MERIS Case2Regional Processor User Manual

Version 1.1

November 2006

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1 PART I: OVERVIEW

The Case2 Regional processor has been developed as a joint effort between GKSS Research Centre, Institute for Coastal Research, and Brockmann Consult, under contract of the European Space Agency ESA. Co-investigators in form of sub-contractors are the Norwegian Institute for Water Research (NIVA) and the Institute of Ocean Sciences (IOS), BC, Canada.

The Case2Regional Processor is producing Level 2 data from MERIS Level 1b data for regional coastal waters. This includes an algorithm for atmospheric correction and an algorithm to derive properties of the water such as the inherent optical properties (IOP's) absorption and scattering and the concentrations of total suspended matter (TSM) and chlorophyll from the water leaving radiance reflectance spectra (i.e. after atmospheric correction).

The processor software has been developed as BEAM processor. It can be downloaded free of charge from the BEAM Plug-In page. It can be run either in batch-mode or from within the VISAT BEAM tool.

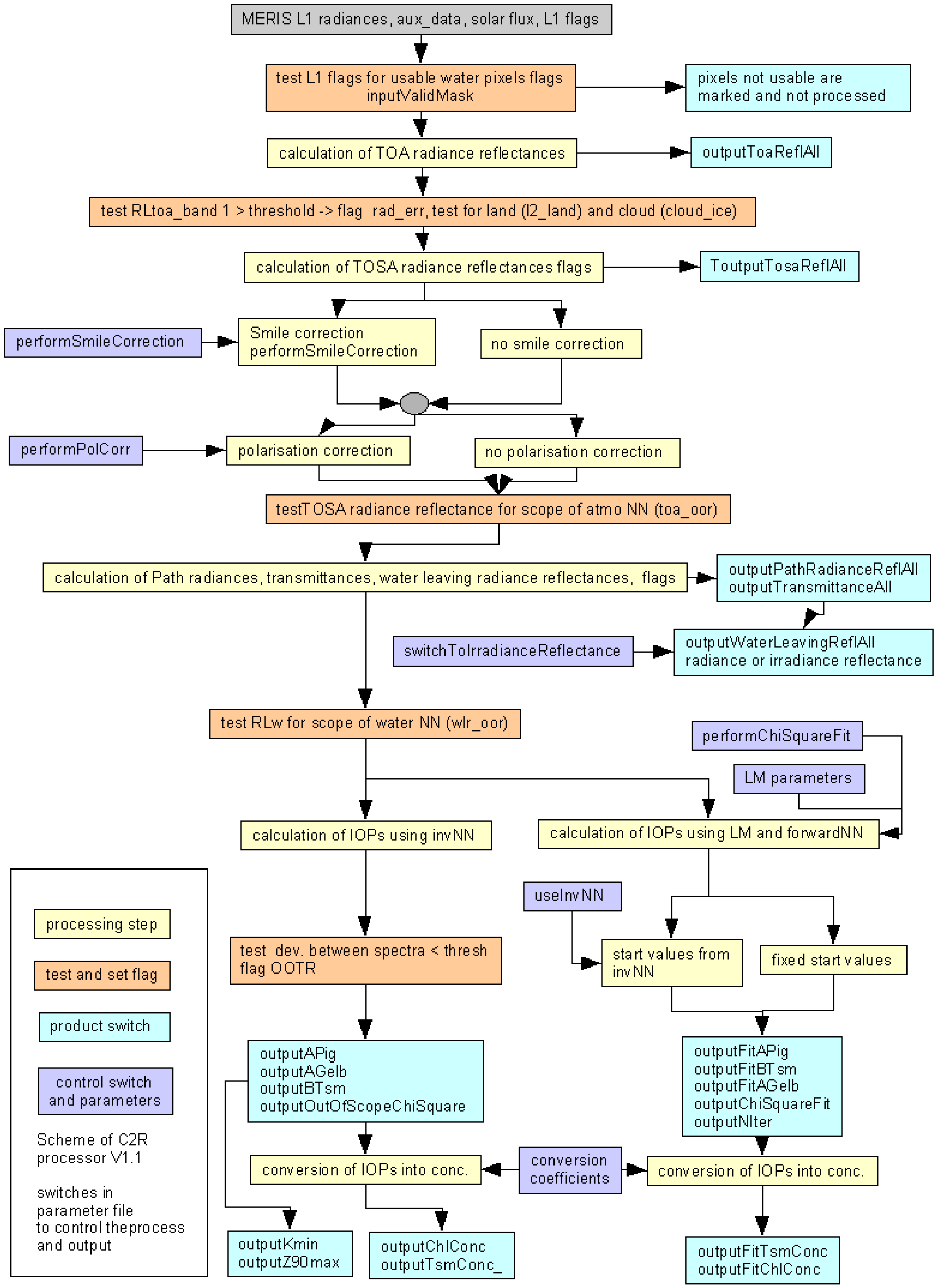
1.1 Algorithm Overview

The Case2Regional Processor includes two major parts: an atmospheric correction and the retrieval of water constituents.

The atmospheric correction includes as a first step the calculation of the top of standard atmosphere (TOSA) radiance reflectance with respect to the surface atmospheric pressure and column ozone content. In this correction step only the differences between the surface pressure and ozone content, as given in the MERIS product, and the standard pressure (1013.25 hPa) and ozone content of 350 Dobson Units respectively are considered. The TOSA radiance reflectances of MERIS bands 9, 10, 12, 13 together with the angles (sun zenith, viewing zenith, azimuth difference between sun and viewing direction) are then the input to the atmospheric correction neural network, which is used to determine the path radiances and transmittances for MERIS bands 1-9. In the final step these are used to compute the water leaving radiance reflectances of MERIS bands 1-9.
The atmospheric correction can be performed with and without a correction of the polarisation effect.

For the retrieval of IOPs and water constituents two different procedures are included in the processor. The first alternative is based on an inverse neural network, which is used to determine three IOPs from the water leaving radiance reflectances, i.e. the absorption of algal pigments (a_pig_443), the absorption of yellow substances (a_gelb_443) and the scattering of all particles (b_tsm). The second alternative uses a forward neural network within an optimization procedure based on the Levenber-Marquard algorithm. Using this second alternative one can achieve a better fit between the water leaving radiance reflectance spectrum as produced by the forward network and that as produced by the atmospheric correction procedure. The first guess can be the result of the backward network or a mean constant value. However, due to the optimization loop this procedure is slower. Both procedures can run in parallel. In both cases the IOPs are converted into concentrations of water constituents (Chlorophyll-a, TSM) using simple exponential equations, which coefficients are provided in the parameter file and can be selected.

An overview about the flux of information and the parameters in the parameter file to control the flux and the output as well as about the tests and flags is given in Fig. xx.



1.2 Atmospheric correction

The atmospheric correction is based on the idea that the path radiances as well as the transmittances of the first 9 MERIS bands (412 -708 nm) can be derived from the top of atmosphere directional radiance reflectance of 4 MERIS bands in the near infrared spectral range (708 - 870 nm) and that the relationship between these variables can be described by a neural network. We assume that the variability of the path radiances and transmittances of all bands, for a standard atmosphere, depend on (1) the aerosol types and their concentrations in different layers of the atmosphere, (2) on thin cirrus clouds, and on (3) the specular reflectance of scattered light at the sea surface (sky light glitter) and on the specular reflectance of direct sun light at the sea surface (sun glint), both of which are wind dependent, and finally (4) on the scattering of particles in water. By knowing the reflectance in the 4 NIR bands it is possible to determine the path radiance and transmittance of first 9 MERIS bands, which are used for water remote sensing. Since the absorption of pure water in the NIR bands is very high, the contribution of other water constituents to the total absorption can be neglected. In turbid water the 4 NIR bands might also be affected by the scattering of particles in water. Thus an algorithm, as we provide here for case 2 water, has to take this effect into account. The techniques we have used to determine the path radiances and transmittances from these 4 NIR bands is a neural network. It is trained by simulated top of standard atmosphere directional radiance reflectances. Input to the neural network are the reflectances in the 4 NIR bands as well as the solar and viewing zenith angel and the difference between solar and viewing azimuth angle. Output of the NN are the 9 path radiances and transmittances of the first 9 MERIS bands. This information can then be simply used to compute the directional water leaving radiance reflectances for these 9 bands. The NN is applied to the reflectances top of a standard atmosphere (TOSA). These reflectances are derived from the Top of Atmosphere (TOA) radiance reflectances by taking the difference between the standard and actual surface pressure into account to correct for the scattering of air molecules (Rayleigh scattering) of this correction layer. In the same way the difference between the standard and actual ozone concentration is used in this correction layer (details s. ATBD Atmospheric correction). The correction for these two deviations from a standard atmosphere is performed by an analytical algorithm. This algorithm converts TOA radiance reflectances into TOSA radiance reflectances, which are the input to the NN. Furthermore, we have included in this correction procedure an optional (s. parameter file) correction for the spectral deviations of the individual pixels of each camera due to the remaining misalignment of the cameras (in other papers called "smile correction"). This misalignment has mainly an effect on the path radiance calculation (scattering by air molecules) and on the solar irradiance at top of atmosphere. A further, experimental, add on is a special neural network for taking the influence of the polarisation of light by air molecules into account for the atmospheric correction. Also this procedure can be optionally switched on by a parameter. Output products of the atmospheric correction are the TOSA radiance reflectances, the path radiances, the transmittances and the water leaving radiances. The inclusion of all of these variables in the output product file can be selected in the parameter file band by band individually.

