C2RCC

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4 EOMasters

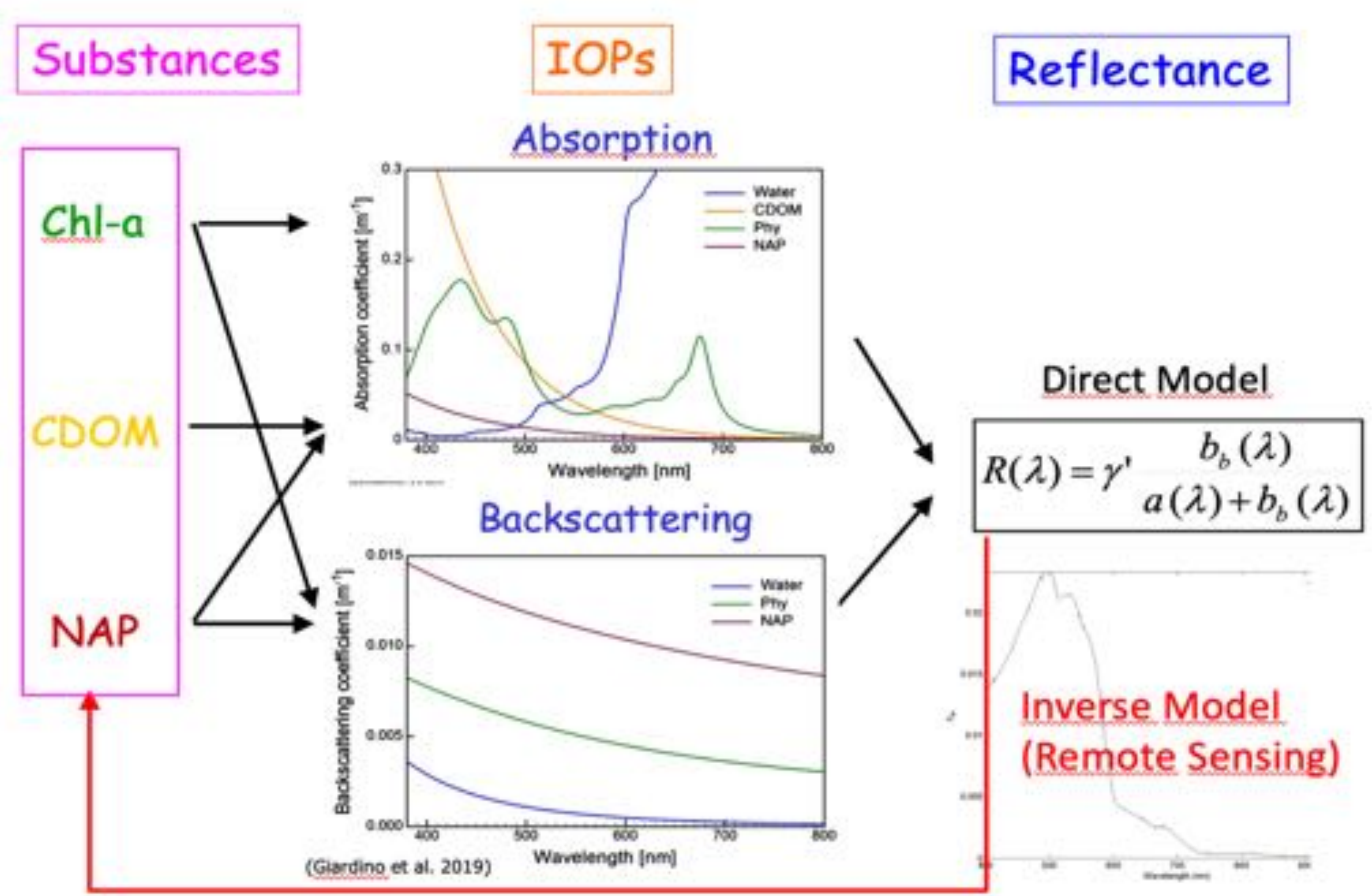
IOCCG Summer Lecture Series 2024

C2RCC Introduction

Case-2 Regional CoastColour

- The Secrets of C2RCC – Development
- Design of C2RCC
- Processing with SNAP

From substances to IOPs to AOPs



Ana Dogliotti

From AOPs to IOPs to substances: inverse modelling

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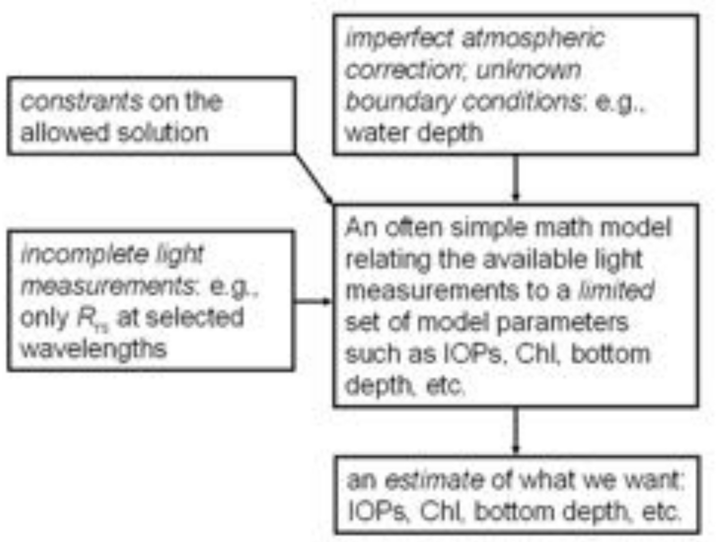
The conceptual process involved in solving a remote-sensing inverse radiative transfer problem



Most popular techniques:
"*Inversions are always based on an assumed model that relates what is known to what is desired.*"

