Fraunhofer
IME

FRAUNHOFER-INSTITUT FÜR MOLEKULARBIOLOGIE UND ANGEWANDTE OEKOLOGIE IME

ABIWAS 3.0

Calculation of the abiotic degradation of chemicals in water

ABIWAS 3.0

Re-implementation of ABIWAS 2.0 (VB6)

Dr. Judith Klein
Dr. Michael Klein
Dr. Martin Müller

Fraunhofer-Institut für Molekularbiologie und Angewandte Oekologie
in Schmallenberg

Content

1 Summary

The software ABIWAS calculates the abiotic degradation in water. For the use in the regulation of plant protection products only photolysis in water is considered. This program is the reimplementation of ABIWAS 2.0 implemented by Martin Müller in 2002. The program is based on the original publication:

Herrmann, M., D. Büchel, M. Klein: ABIWAS - Programm zur Berechnung des abiotischen Abbaus von Chemikalien in Gewässern, Z. Umweltchem. Ökotox., 5 (1993) 275-276

In OECD 2008, the program ABIWAS is mentioned "to estimate direct photolysis rates and half-life for the test chemical applicable to any types of surface waters (defined by depth and light attenuation), seasons, and latitudes of interest".

2 Model description

The software ABIWAS 3.0 calculates the abiotic degradation of chemicals in water. The abiotic degradation is calculated based on the concentration of chemical in mol/L, the extinction of chemical at wavelength and the quantum yield of substance at wavelength. The input data can be derived according to OECD 2008. Endpoints of the calculation are the half time values (DegT50 min, DegT50, DegT50max) and the corresponding photolysis rates during the year (Figure 1).

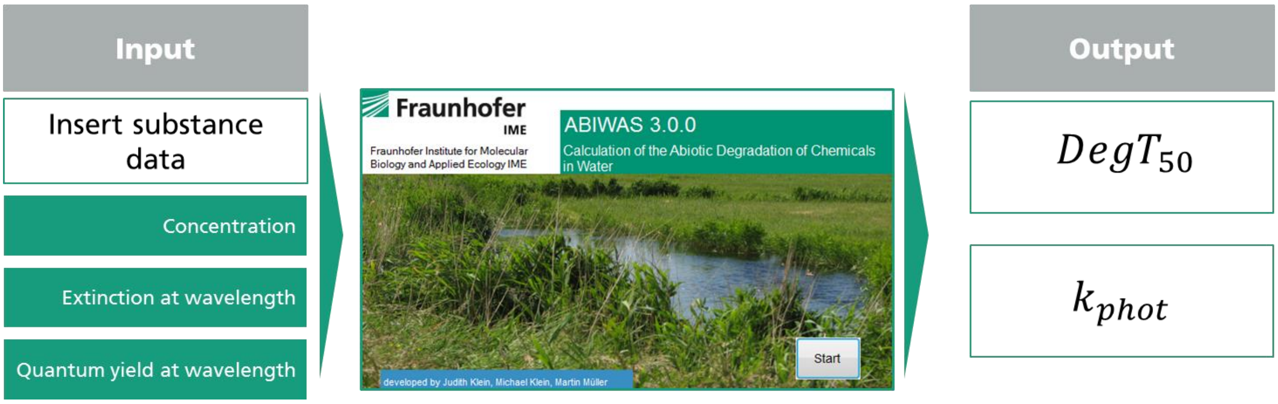


Figure 1: Input and output of the program ABIWAS

2.1 Procedure

The following procedure is implemented in ABIWAS 3.0 for the calculation of the degradation in water.

1. Load and standardize water data (wavelength in nm $\lambda \in [290{,}800]$
2. Load and standardize substance specific data (wavelength in nm $\lambda \in [290{,}800]$)
3. For each month
    a. Load and standardize light intensity data
    b. Calculate half time (DegT50) (max, min, standard)
        i. For each wavelength $\lambda \in [290{,}800]$
            1. Calculate total extinction $\epsilon_{total}(\lambda) = \epsilon_{water}(\lambda) + \epsilon_{substance}(\lambda) \cdot C$ (Assumption: Concentration above zero)
            2. Calculate the temporary variable h1 describing the influence of one wave length to degradation based on substance data $h_1(\lambda) = 0.9 \cdot I(\lambda) \cdot \Phi(\lambda) \cdot \epsilon_{substance}(\lambda)$
            3. Calculate the temporary variable h2 describing the influence of water depth on degradation based on water data:
            $$h_2(\lambda) = \begin{cases} \exp(-\ln(10) \cdot \epsilon_{total}(\lambda) \cdot d), & \text{if} \quad \ln(10) \cdot \epsilon_{total}(\lambda) \cdot d < 40, \\ 0, & \text{else}. \end{cases}$$
            4. Calculate joint h based on substance and water data):
            $$h(\lambda) = \begin{cases} h_1(\lambda) \cdot \dfrac{(1 - h_2(\lambda))}{\epsilon_{total}(\lambda) \cdot d} \cdot \dfrac{1}{n_0}, & \text{if} \quad \epsilon_{total}(\lambda) > 0, \\ 0, & \text{else}. \end{cases}$$
        ii. Calculate photolysis rate (compare OECD 2008):
        $$k_{photolysis} = \sum_{\lambda} h(\lambda) \cdot 1000 \cdot \left(\frac{LH}{24}\right)$$
        iii. Calculate DegT50:

$$DegT_{50} = \frac{\ln(2)}{3600 \cdot 24 \cdot k_{photolyse}}$$

iv. Calculate minimal and maximal DegT50:

$$\underline{DegT_{50}} = 100 \cdot \frac{DegT_{50}}{\overline{I}} \text{ and } \overline{DegT_{50}} = 100 \cdot \frac{DegT_{50}}{\underline{I}}$$

v. Transform DegT50 values to photolysis rate:

$$k_{phot} = \frac{\ln(2)}{DegT_{50}}.$$

In Table 1, and overview of the model parameters and constants is given. For this, unit and domain respectively value as well as a description of parameter/constant are given.