1.3 Retrieval of water constituents and IOPs

Although it is possible to perform the atmospheric correction and retrieval of water constituents in one step with one neural network, we have separated these tasks in order not to involve a specific bio-optical model in the atmospheric correction, so that the use of only the atmospherically corrected data is independent from the optical properties of the water constituents as assumed in a bio-optical model. The retrieval of the water constituents from the directional water leaving radiance reflectances is performed also with a neural network. In this version of the processor we provide two alternatives, the second of which can be selected by a parameter in the parameter file. Both versions can produce the two types of outputs in the same run. In both cases the networks are trained with simulated directional radiance reflectances. Details of the bio-optical model, the simulations and training procedure can be found in Doerffer & Schiller (2007) and in the ATBD.

The first version is a combination of a backward and forward neural network. Input to the backward network are the directional water leaving radiance reflectances of 8 MERIS bands (412 - 708 nm, excluding the fluorescence band at 681 nm). Output of the network are 3 inherent optical properties (IOP), i.e. (1) scattering of all particles, (2) absorption of phytoplankton pigments and (3) absorption of Gelbstoff and bleached particles, all three at MERIS band 2 (442 nm). Bleaching is used in proceesing the water samples to remove the phytoplankton pigments. These IOPs are also input to a forward neural network, which computes the water leaving radiance reflectances. The computed reflectances are then compared with the measured ones (after atmospheric correction). In the case that the sum of the squared deviations between both spectra surmounts a threshold of 4 (can be set in the parameter file) a warning flag is triggered. Furthermore the values of the agreement is also provided as a selectable product. The advantage of this processing version is that it is rather fast.

The second, selectable, alternative is based on an optimization procedure. It uses only the forward neural network. By modifying the three IOPs in the optimization loop an optimum agreement between the simulated and measured spectrum of the the directional water leaving radiance reflectance is searched. If the deviation is below a certain minimum or if the maximum number of iterations is reached, the three IOPs are provided as the result. Furthermore, the remaining Chi2 deviation is also provided. Comparisons between both alternatives have shown that in most cases the remaining deviation is significantly smaller when the optimization procedure is used instead of the backward neural network. However, this alternative requires significantly more computation time and requires a high accuracy in the atmospheric correction.

1.4 Selection of neural networks

For the retrieval of water properties two sets of networks are provided. Tests have shown that for the Levenberg-Marquard procedure the following networks give better results, also when setting useInvNN = false (s. description of parameter file):

```
waterNnInverseFilePath = 45x16x12x8x5_3716.7_invreflcutx3.net
waterNnForwardFilePath = 55x20x15x10_3766.9_forwreflcutx3.net
```

For the standard inversion using only the neural networks without Levenberg-Marquard iteration the following pair of networks has turned out to be better.

```
waterNnInverseFilePath = ./water_net_20020807/60x20x5_639.4.net
waterNnForwardFilePath = ./water_net_20020807/15x20_144.8.net
```

Future versions will provide more networks dedicated to different types of water.

2 PART II: INSTALLATION

2.1 Software Download

The Case2 Regional Processor is a Java program that can be downloaded free of charge from the BEAM Plug-In page.

http://www.brockmann-consult.de/beam/plugins.html

2.2 Installation of the Plug-In

1. Download and unzip the plug-in ***Case2Regional.zip*** archive. It will contain a Case2Regional.jar file, which is the actual plug-in, and a readme.txt and .pdf file. The plug-in also requires auxiliary data, which is stored in a sub-directory called auxdata.
2. The plug-in is installed by copying the Case2Regional.jar file into the extensions sub-directory of your BEAM installation directory.
3. The auxdata sub-directory has to be copied into the auxdata sub-directory of your BEAM installion directory.
4. Please make sure to scan the readme (if any) for extra installation notes (txt file) and hints for using the processor (pdf file).
5. All BEAM plug-ins have to be re-installed if you install a new BEAM version on your computer.

2.3 Hardware Requirements

- A computer with an operating system for which a Java Virtual Machine is available.
- Minimum RAM to start the processor: 128MB. However, the processing requirements depend of the size of the MERIS product to be processed. It is recommended to have at least 256MB RAM for a 1121x1121 pixel scene. For typical work with MERIS products, BEAM and the Case2Regional processor it is recommended to have 1GB RAM.
- Hard Disk requirements:100MB for BEAM and the Case2Regional Processor
- Graphic board: no specific requirements
- Processor: minimum requirement is 1GHz, recommended 2GHz or better

2.4 Software Requirements

- BEAM 3.x (http://www.brockmann-consult.de/beam/downloads.html)
- Java VM (is part of the BEAM installation)
- Case2Regional Plug-In (http://www.brockmann-consult.de/beam/plugins.html)

3 PART III: USING THE PROCESSOR

3.1 Operation of the Case2 Regional processor

The Case2Regional Processor works with MERIS FR and RR products as input. It generates a MERIS Case2Regional Level 2 Product.

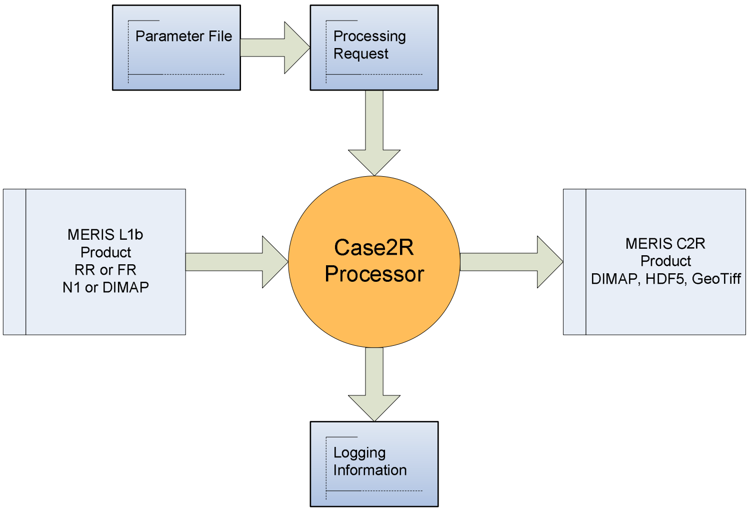


Figure 1: Schematic of the external interfaces of the Case2Regional Processor

The Processor is a self-standing Java application. It is invoked with a processing request. This processing request contains the specification of

- The name and location of the input product to be processed
- The name, location and format of the output product to be generated
- Specification of logging requirements
- The name and location of a parameter file, that contains a detailed specification of parameters influencing the algorithm

The processing request can either be configured using a graphical user interface (GUI) or by writing a text file (XML format). The GUI can be used to write the XML file.

The parameter file, which is referenced in the processing request, is also a text file. This can be edited also from within the GUI, but it may also be changed using a plain text editor.

Both files, the processing request file and the parameter file, may also be generated by another program, for example for automated batch-processing.

