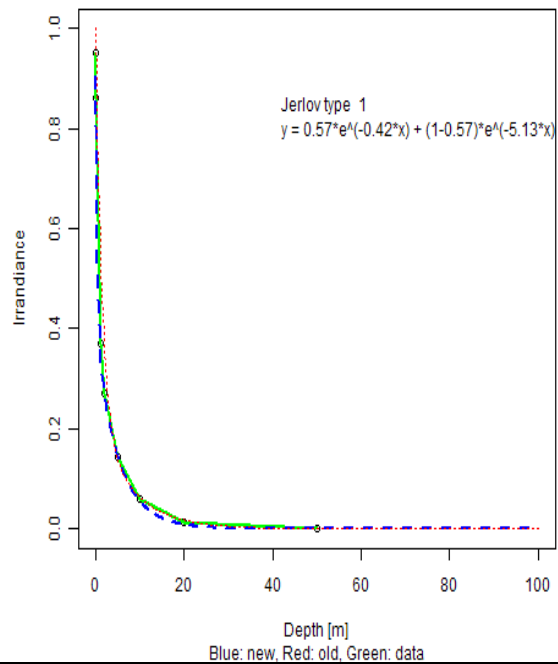
Fitted double exponential function



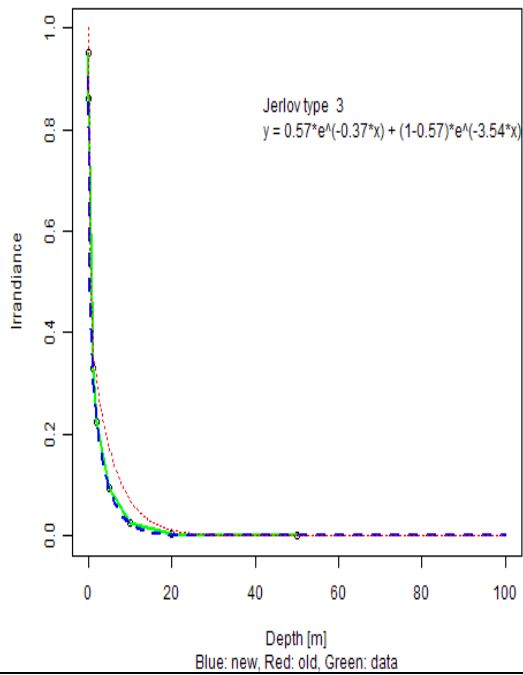
Fitted double exponential function



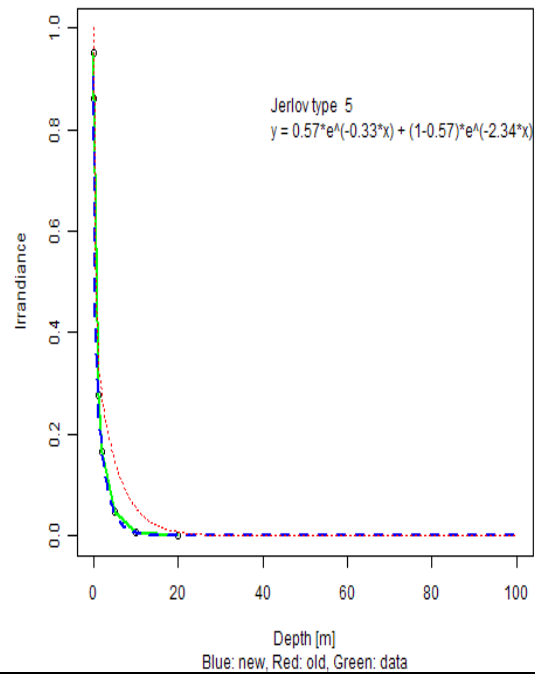
Fitted double exponential function



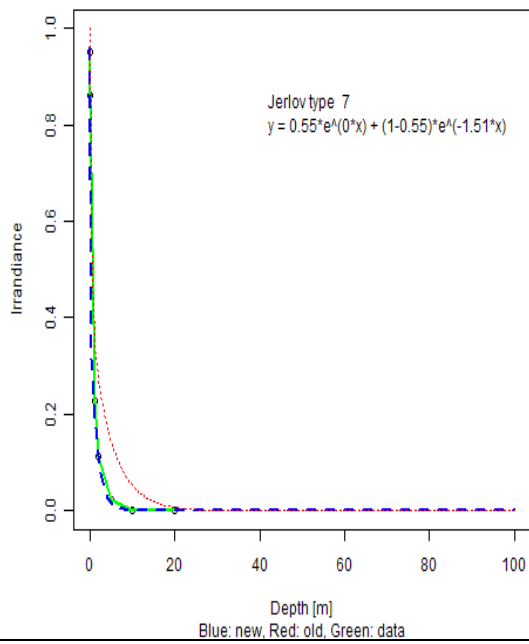
Fitted double exponential function



Fitted double exponential function



Fitted double exponential function



Discussion

Using the standard Gauss-Newton algorithm and adding the surface point (0m, 1) most of the results from Paulson and Simpson 1977 can be exactly reproduced, which gives us some confidence in the overall procedure. Also the results from the IDL *curvefit* routine are reproduced when using the standard algorithm of the *nls* function. This algorithm has however proven to be not very stable, so that a provision of good initial parameters is an absolute must before any successful parameter estimation. Providing just some arbitrary initial parameters the standard *nls* algorithm is failing with numerical errors. Much more robust and also achieving finally much smaller residual errors is the “plinear” algorithm which was used in the end exclusively.

By applying this algorithm the goodness of fit (smaller residuals) and therefore the performed parameter estimates could be all improved compared to the old Paulson and Simpson 1977 fits. Nevertheless as can be seen from table 2 specifically the coefficients from the new coastal water types could not be estimated with a statistical error probability of less than 0.05 (which was the intended target threshold). Indeed as in these waters most of the absorption takes place very near to the surface the use of a double exponential function seems not to be justified anymore (see the fit of Jerlov type 7, which gives $g_1=0.0$). But considering the still very small (and of comparable magnitude to the other fits) residual errors of the fits these values can still be confidently used for approximating the corresponding irradiance profile in the water. This way the usage of different functional forms for representing the irradiance for different water types in the hydrodynamic model can be avoided.