Table 1: Overview of the model parameters and constants including their unit, domain respectively value, and description

Parameter	Unit	Domain/Value	Description
ϵ_x	-	$\mathbb{R}_+$	Extinction coefficient with respect to x (water or substance)
λ	nm	$[290,800]$	Wavelength
C	mol/L	$\mathbb{R}_+$	Concentration of substance
I		$\mathbb{R}_+$	Intensity over a 1 nm interval centered at wavelength λ
Φ		$[0,1]$	quantum yield
d	cm	$\mathbb{R}_+$	Water depth
n_0	1/g	$6.023E + 23$	Loschmidt constant (number per gram)
LH	h	$[0,24]$	Light hours per day

The light data (extinction coefficients, intensity, and light hours per day) depend on the month. The DegT50 values are calculated for each month separately.

The extinction of coefficient with respect to the substance, the concentration of substance and quantum yield is entered in the programme by the user.

2.2 Scenario

The implemented standard scenario in ABIWAS 3.0 contains light data based on central Europe (55°). Water data is given without absorption (extinction equal to zero) or equal to the extinction of distilled water (Figure 2).

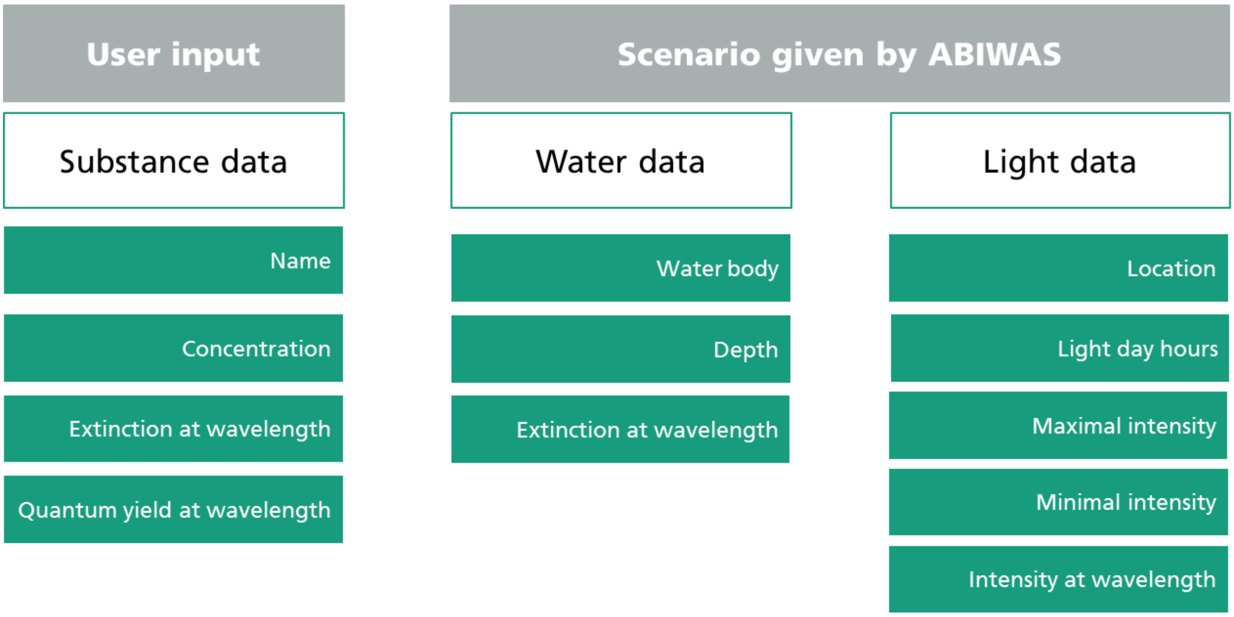


Figure 2: Data sets used in ABIWAS

3 Evaluation

The use of ABIWAS for the evaluation of abiotic degradation is proposed in OECD guideline 316 "Phototransformation of Chemicals in Water – Direct Photolysis" (OECD 2008).

3.1 Regulatory endpoints

The regulatory endpoints are the photolysis rate constant k_{phot} and half-life $DegT_{50}$ (Figure 1, OECD 2008).

$$DegT_x = \frac{\ln\left(\frac{100}{100 - x}\right)}{k_{phot}}$$

$$DegT_{50} = \frac{\ln(2)}{k_{phot}}.$$

4 Working with ABIWAS 3.0

4.1 Installing ABIWAS 3.0

The program ABIWAS is available at the software website of the Fraunhofer Institute for Molecular Biology and Applied Ecology IME. Permanently, the program and associated material is linked to the download area http://software.ime.fraunhofer.de/abiwas/.

Please download the installer "abiwas_setup_xxxxxxxx.exe" and follow the instructions. After installing ABIWAS successfully, the start form of the program appears.

4.2 Working with ABIWAS

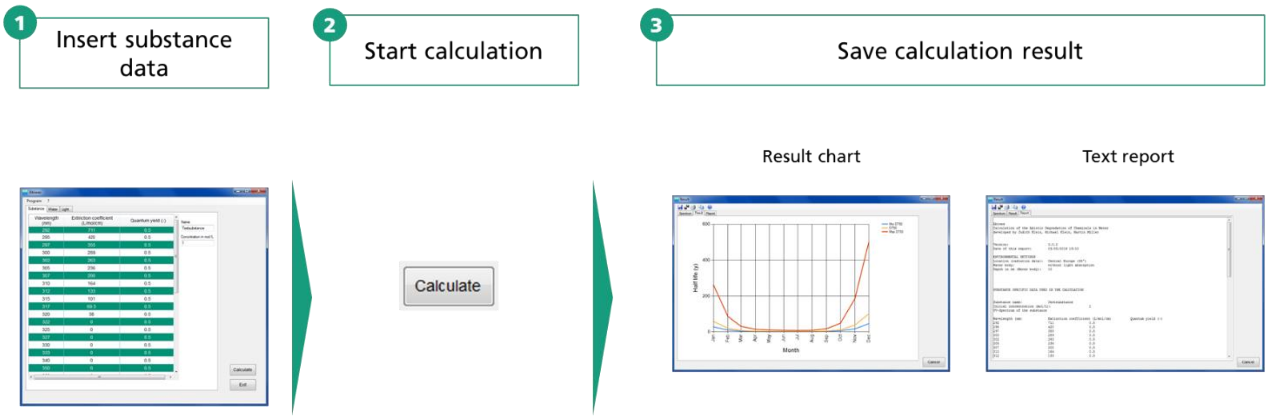


Figure 3: Procedure- The user has to fulfill three steps for the abiotic degradation calculation.