The following table gives an overview, how the Case2Regional can be invoked and which files are required:

Launch type	Processing Request	Parameter file
VISAT	GUI	Parameter file, can be edited in the GUI
Command line using the GUI	GUI	Parameter file, can be edited in the GUI
Command line without GUI	Processing Request file	Parameter file

Example of a Processing Request File:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<RequestList>
    <Request type="MERISC2R">
        <Parameter name="output_format" value="BEAM-DIMAP" />
        <Parameter name="log_prefix" value="merisc2r" />
        <Parameter name="log_to_output" value="false" />
        <Parameter name="property_file" value="C:\default-parameters.txt" />
        <InputProduct URL="file:C:\MER_RR__1PQBCM20030715.dim" />
        <OutputProduct URL="file:C:\C2R2_20030715.dim" format="BEAM-DIMAP" />
    </Request>
</RequestList>
```

Example of a Parameter File[1]:

```
#
# Parameter file for the MERIS Case II Regional Processor
#

#
#(1)
waterNnInverseFilePath = 45x16x12x8x5_3716.7_invreflcutx3.net
waterNnForwardFilePath = 55x20x15x10_3766.9_forwreflcutx3.net
atmCorrNnFilePath      = 10x20_155.2.net
polCorrNnFilePath      = 18_518.1.netPolEffekt
#
#(2)
inputValidMask = not l1_flags.INVALID and not l1_flags.SUSPECT and not
             l1_flags.LAND_OCEAN and not l1_flags.BRIGHT and not l1_flags.COASTLINE
#
#(3)
performSmileCorrection = false
#
#(4)
outputAPig = false
outputAGelb = false
outputBTsm = false
#
#(5)
outputChlConc = false
outputTsmConc = false
#
#(6)
outputAngstrom = false
outputTau = false
#
#(7)
outputOutOfScopeChiSquare = true
#
#(8)
chiSquareFit = true
outputFitAPig = true
outputFitBTsm = true
```

[1] All entries of the parameter file are explained in section 3.2.3.