Conclusion

New estimates for the parameters a , g_1 and g_2 could be presented for the classical as well as for different new coastal water types. The goodness of fit and therefore the estimated parameters could be improved by applying the R function *nls*, hence it is recommended to use the here derived new parameters for applications within regional modelling.

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Appendix: Copy of table with original values from Jerlov 1976, used for the parameter estimates

TABLE XXVIII										
Percentage of total irradiance (300–2,500 nm) from sun and sky ¹										
Depth (m)	Oceanic water					Coastal water				
	<i>I</i>	<i>IA</i>	<i>IB</i>	<i>II</i>	<i>III</i>	<i>I</i>	<i>3</i>	<i>5</i>	<i>7</i>	<i>9</i>
0	100	100	100	100	100	100	100	100	100	100
1	44.5	44.1	42.9	42.0	39.4	36.9	33.0	27.8	22.6	17.6
2	38.5	37.9	36.0	34.7	30.3	27.1	22.5	16.4	11.3	7.5
5	30.2	29.0	25.8	23.4	16.8	14.2	9.3	4.6	2.1	1.0
10	22.2	20.8	16.9	14.2	7.6	5.9	2.7	0.69	0.17	0.052
20						1.3	0.29	0.020		
25	13.2	11.1	7.7	4.2	0.97					
50	5.3	3.3	1.8	0.70	0.041	0.022				
75	1.68	0.95	0.42	0.124	0.0018					
100	0.53	0.28	0.10	0.0228						
150	0.056			0.00080						
200	0.0062									

¹ For oceanic water the solar altitude is 90°; for coastal water 45°.

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EUR 24658 EN – Joint Research Centre – Institute for Environment and Sustainability

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Author: Adolf Konrad Stips

Luxembourg: Publications Office of the European Union

2010 – 14 pp. – 21.0 x 29.7 cm

EUR – Scientific and Technical Research series – ISSN 1018-5593

ISBN 978-92-79-18924-1

doi:10.2788/80912

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