Procedure:

1. Insert substance data
    a. Wavelength in nm
    b. Extinction coefficient
    c. Quantum yield
2. Start calculation
3. Save the calculation results

By starting the program ABIWAS, a start screen appears (Figure 4). Clicking at start the proper program is started.

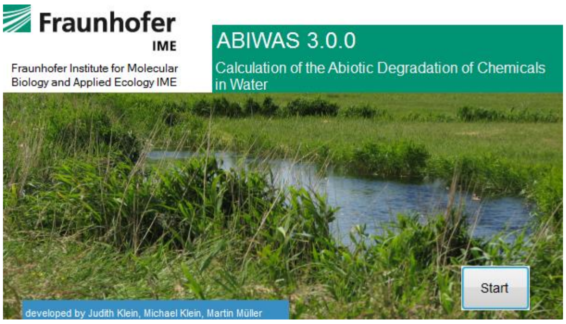


Figure 4: Start screen of the program ABIWAS

The main form of the program ABIWAS 3.0 includes a tab control containing the substance specific data, as well as water data and light data (Figure 5). The user shall insert the experimental substance specific data (name of substance, concentration of substance, wavelength, extinction coefficient, quantum yield) as presented in Figure 5. Experimental data (Figure 5) can be entered manually or by copy paste (CTRL-C,CTRL-V) from EXCEL. Calculation is only possible if experimental data is entered.

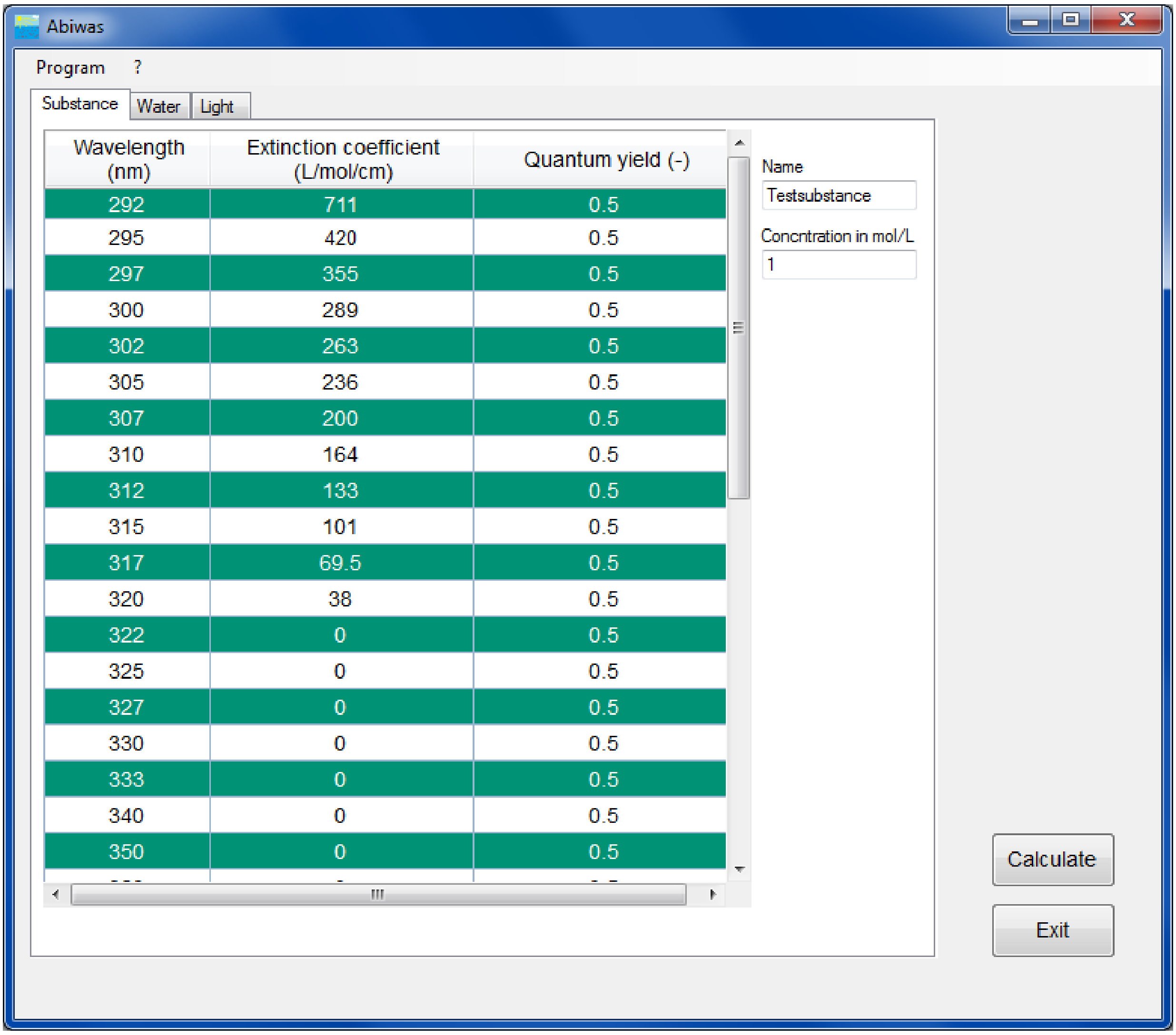


Figure 5: Main form of the ABIWAS 3.0

Figure 6 shows the tab pages “Water” and “Light”. The user can choose the water body between “without light absorption” and “distilled water”. However, the user is not able to add additional water bodies. The light tab page contains the light data (wavelength, intensity) for each month. The data corresponds to the radiation of Central Europe (55°). In addition to that the light day hours, the maximum intensity and minimum intensity are given for each month. Again, the data is fixed and cannot be modified by the user.