```
outputFitTsmConc = true
outputFitChlConc = true
outputFitAGelb = true
outputChiSquareFit = true
outputNIter = true
#
#(9)
useInvNN = false
nIterMax = 30
nu = 2.0
tau = 0.05
eps1 = 0.01
eps2 = 0.0003
#
#(10)
usePolCorr = false
#
#(11)
tsmConversionFactor = 1.73
tsmConversionExponent = 1.0
#
#(12)
chlConversionFactor = 21.0
chlConversionExponent = 1.04
#
#(13)
maxWaterToaRadRefl14 = 0.02
maxLandToaRadRefl14 = 0.2
#
#(14)
# flag = true if chi-square > thres, false else
spectrumOutOfScopeThreshold = 4.0
#
#(15)
outputPathRadianceReflAll = true
#
#(16)
outputIrradianceReflectance = false
#
#(17)
outputWaterLeavingReflAll = true
#
#(18)
outputTransmittanceAll = true
#
#(19)
outputToaReflAll = true
#
#(20)
outputTosaReflAll = true
#
```

3.2 Launching the processor from within VISAT

The Case2Regional Processor appears under the VISAT menu “Tools” → “MERIS Case-2 Regional Processor …”. Clicking on this entry starts the graphical user interface. This interface has two tabs

- The input- output parameters tab to specify the file to be processed and the format, name and location of the generated output product
- The processing parameters tab to specify the parameters that influence the processing

3.2.1 The Meris Case-2 Regional Processing Parameters tab

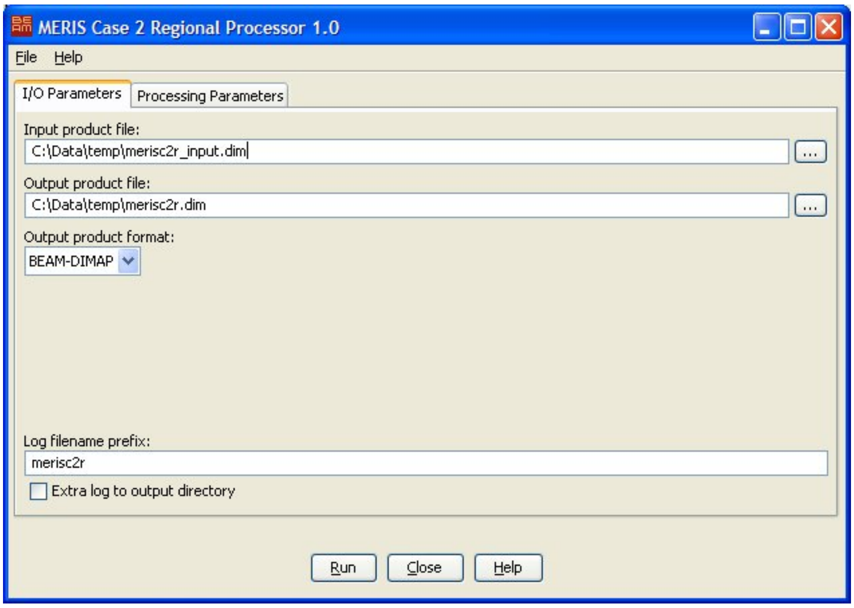


Figure 2: Snapshot of the Processing Parameters tab.

1. **Input product file**: Select the input product file by either typing the product path into the text field or by pressing the file selection button ... to invoke a standard file dialog.
2. **Output product file**: Select the output product file by either typing the product path into the text field or by pressing the file selection button ... to invoke a standard file dialog.
3. **Output product format**: Select one of the available output product formats.
4. **Log filename prefix**: Select the prefix of the log file.
5. **Extra log to output directory**: Select whether to write an additional log file to the directory selected for the output product.

3.2.2 The Meris Case-2 Regional Processing Parameters tab

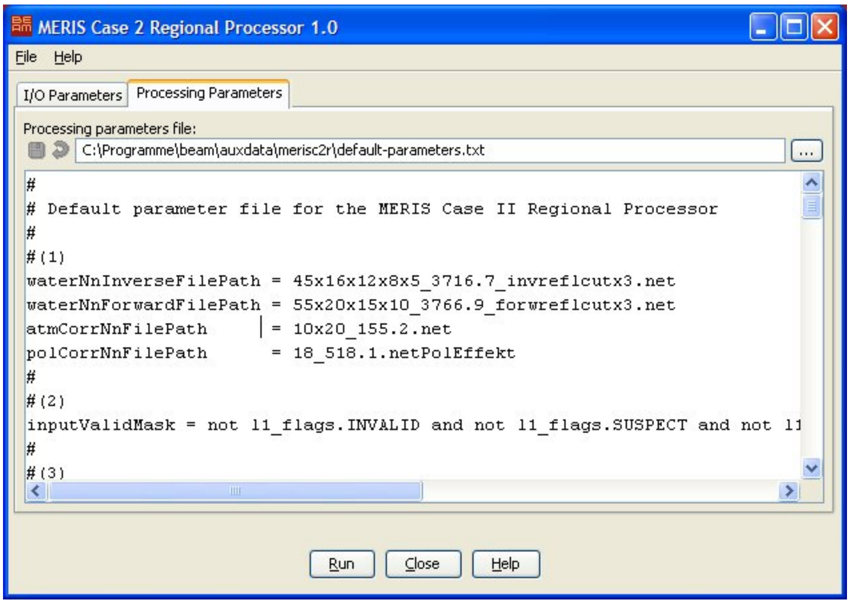


Figure 3: snapshot of the processing parameters tab

1.  Saves the edited parameters to a file.
2.  Resets the edited parameters text to the default text.
3. One can select a file where the processing parameters are stored. This file has to be a *.txt or a *.properties file.

In the text field one can edit and adjust the processing parameters for the current run of the processor.

3.2.3 Description of the Processing Parameters

Parameter	Description
waterNnInverseFilePath, waterNnForwardFilePath, atmCorrNnFilePath, polCorrNnFilePath	Paths and names of the neural network files: if no path is given (just the name) the files are assumed to be in *${BEAM-HOME}\auxdata\merisc2r*.
inputValidMask	A logical expression which defines the valid pixels for the processing (from L1 flags). Pixels which are not valid are skipped by the processor.
performSmileCorrection	Switch the smile (camera alignment) correction on and off.
outputAPig, outputAGelb, outputBTsm	Select which of the IOP products shall be included in the output file. All are given for MERIS band 2 (443 nm). outpuAPig := absorption coefficient of phytoplankton pigments outputAGelb := absorption coefficient of yellow substance and of all particles after bleaching outputBTsm := scattering coefficient of all particles
outputChlConc,	Select which of the concentrations shall be included in the

outputTsmConc	putput file. outputChlConc := chlorophyll concentration (mg m-3) outputTsmConc := total suspended matter (including phytoplankton) dry weight (g m-3)
outputAngstrom outputTau	Select if the angstrom coefficient and the aerosol optical thickness shall be computed and provided as
outputKmin outputZ90max	Select if the minimum attenuation coefficient for downwelling irradiance and the inverse, the signal depth z90, shall be computed. Kmin is calculated as the mean from those 3 bands which have minimum K values. Z90 describes the depth from which 90% of the reflected light just below the water surface stems from.
outputOutOfScopeChiSquare	Controls the Output of the chi2 value, i.e. the squared difference between measured and simulated water leaving radiance reflectances, shall be included in the product. A low value in the product indicates a higher success in the retrieval and that the conditions, which have led to the measured spectrum, are in (sufficient) agreement with the conditions and the bio-optical model used in the simulations for training the neural network. A value above 4.0 triggers the out of training range == out of scope flag, The threshold can be changed in the parameter file s. spectrumOutOfScopeThreshold.
chiSquareFit, outputFitAPig, outputFitBTsm, outputFitTsmConc, outputFitChlConc, outputFitAGelb, outputChiSquareFit, outputNIter	Perform the optimization fitting algorithm, this has to be set true if the IOPs and concentrations shall be computed alternatively or in addition using the optimization procedure. However, this procedure requires more computation time, but the results are normally improved, provided a good atmospheric correction.
useInvNN, nIterMax, nu, tau, eps1, eps2	Parameters used to control the optimization. Please leave them unchanged presently. For details s. technote *LMpars_hs_20061106.pdf*
usePolCorr	Controls if the polarisation correction should be included in the atmospheric correction procedure. This part is presently experimentally and has not been verified so far.
tsmConversionFactor, tsmConversionExponent	Factors for converting particle scattering into total suspended matter dry weight. Ctsm (g m-3) = tsmConversionFactor * b443^tsmConversionExponent
chlConversionFactor, chlConversionExponent	Factors for converting absorption of phytoplankton pgiment at 443 into chlorophyll concentration. Chlorophyll (mg m-3) = chlConversionFactor a_pig443^chlConversionExponent
spectrumOutOfScopeThreshold	The out of scope (= out of training range) flag will be set if the chi2 value is above the given threshold.
outputPathRadianceReflAll	outputPathRadianceReflAll sets the default value for all

outputPathRadianceRefl.[1 - 9]	values of the outputPathRadianceRefl.{X}. outputPathRadianceRefl.{X} defines (separately for each band) if path radiance reflectance shall be included in output product.
outputWaterLeavingReflAll outputWaterLeavingRefl.[1 - 9]	outputWaterLeavingReflAll sets the default value for all values of outputWaterLeavingRefl. outputWaterLeavingRefl.{X} defines (separately for each band) if path radiance reflectance shall be included in output product.
outputTransmittanceAll outputTransmittance.[1 - 9]	outputTransmittanceAll sets the default value for all values of outputTransmittance. outputTransmittance.{X} defines (separately for each band) if path radiance reflectance shall be included in output product.
outputToaReflAll outputToaRefl.[1 - 15]	outputToaReflAll sets the default value for all values of outputToaRefl. outputToaRefl.{X} defines (separately for each band) if path radiance reflectance shall be included in output product.
outputTosaReflAll outputTosaRefl.[1 – 10, 12,13]	outputTosaReflAll sets the default value for all values of outputTosaRefl. outputTosaRefl.{X} defines (separately for each band) if path radiance reflectance shall be included in output

3.3 Launching the processor from the command line with graphical user interface

During installation, shell scripts for Windows and Unix/Linux are copied into the extension directory of the BEAM installation.

Important: the `beam_home` variable of shell/batch file needs to be adapted to the local path.

These shell scripts can be called from a command line. If the “- i” is specified, the user interface as explained in section 3.2 is invoked. Optionally, a request file can be specified. If no request file is specified, the defaults will be used.

Operating system	command line string
Unix/Linux	merisc2r.sh –i <request-file.xml>
Windows	merisc2r.bat –i <request-file.xml>

3.4 Launching the processor from the command line without graphical user interface

During installation, shell scripts for Windows and Unix/Linux are copied into the extension directory of the BEAM installation. These files may be copied to any other location.

Important: the `beam_home` variable of shell/batch file needs to adapted to the local path.

These shell scripts can be called from a command line. A request file has to be specified. Then the processor does not require any interactive user input. These files may be copied to any other location.

Operating system	command line string
Unix/Linux	merisc2r.sh request-file.xml
Windows	merisc2r.bat request-file.xml

3.5 The output product

The output generated by the Case2Regional processor includes meta data, flag codings, tie-point grids and bands.

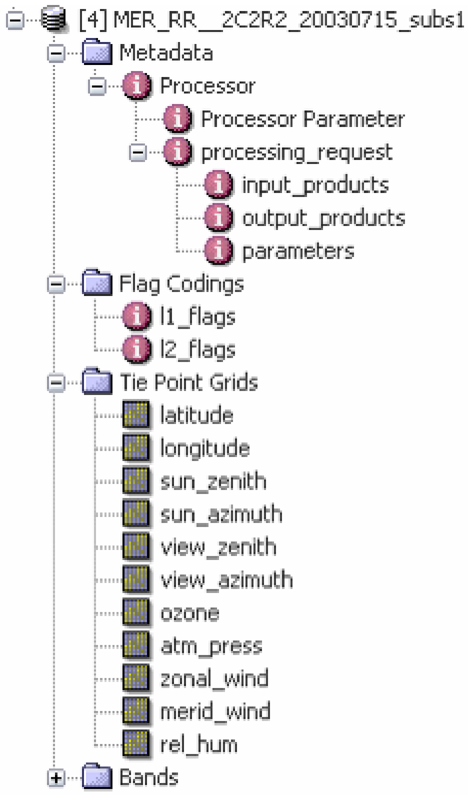


Figure 4: Structure of a Case2Regional output product. The bands section has not been expanded because its contents depends on the specification of the parameter file.

3.5.1 Meta data

As meta data are included

- Processor: Name, Version and copyright information
- Processor parameter: a listing of the parameters as specified in the processing parameters tab of the processing request. This corresponds to the content of the parameter-file.
- Processing request: the input and output details of the processing request. This corresponds to the content of the processing-request-file.

3.5.2 Flag Coding

The Case2Regional product includes several flags (binary values). All flags of the MERIS L1b input product are copied into the output product (l1_flags). Additionally, the Case2Regional processor is generating additional flags (l2_flags). The following table lists all flags:

Flag Name	Source	Description
COSMETIC	MERIS L1b Input Product	Pixel is cosmetic
DUPLICATED		Pixel has been duplicated (filled in)
GLINT_RISK		Pixel has glint risk
SUSPECT		Pixel is suspect
LAND_OCEAN		Pixel is over land, not ocean
BRIGHT		Pixel is bright
COASTLINE		Pixel is part of a coastline
INVALID		Pixel is invalid
RAD_ERR	Case2R Algorithm	TOAR out of valid range
LAND		Land pixels
CLOUD_ICE		Cloud or ice
SUNGLINT		Sunglint risk
ANCIL		Missing/OOR auxiliary data
TOA_OOR		TOAR out of scope
WLR_OOR		WLR out of scope
SOLZEN		Large solar zenith angle
SATZEN		Large spacecraft zenith angle
ATC_OOR		Atmospheric correction out of range
CONC_OOR		Concentration out of training range
OOTR		Water leaving reflectance out of training range
WHITECAPS		Windspeed > 12 m/s -> high risk of white caps
INVALID		Invalid Level 2 product

Description of flags

3.5.2.1 rad_err

This flag is switched on under hazy conditions, when the aerosol optical thickness surmounts a certain degree for which the neural network has not been trained. It is simply checked by the toa radiance reflectance in Meris band 1. Under these hazy conditions the separation between reflectance caused by the atmosphere or by turbid water can fail.

3.5.2.2 l2_land

Although the land is flagged already by the level 1 land flag and the coastline flag, conditions occur like dry fallen tidal flats, which are not included in the L1 flag. With the l2_land flag we test if the radiance reflectance in MERIS band 13 (865 nm) is above a threshold, which is provided and can be changed in the parameter file. Also the rim of clouds maybe flagged.

3.5.2.3 cloud_ice

This flag indicates very high radiance reflectance indicating clouds, ice or snow. Normally it should not appear, because these pixels should have been excluded from water processing by the L1 bright flag. The algorithm works as for l2_land, the threshold is provided in the parameter file.

3.5.2.4 sunglint

This flag is presently not implemented. Sunglint is corrected as far as presently possible by the atmsopheric correction procedure.

3.5.2.5 ancil

This flag indicates unreasonable data for ozone or pressure, which are used in the atmospheric correction procedure.

3.5.2.6 toa_oor

This flag is on when the input radiance reflectances (top of standard atmosphere, tosa) in one or more bands are out of the atmosphere neural network training range.

3.5.2.7 wlr_oor

This flag is on when the input water leaving radiance reflectances (as result of the atmospheric correction) in one or more bandds are out of the water neural network training range.

3.5.2.8 solzen

Flag is on if the solar zenith angle is out of the neural network training range.

3.5.2.9 satzen

Flag is on if the viewing zenith angle is out of the neural network training range.

3.5.2.10 atc_oor

Flag is on if the output of the atmospheric correction neural network (path radiance reflectances and transmittances) in one or more bands are not within the expected range.

3.5.2.11 conc_oor

Flag is on if the output of the water neural network, i.e. the inherent optical properties a_pig, b_tsm, a_yellow, are not within the expected range.

3.5.2.12 ootr

This flag indicates that the water leaving radiance reflectance as submitted to the water NN is outside the range of the spectra used for training of the NN. Flag is on if the sum of the squared deviations between the water leaving radiance reflectances (i. e. after atmospheric correction) and the water leaving radiance reflectances as simulated with the forward NN surmounts a certain threshold, which is given in the parameter file and which can be changed, s. spectrumOutOfScopeThreshold. The degree of the deviation is also provided as the output product chi_square (set outputOutOfScopeChiSquare = true in parameter file).

3.5.2.13 whitecaps