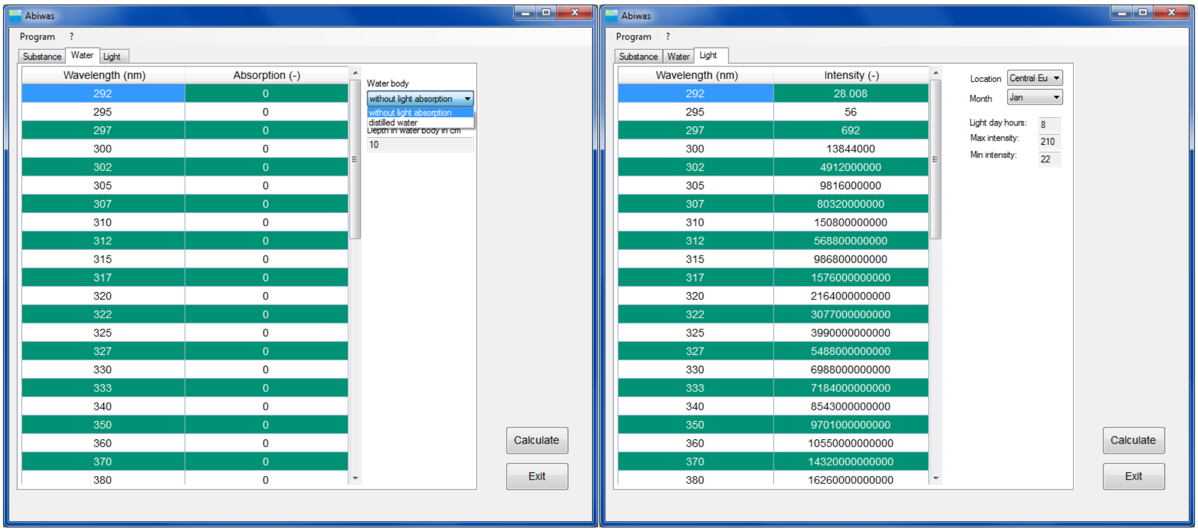


Figure 6: Tab pages “Water” (left) and “Light” (right) of main form

The result of the calculation is represented as

1. Input Chart (Figure 7): Visual representation of by user entered substance specific data, the change of extinction coefficient with respect to wavelength (nm)
2. Result Chart (Figure 10): Change of half-time DegT50 values (DegT50, minimal and maximal DegT50) in time (month)
3. Report (Figure 11): Text file containing experimental input data and result of calculation

The program enables the user to save, copy into clipboard and print the results by clicking at the menu items “Save”, “Save All”, “Print” and “Copy”.

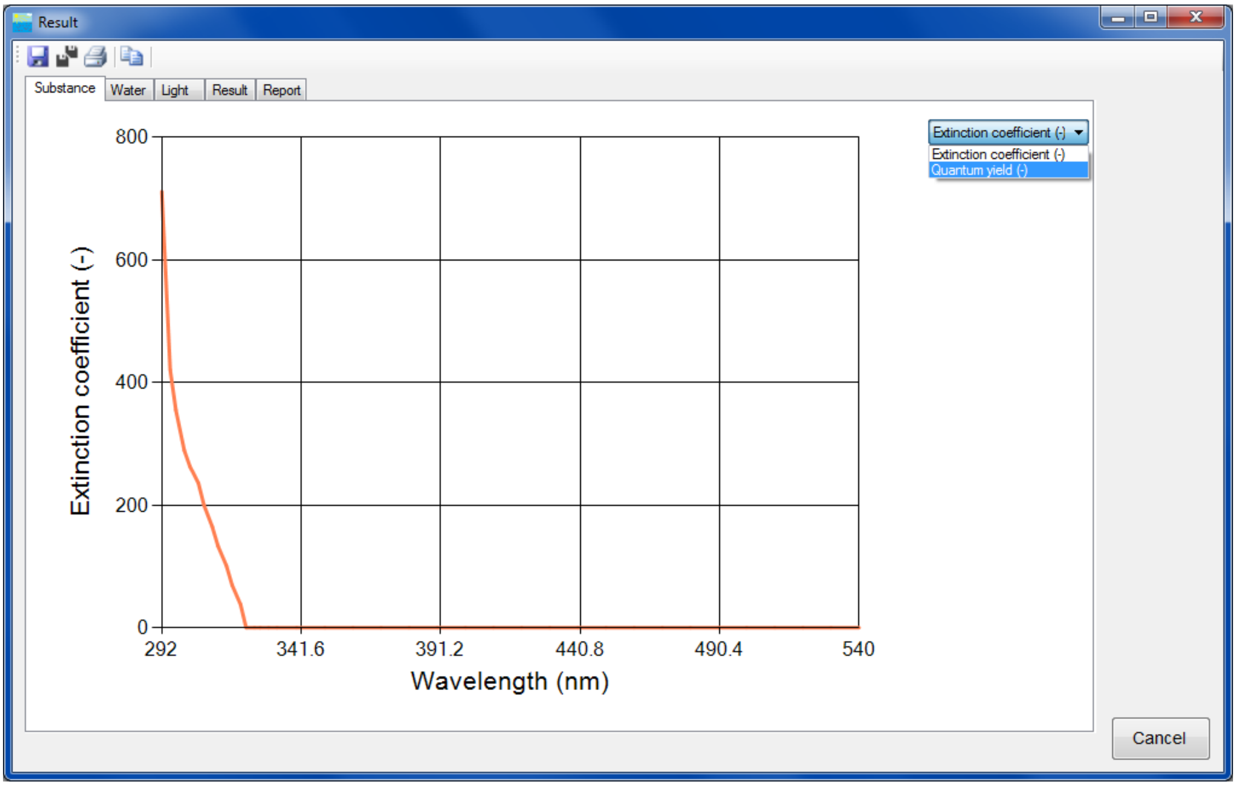


Figure 7: Input chart: substance specific data entered by user, extinction coefficient and quantum yield of the test substance depending on wavelength in nm