This flag is triggered if the windspeed as provided with the MERIS product surmounts 12 m/s, which is about Beaufort 6. Note that whitecapping starts at wind speeds around 7 m/s (Beaufort 4). Large white patches , which may have a significant influence on the reflectance of the ocean, occur at wind speeds above 11 m/s (Beaufort 6). In coastal waters, the foam coverage can be influenced also by organic material and thus, at high concentrations, may be formed even at lower windspeeds.

3.5.2.14 l2_invalid

This is the master flag, which goes on if any of the flags OOTR, wlr_oor, toa_oor, l2_land, cloud_ice, rad_err, WHITECAPS has been triggered.

3.5.3 Tie-point grids

Important tie-point grid values of the MERIS L1b input product are copied into the output product. The values are specified on a 16km x 16km raster, i.e. a 16 x 16 pixel subsampling for RR products and a 64 x 64 pixels subsampling for FR products[2].

These tie-point grids are included:

- latitude and longitude (decimal degrees)
- viewing geometry: sun and viewing zenith and azimuth angles (decimal degrees)
- ECMWF meteorology values: ozone (Dobson Units), atmospheric pressure at sea level (hPa), zonal and meridional wind speed (m/s), relative humidity (%).

3.5.4 Bands

The bands which are written into the output product can be specified in the processing parameters. There are spectral bands which give values at certain wavelengths (e.g. water leaving reflectances), and other geophysical, scalar values (e.g. chlorophyll concentration). Two bands with L1b and L2 flags are always written.

The following table lists all possible choices:

[2] BEAM/VISAT takes care of the subsampling and interpolates the values to the pixel grid.

Band Name	Spectral Bands	Description
toa_reflec_i	i = 1 … 15	Top of atmosphere reflectance
tosa_reflec_i	i = 1 … 1,12, 13	Top of standard atmosphere reflectance (toa_reflectance but for standard air pressure, humidity and ozone content)
path_i	**i** = 1 … 9	Atmospheric path reflectance
trans_i	**i** = 1 … 9	Downwelling irradiance transmittance (`Ed_BOA/Ed_TOSA`) `Ed` … downwelling irradiance `BOA` … bottom of atmosphere `TOSA` … top of standard atmosphere
reflec_i	i = 1 … 9	Water leaving radiance reflectance
angstrom	Scalar	Aerosol angstrom coefficient, calculated between 620nm and 681nm
tau		Aerosol optical depth at 681nm
a_gelbstoff	scalar	Gelbstoff absorption at 442nm (without optimisation)
b_tsm	scalar	Total suspended matter scattering (without optimisation)
a_pig	scalar	Pigment absorption at 442nm (without optimisation)
a_total	scalar	Total absorption of water constituents (without opt.)
k_min	scalar	Downwelling irradiance attenuation coefficient, mean of those 3 bands with minimum k values
z_90	scalar	Signal depth -> depth from which 90% of surface reflectance stems from; == 1/k_mean
tsm	scalar	Total suspended matter dry weight concentration (without optimisation)
chl_conc	scalar	Chlorophyll-a concentration (without optimisation)
chiSquare	scalar	Sum of deviation of measured (after atmospheric correction) and modelled water leaving radiance reflectances (without optimisation)
gelbstoffFit	scalar	Gelbstoff absorption at 442nm after optimisation procedure
b_tsmFit	scalar	Total suspended matter scattering after optimisation procedure
a_pigFit	scalar	Pigment absorption at 442nm after optimisation procedure
Tsm_concFit	scalar	Total suspended matter dry weight concentration after optimisation procedure
chl_concFit	scalar	Chlorophyll-a concentration after optimisation procedure
chiSquareFit	scalar	Sum of deviation of measured and modelled top of atmospherie reflectances after optimisation procedure
Niter	Scalar	Number of iterations used during the optimisation
L2flags	Flags band	Case2Regional specific flags, see 3.5.2
L1flags	Flags band	MERIS L1b flags, see 3.5.2

4 PART IV: APPLICATION EXAMPLE

In this part we will demonstrate how the Case2Regional processor is applied to MERIS scene. The selected scene is orbit 7176, 15.7.2003, passing over the North Sea and the Baltic Sea. The visual inspection of the L1b RGB shows the following features:

- North Sea
  - free of sun glint
  - no clouds
  - little haze in the German Bight
  - bright features in the Skagerrak, probably Coccolithophores bloom
  - bright spot off the Dutch coast, probably Coccolithophores bloom

- Kattegat
  - the water is already significantly darker than in the North Sea, probably due to higher amount of yellow substance
  - close to the centre of the image (nadir view) and probably affected by sun glint, although not visible

- Baltic Sea
  - large and intense cyanobacteria bloom in the central Baltic Sea
  - some in the Western Baltic Sea
  - sun glint in the Western Baltic Sea

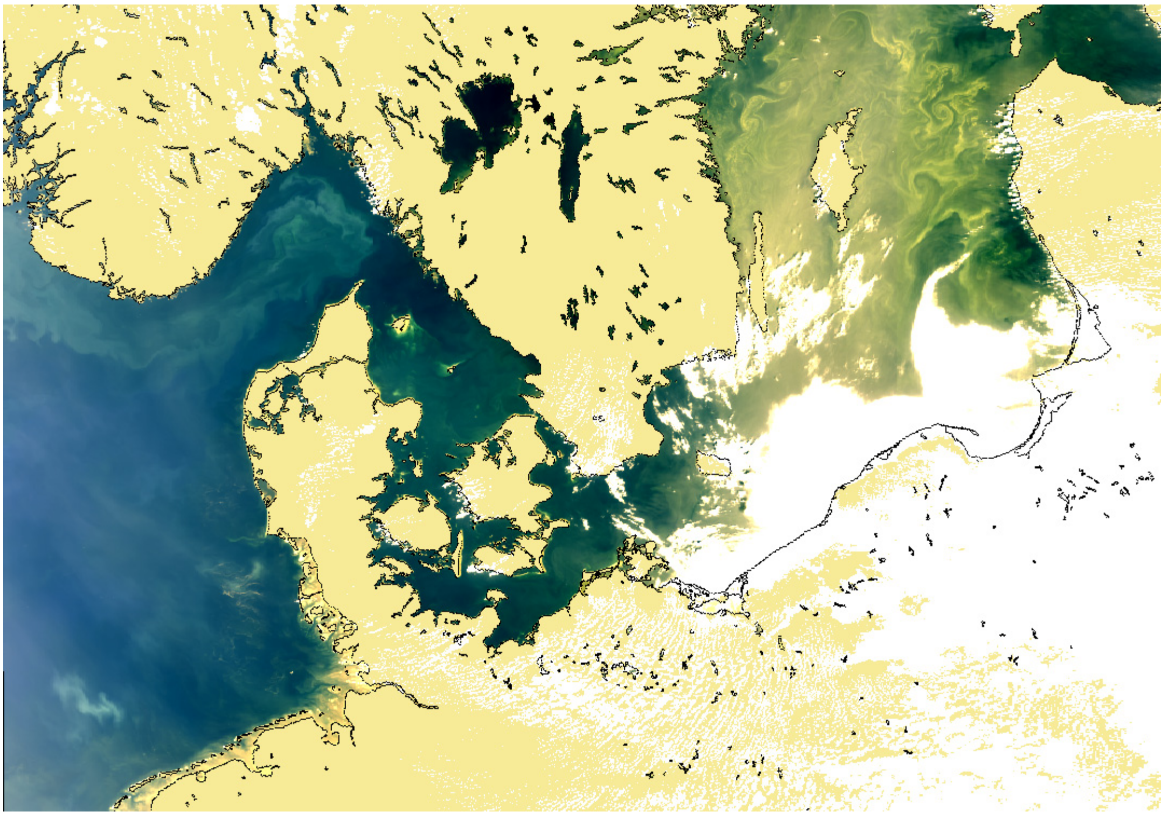


Figure 5: L1b RGB of MERIS orbit 7176, 15.7.2003.

4.1 Run 1: Default Parameter Set

The default parameter set (see Annex 1) that is delivered with the Case2Regional processor has the main following main characteristics. Please note the optimisation is activated which causes a comparable long processing time.

- Processed are only valid, non bright water pixels
  `inputValidMask = not l1_flags.INVALID and not l1_flags.SUSPECT and not l1_flags.LAND_OCEAN and not l1_flags.BRIGHT and not l1_flags.COASTLINE`
  Comments:
  - the inputValidMask is an arithmetic expression in which all MERIS L1b flags but also logical expression using the radiance bands can be used.
  - the L1b-Bright flag is more than a cloud flag: it identifies every pixel which radiance value in the blue exceeds a certain threshold, including ice, snow, clouds, bright sands. Over water, it is a reasonable approximation for a cloud and ice flag, but it certainly misses thin clouds.
  - It is important to exclude non water pixels from the processing in order to avoid unnecessary long processing time.

- The smile correction is not performed
  ```
  performSmileCorrection = false
  ```

- The optimization loop is switched on and the fitted IOPs, concentrations, the ChiSquare and the number of iterations after completing the optimization are written into the output product:
  ```
  chiSquareFit = true
  outputFitAPig = true
  outputFitBTsm = true
  outputFitTsmConc = true
  outputFitChlConc = true
  outputFitAGelb = true
  outputChiSquareFit = true
  outputNIter = true
  ```
  The retrieved IOPs and concentrations before the optimization are not written into the output product:
  ```
  outputAPig = false
  outputAGelb = false
  outputBTsm = false
  outputChlConc = false
  outputTsmConc = false
  ```

- Aerosol information is not written into the output product
  ```
  outputAngstrom = false
  outputTau = false
  ```

- The polarization correction is not applied
  ```
  usePolCorr = false
  ```

- The conversion factors to transform IOPs into concentrations are derived from North Sea water samples
  ```
  tsmConversionFactor = 1.73
  tsmConversionExponent = 1.0
  chlConversionFactor = 21.0
  chlConversionExponent = 1.04
  ```

- The threshold applied to the ChiSquare values in order to flag out-of-scope spectra is set to 4.0.

  ```
  spectrumOutOfScopeThreshold = 4.0
  ```

- The irradiance reflectance (corresponds to standard MERIS L2 water reflectance) is not written into the product instead of the radiance reflectance

  ```
  outputIrradianceReflectance = false
  ```

- The following spectral bands are written into the output product: atmospheric path radiance reflectance, water leaving radiance reflectances, atmospheric transmittances, top-of-standard atmosphere reflectance.

  ```
  outputPathRadianceReflAll = false
  outputPathRadianceRefl.1 = true
  outputPathRadianceRefl.2 = true
  …
  outputWaterLeavingReflAll = false
  outputWaterLeavingRefl.1 = true
  outputWaterLeavingRefl.2 = true
  …
  outputTransmittanceAll = false
  outputTransmittance.1 = true
  outputTransmittance.2 = true
  …
  outputTosaReflAll = false
  outputTosaRefl.1 = true
  outputTosaRefl.2 = true
  …
  ```

  Comment: with setting parameter output<variable>All=false the output for all bands is disables, i.e. it is used as a master switch. If it is set true, then the setting for the individual bands is used. Default is false, i.e. if a band is not included in the list it is set false. The consequence is that if <variable>All is set true, but none of the individual bands is set true no band would appear in the product.

The output product written with default parameters contains the following bands:

- Water leaving radiance reflectances
- Atmospheric path radiance reflectances
- Downwelling irradiance transmittances
- Top-of-atmosphere radiance reflectances
- Top-of-standard atmosphere radiance reflectances
- ChiSquare out of scope
- Gelbstoff absorption (fitted, i.e. after optimization)
- Scattering of total suspended matter (fitted, i.e. after optimization)
- Pigment absorption (fitted, i.e. after optimization)
- Total suspended matter concentration (fitted, i.e. after optimization)
- Chlorophyll-a concentration (fitted, i.e. after optimization)
- ChiSquare after the fit (fitted, i.e. after optimization)
- Number of iterations in the optimisation

Figure 6 shows an image of the water leaving reflectance in band 1 (412.5nm). The Level 1b bright and land flag are overlaid. Because the processing was excluded for these pixels, there are no data below this flag. In brown is overlaid the Leve 2 land flag. This identifies correctly additional land surfaces, such as the intertidal (here dry) areas along the German coast; however, it masks also cloud borders. The Level 2 cloud_ice flag should identify this, but it doesn't. In this example this flag is never raised. Some adjustment of the threshold seems necessary. The first impression is that the reflectances look reasonable everywhere. The OOTR flag indicates some problematic areas in German Bight and especially in the cloudy / sun glint area in the Western Baltic Sea (Figure 7). No other out-of-range flags are raised.

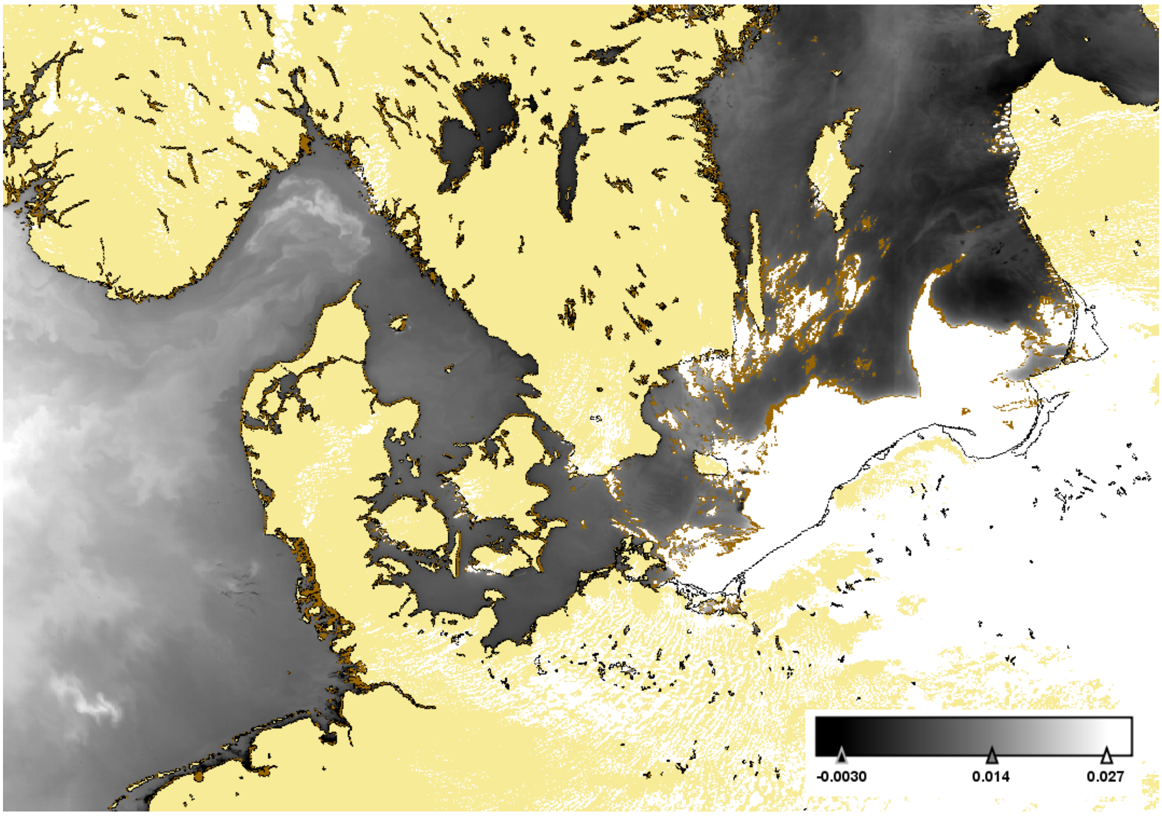


Figure 6: Water leaving radiance reflectance at 412nm (band 1). The following flags are overlaid: yellow: L1b Land; white: L1b bright; brown: L2 land

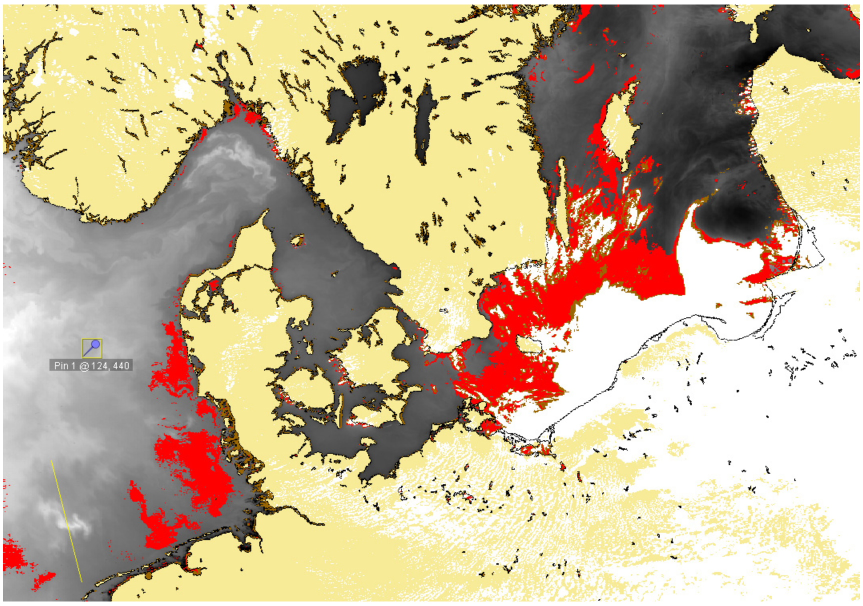


Figure 7: Same as Figure 6 but with the OOTR flag overlaid in red (water leaving reflectance out of training range). The pixel which is investigated further is indicated with a pin, and the transect with a yellow line in the North Sea.

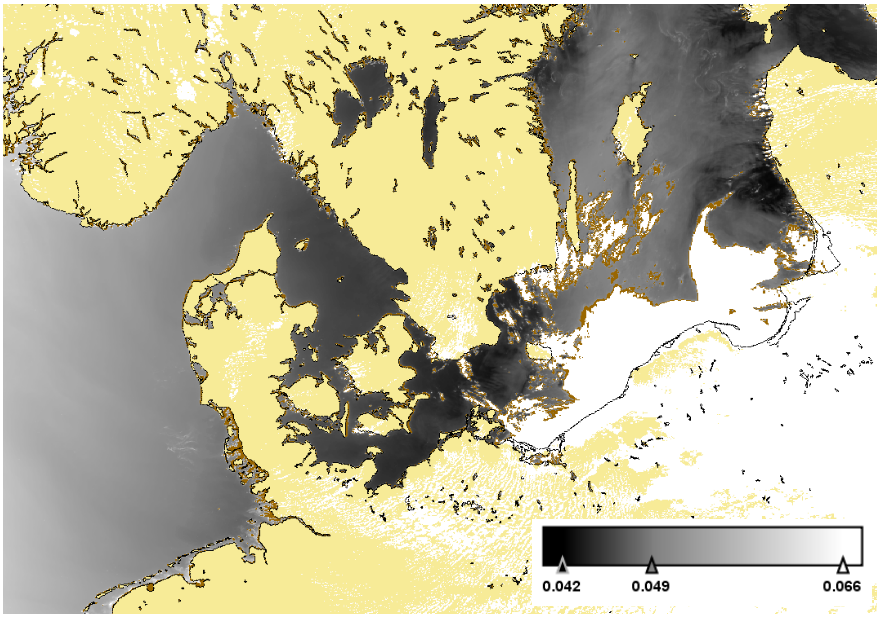


Figure 8: Atmospheric path radiance, band 1 (412.5nm)

The investigation of the spectral bands permits an assessment of the performance of the atmospheric correction. Figure 8 shows the image of the path reflectance in band 1. The pattern is smooth, and no small scale structure as in the water leaving reflectance could be seen. Figure 9 and Figure 10 show the spectra at an arbitrary pixel in the central North Sea (see Figure 7) and the reflectance values of band 2 (442nm) along a transect off the Dutch coast (shown in 7), which passes a bright spot, probably a cocolithophores bloom. Both graphs demonstrate the good decoupling of the atmospheric signal from the water leaving reflectance.

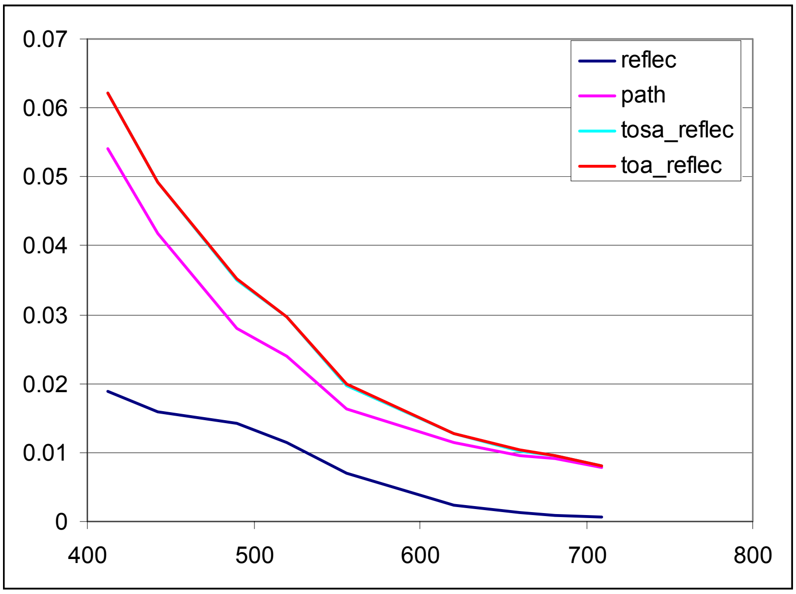


Figure 9: Top of atmosphere, path radiance and water leaving reflectance at the Pin location.

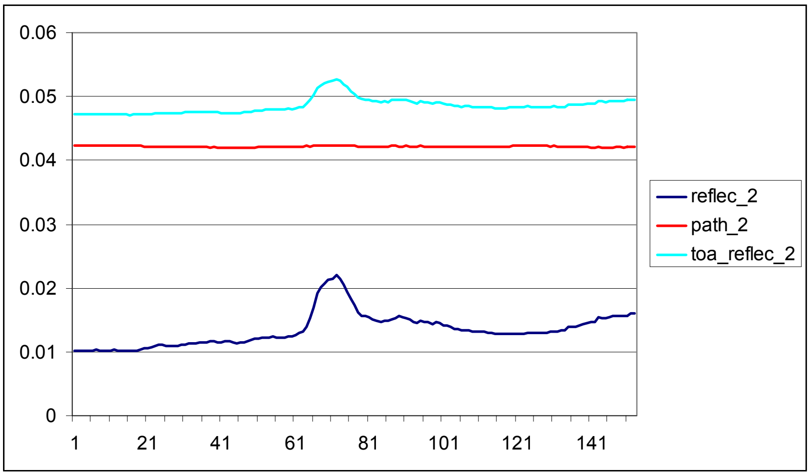


Figure 10: Top of atmosphere reflectance, path reflectance and water leaving reflectance along the transect shown in Figure 7.

The pigment absorption is shown in Figure 11. The OOTR flagged pixels have not been masked out, although they are indicated as invalid.

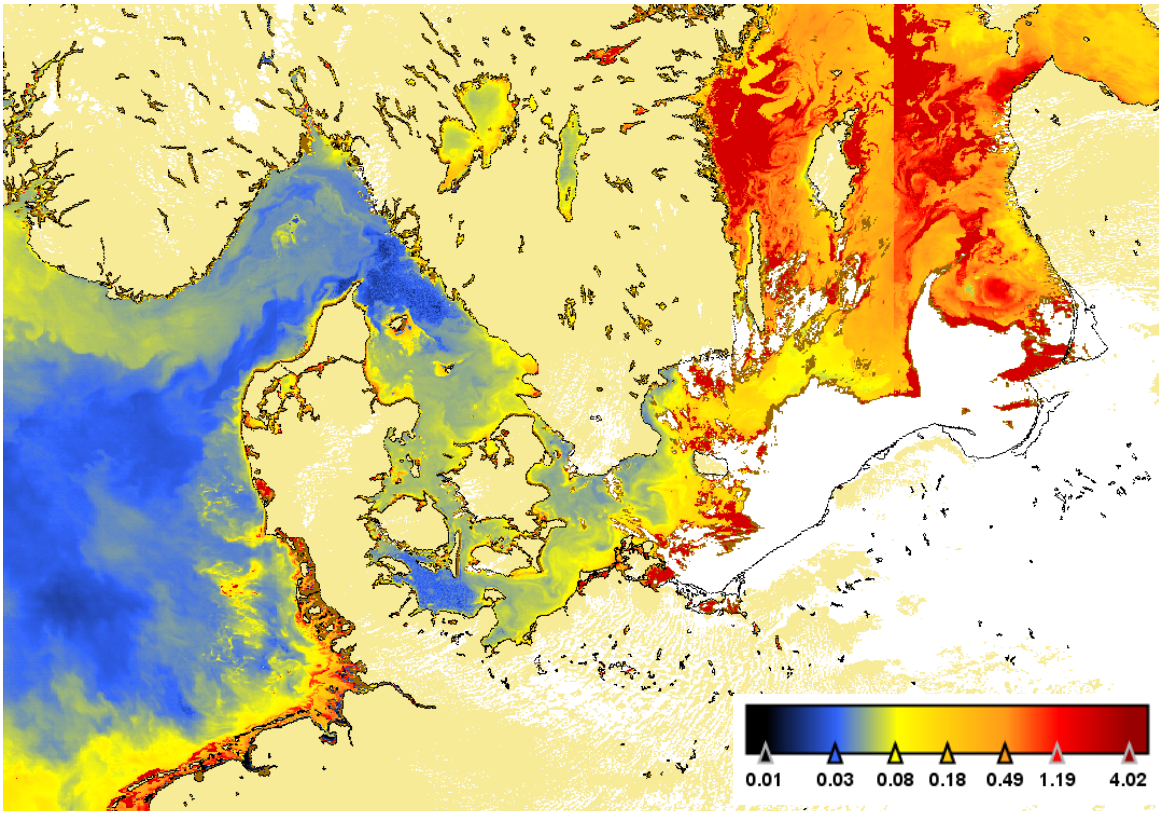


Figure 11: Pigment absorption.

To be completed: comparison with optimization turned off, smile correction turned on; polarization turned on.

5 ANNEX 1: DEFAULT PARAMETER FILE