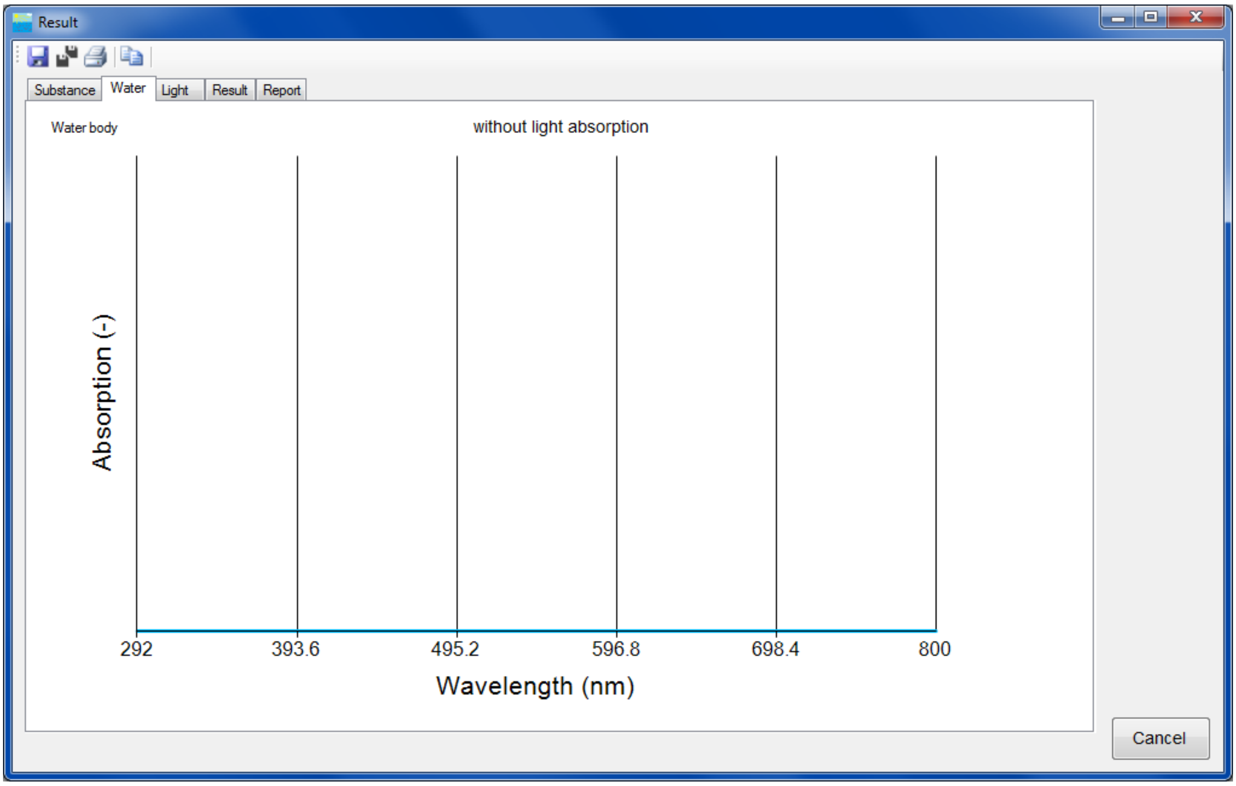


Figure 8: Input chart: water specific data absorption depending on wavelength in nm and the chosen water body