```
#
# Default parameter file for the MERIS Case II Regional Processor
#

#
#(1)
waterNnInverseFilePath = ./water_net_20020807/60x20x5_639.4.net
waterNnForwardFilePath = ./water_net_20020807/15x20_144.8.net
atmCorrNnFilePath      = 10x20_155.2.net
polCorrNnFilePath      = 18_518.1.netPolEffekt

#
#(2)
inputValidMask = not l1_flags.INVALID and not l1_flags.SUSPECT and not
l1_flags.LAND_OCEAN and not l1_flags.BRIGHT and not l1_flags.COASTLINE

#
#(3)
performSmileCorrection = true

#
#(4)
outputAPig = true
outputAGelb = true
outputBTsm = true
outputATotal = true

#
#(5)
outputKmin = true
outputZ90max = true

#
#(6)
outputChlConc = true
outputTsmConc = true

#
#(7)
outputAngstrom = true
outputTau = true

#
#(8)
outputOutOfScopeChiSquare = true

#
#(9)
performChiSquareFit = false
outputFitAPig = true
outputFitBTsm = true
outputFitTsmConc = true
outputFitChlConc = true
outputFitAGelb = true
outputChiSquareFit = true
outputNIter = true
```

```
#
#(10)
useInvNN = false
nIterMax = 30
nu = 2.0
tau = 0.05
eps1 = 0.01
eps2 = 0.0003

#
#(11)
performPolCorr = true

#
#(12)
tsmConversionFactor = 1.73
tsmConversionExponent = 1.0

#
#(13)
chlConversionFactor = 21.0
chlConversionExponent = 1.04

#
#(14)
maxWaterToaRadRefl14 = 0.02
maxLandToaRadRefl14 = 0.2

#(15)
# flag = true if chi-square > thres, false else
spectrumOutOfScopeThreshold = 4.0

#
#(16)
outputPathRadianceReflAll = false
outputPathRadianceRefl.1 = true
outputPathRadianceRefl.2 = true
outputPathRadianceRefl.3 = true
outputPathRadianceRefl.4 = true
outputPathRadianceRefl.5 = true
outputPathRadianceRefl.6 = true
outputPathRadianceRefl.7 = true
outputPathRadianceRefl.8 = true
outputPathRadianceRefl.9 = true

#
#(17) set true if you want water leaving irradiance reflectance instead of
radiance reflectance
switchToIrradianceReflectance = false

#
#(18)
outputWaterLeavingReflAll = false
outputWaterLeavingRefl.1 = true
outputWaterLeavingRefl.2 = true
outputWaterLeavingRefl.3 = true
outputWaterLeavingRefl.4 = true
outputWaterLeavingRefl.5 = true
outputWaterLeavingRefl.6 = true
outputWaterLeavingRefl.7 = true
outputWaterLeavingRefl.8 = true
outputWaterLeavingRefl.9 = true
```

```
#
#(19)
outputTransmittanceAll = false
outputTransmittance.1 = true
outputTransmittance.2 = true
outputTransmittance.3 = true
outputTransmittance.4 = true
outputTransmittance.5 = true
outputTransmittance.6 = true
outputTransmittance.7 = true
outputTransmittance.8 = true
outputTransmittance.9 = true

#
#(20)
outputToaReflAll = false
outputToaRefl.1 = true
outputToaRefl.2 = true
outputToaRefl.3 = true
outputToaRefl.4 = true
outputToaRefl.5 = true
outputToaRefl.6 = true
outputToaRefl.7 = true
outputToaRefl.8 = true
outputToaRefl.9 = true
outputToaRefl.10 = true
outputToaRefl.11 = true
outputToaRefl.12 = true
outputToaRefl.13 = true
outputToaRefl.14 = true
outputToaRefl.15 = true

#
#(21)
outputTosaReflAll = false
outputTosaRefl.1 = true
outputTosaRefl.2 = true
outputTosaRefl.3 = true
outputTosaRefl.4 = true
outputTosaRefl.5 = true
outputTosaRefl.6 = true
outputTosaRefl.7 = true
outputTosaRefl.8 = true
outputTosaRefl.9 = true
outputTosaRefl.10 = true
outputTosaRefl.11 = false
outputTosaRefl.12 = true
outputTosaRefl.13 = true
outputTosaRefl.14 = false
outputTosaRefl.15 = false
```