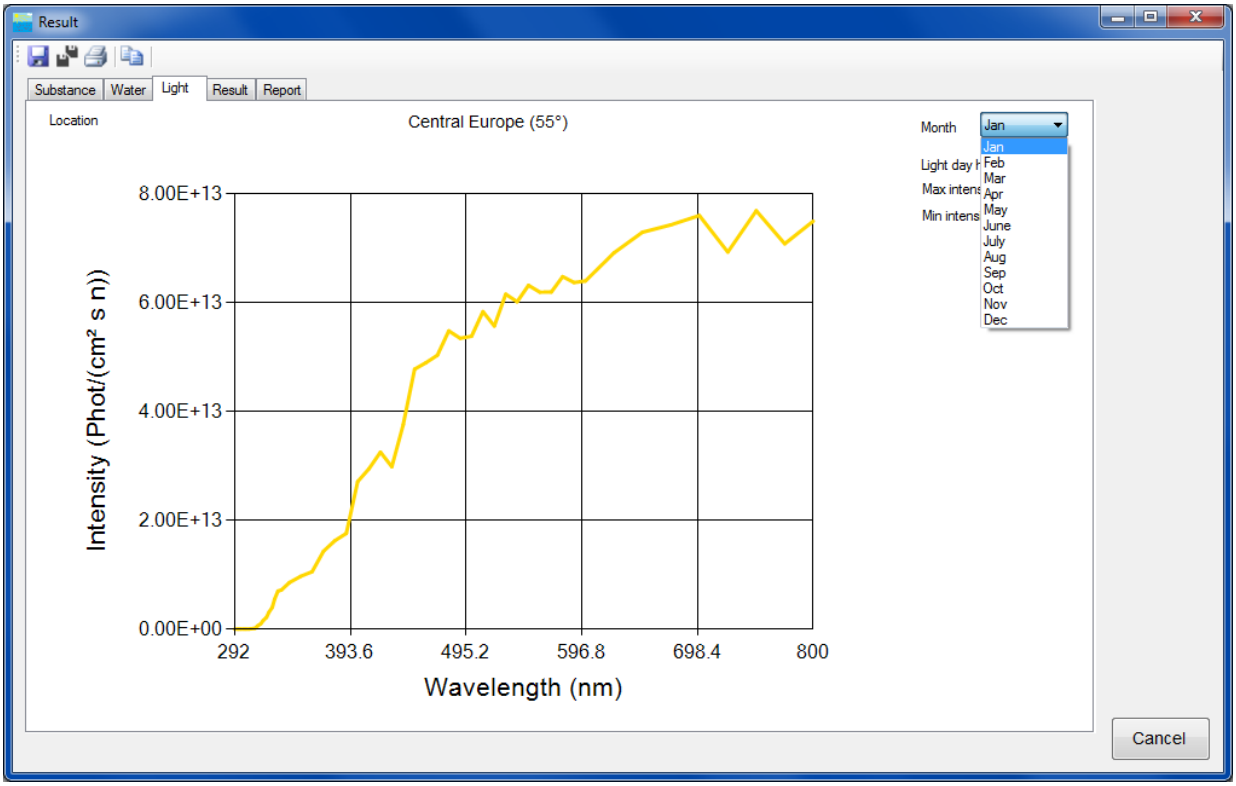


Figure 9: Input chart: light specific data intensity depending on wavelength in nm and the chosen month

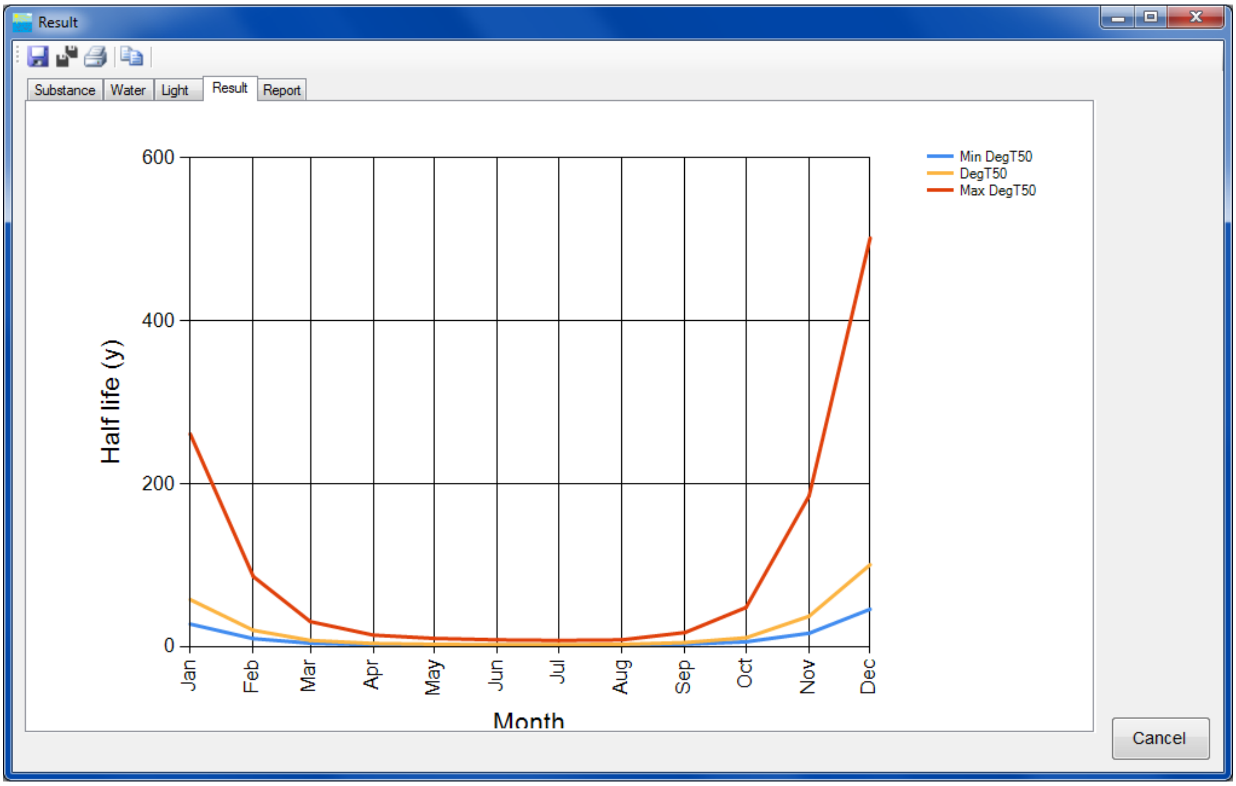
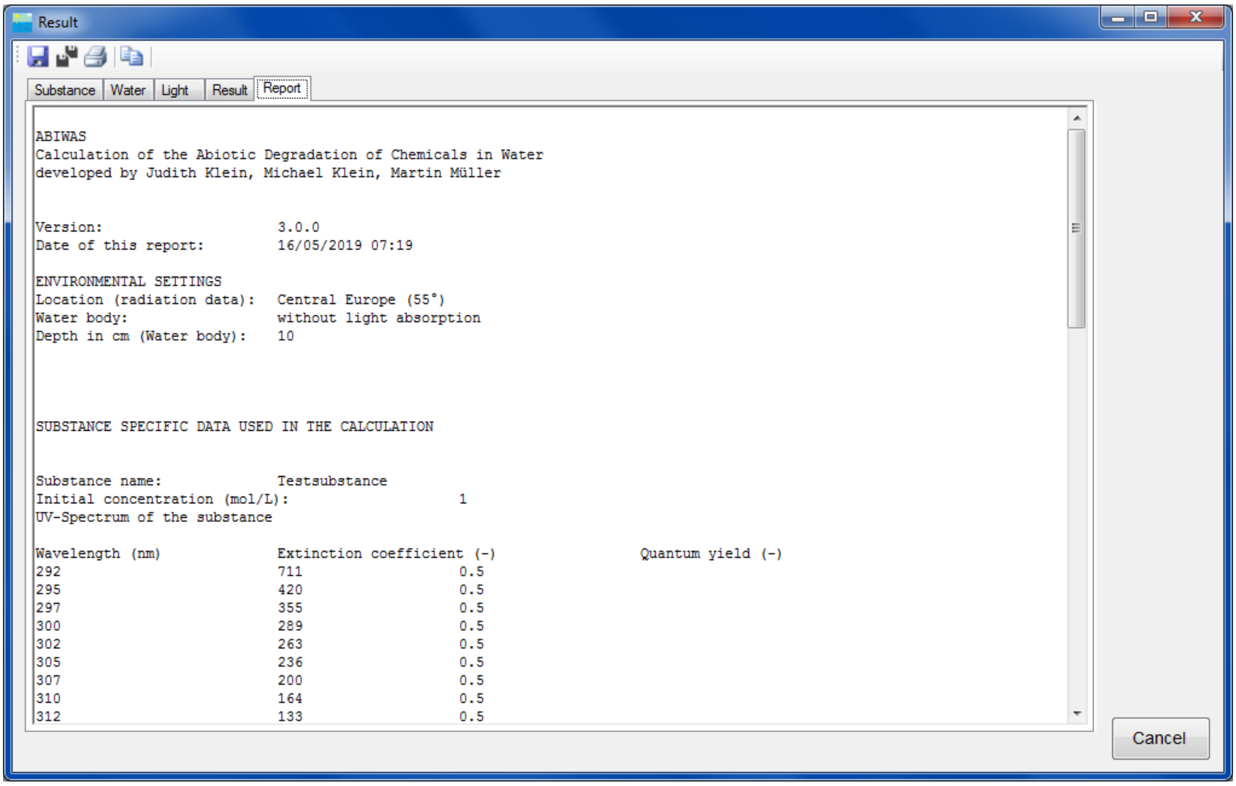


Figure 10: Result chart - Half-time values (DegT50, minimal DegT50, and maximal DegT50) per month



ABIWAS
Calculation of the Abiotic Degradation of Chemicals in Water
developed by Judith Klein, Michael Klein, Martin Müller

Version: 3.0.0
Date of this report: 16/05/2019 07:19

ENVIRONMENTAL SETTINGS
Location (radiation data): Central Europe (55°)
Water body: without light absorption
Depth in cm (Water body): 10

SUBSTANCE SPECIFIC DATA USED IN THE CALCULATION

Substance name: Testsubstance
Initial concentration (mol/L): 1
UV-Spectrum of the substance

Wavelength (nm)	Extinction coefficient (-)	Quantum yield (-)
292	711	0.5
295	420	0.5
297	355	0.5
300	289	0.5
302	263	0.5
305	236	0.5
307	200	0.5
310	164	0.5
312	133	0.5

Figure 11: Text report file containing the input data as well as the calculation result (DegT50 values)

5 Result of test simulation using ABIWAS 3.0

The aim of this chapter is to show the performance of the software ABIWAS 3.0. For testing, we use a hypothetical test data set (Table 2).

5.1 Input Data

As test substance data, we use the data given in Table 2. Wavelength is given in a range of wavelength in $[292{,}540]$. The program standardizes the data to $[290{,}800]$ (linear interpolation, step size 1nm, beyond the range extinction coefficient and quantum yield are set to zero).

Table 2: Substance specific input data - extinction coefficient and quantum yield of test substance with respect to wavelength in nm

Wavelength	Extinction coefficient	Quantum yield
292	711	0.5
295	420	0.5
297	355	0.5
300	289	0.5
302	263	0.5
305	236	0.5
307	200	0.5
310	164	0.5
312	133	0.5
315	101	0.5
317	69.5	0.5
320	38	0.5
322	0	0.5
325	0	0.5
327	0	0.5
330	0	0.5
333	0	0.5
340	0	0.5
350	0	0.5
360	0	0.5
370	0	0.5
380	0	0.5
390	0	0.5
400	0	0.5
410	0	0.5
420	0	0.5
430	0	0.5
440	0	0.5
450	0	0.5
460	0	0.5
470	0	0.5
480	0	0.5
490	0	0.5
500	0	0.5
510	0	0.5

520	0	0.5
530	0	0.5
540	0	0.5

As water body the option “without light absorption” is chosen with 10 cm water depth. The light data corresponds to “Central Europe (55°).

5.2 Results

In Table 3, a summary of results is given, namely the half-live values (DegT50, minimal and maximal DegT50) for each month. The results are obtained choosing above described options as well as substance specific input data given in Table 2.

Table 3: Result of test simulation using the input data given in Table 2

Month	Min half life (y)	Half life (y)	Max half life (y)
Jan	27.3	57.34	260.63
Feb	9.38	19.69	85.6
Mar	3.83	7.28	30.33
Apr	1.91	3.44	13.76
May	1.51	2.41	9.66
June	1.33	1.99	7.96
July	1.46	2.19	7.31
Aug	1.58	2.37	7.91
Sep	2.68	4.56	16.89
Oct	5.52	10.49	47.67
Nov	16.07	36.95	184.75
Dec	45.56	100.22	501.11

The outputs coincide to the data obtained using the VB6 implementation ABIWAS 2.0. Detailed output (text reports) from ABIWAS 2.0 and ABIWAS 3.0 are given in appendix A.

A Supplementary Material

A.1 Documentation of model output: ABIWAS 2.0

Calculation of the Abiotic Degradation in Water

developed by Michael Klein and Martin Müller

Program version:	2.1
Date of this simulation:	03/05/2019, 12:27:52
Location used for radiation data:	Central Europe (55°)
Water body:	without light absorption
Depth of the water body (cm):	10

____
Signature of operator

SUBSTANCE SPECIFIC DATA USED IN THE CALCULATION

Substance name: test compound
Initial concentration (mol/L): 1

UV-Spectrum of the substance

Wavelength (nm)	Extinktion	Quantumyield
292	711	0.5
295	420	0.5
297	355	0.5
300	289	0.5
302	263	0.5
305	236	0.5
307	200	0.5
310	164	0.5
312	133	0.5
315	101	0.5
317	69.5	0.5
320	38	0.5
322	0	0.5
325	0	0.5
327	0	0.5
330	0	0.5
333	0	0.5
340	0	0.5
350	0	0.5
360	0	0.5
370	0	0.5
380	0	0.5
390	0	0.5
400	0	0.5
410	0	0.5
420	0	0.5
430	0	0.5
440	0	0.5
450	0	0.5
460	0	0.5
470	0	0.5
480	0	0.5
490	0	0.5
500	0	0.5
510	0	0.5
520	0	0.5
530	0	0.5
540	0	0.5
541	0	0

RESULTS OF THE CALCULATION

Month	**min. Half life**	**Half life**	**max. Half life**
January	**27.3 y**	**57.3 y**	**261 y**
February	**9.38 y**	**19.7 y**	**85.6 y**

March	**3.83 y**	**7.28 y**	**30.3 y**
April	**1.91 y**	**3.44 y**	**13.8 y**
May	**1.51 y**	**2.41 y**	**9.66 y**
Juned	**1.33 y**	**1.99 y**	**7.96 y**
July	**1.46 y**	**2.19 y**	**7.31 y**
August	**1.58 y**	**2.37 y**	**7.91 y**
September	**2.68 y**	**4.56 y**	**16.9 y**
October	**5.52 y**	**10.5 y**	**47.7 y**
November	**16.1 y**	**37.0 y**	**185 y**
December	**45.6 y**	**100 y**	**501 y**

A.2 Documentation of model output: ABIWAS 3.0

ABIWAS
Calculation of the Abiotic Degradation of Chemicals in Water
developed by Judith Klein, Michael Klein, Martin Müller

Version: 3.0.0
Date of this report: 16/05/2019 08:11

ENVIRONMENTAL SETTINGS

Location (radiation data): Central Europe (55°)
Water body: without light absorption
Depth in cm (Water body): 10

SUBSTANCE SPECIFIC DATA USED IN THE CALCULATION

Substance name: Testsubstance
Initial concentration (mol/L): 1

UV-Spectrum of the substance

Wavelength (nm)	Extinction coefficient (-)	Quantum yield (-)
292	711	0.5
295	420	0.5
297	355	0.5
300	289	0.5
302	263	0.5
305	236	0.5
307	200	0.5
310	164	0.5
312	133	0.5
315	101	0.5
317	69.5	0.5
320	38	0.5
322	0	0.5
325	0	0.5
327	0	0.5
330	0	0.5
333	0	0.5
340	0	0.5
350	0	0.5
360	0	0.5
370	0	0.5
380	0	0.5
390	0	0.5
400	0	0.5

410	0	0.5
420	0	0.5
430	0	0.5
440	0	0.5
450	0	0.5
460	0	0.5
470	0	0.5
480	0	0.5
490	0	0.5
500	0	0.5
510	0	0.5
520	0	0.5
530	0	0.5
540	0	0.5

RESULTS OF THE CALCULATION

Half-lifes

Month	Min DegT50	Unit	DegT50	Unit	Max DegT50	Unit
Jan	27.30	y	57.34	y	260.63	y
Feb	9.38	y	19.69	y	85.60	y
Mar	3.83	y	7.28	y	30.33	y
Apr	1.91	y	3.44	y	13.76	y
May	1.51	y	2.41	y	9.66	y
June	1.33	y	1.99	y	7.96	y
July	1.46	y	2.19	y	7.31	y
Aug	1.58	y	2.37	y	7.91	y
Sep	2.68	y	4.56	y	16.89	y
Oct	5.52	y	10.49	y	47.67	y
Nov	16.07	y	36.95	y	184.75	y
Dec	45.56	y	100.22	y	501.11	y

Photolysis rates

Month	Min k_phot	Unit	k_phot	Unit	Max k_phot	Unit
Jan	0.025	1/y	0.012	1/y	0.003	1/y
Feb	0.074	1/y	0.035	1/y	0.008	1/y
Mar	0.181	1/y	0.095	1/y	0.023	1/y
Apr	0.363	1/y	0.201	1/y	0.050	1/y
May	0.459	1/y	0.287	1/y	0.072	1/y
June	0.523	1/y	0.348	1/y	0.087	1/y
July	0.474	1/y	0.316	1/y	0.095	1/y
Aug	0.438	1/y	0.292	1/y	0.088	1/y
Sep	0.258	1/y	0.152	1/y	0.041	1/y
Oct	0.126	1/y	0.066	1/y	0.015	1/y
Nov	0.043	1/y	0.019	1/y	0.004	1/y
Dec	0.015	1/y	0.007	1/y	0.001	1/y

List of abbreviations and definitions

Abbreviation	Description
DegT50	Disappearance time, the time within which the concentration of substance is reduced by 50%, half-life in a medium due to degradation (transformation) and other processes
FOCUS	FOrum for the Co-ordination of pesticide fate models and their USe
LOD	limit of detection
LOQ	limit of quantification
SFO	single first order kinetics

Term	Definition
Intensity	"Traditional term indiscriminately used for photon flux, fluence rate, irradiance, or radiant power. In terms of an object exposed to radiation, the term should now be used only for qualitative descriptions." (OECD 2008)
Photodegradation	"The photochemical transformation of a molecule into fragments, usually in an oxidation process. This term is widely used in the destruction (oxidation) of pollutants by UV-based processes." (OECD 2008)
Quantum Yield	"The number of defined events which occur per photon absorbed by the system." (OECD 2008)
Wavelength	"The distance, measured along the line of propagation, between two corresponding points on adjacent waves. The wavelength depends on the medium in which the wave propagates." (OECD 2008)

References

Herrmann, M., Büchel, D. and Klein, M. „ABIWAS – Programm zur Berechnung des abiotischen Abbaus von Chemikalien in Gewässern“. Z. Umweltchem.Ökotox., 5 (1993), 275–276.

OECD (2008), *Test No. 316: Phototransformation of Chemicals in Water – Direct Photolysis*, OECD Guidelines for the Testing of Chemicals, Section 3, OECD Publishing, Paris, https://doi.org/10.1787/9789264067585-en.