https://www.oceanopticsbook.info/view/remote-sensing/inverse-problems

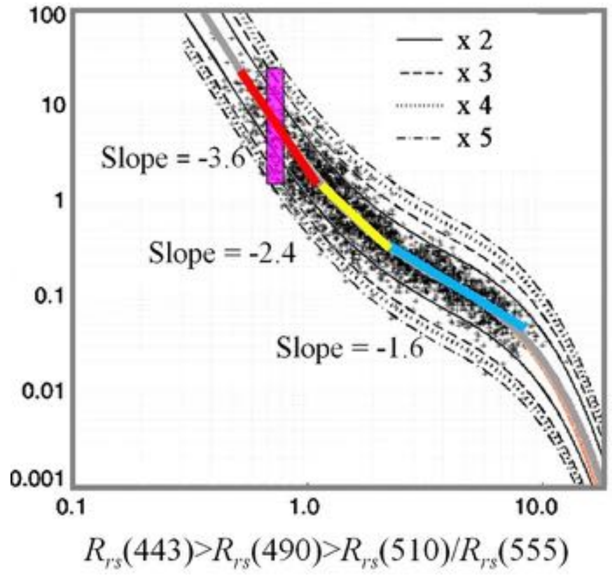
Some techniques that give possible accurate solutions

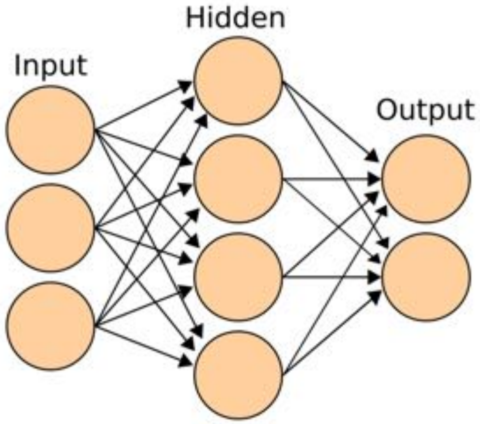
1. Numerical modelling: by solving the radiative transfer equation→ HydroLight, 6S, MODTRAN, Monte Carlo simulations, Mie theory.

2. Semi-analytical models: Quasi-Analytical Algorithm (QAA), Garver-Siegel-Maritorena (GSM) model, HOPE, GIOP...

3. Empirically: build relationships with in-situ data (regression). E.g. Chlorophyll-a determination with polynomial algorithms (OC4ME).

4. Machine learning/deep learning: Case 2 Regional Coast Colour (C2RCC) based on neural net technologies.





Case 2 Regional (CoastColour)

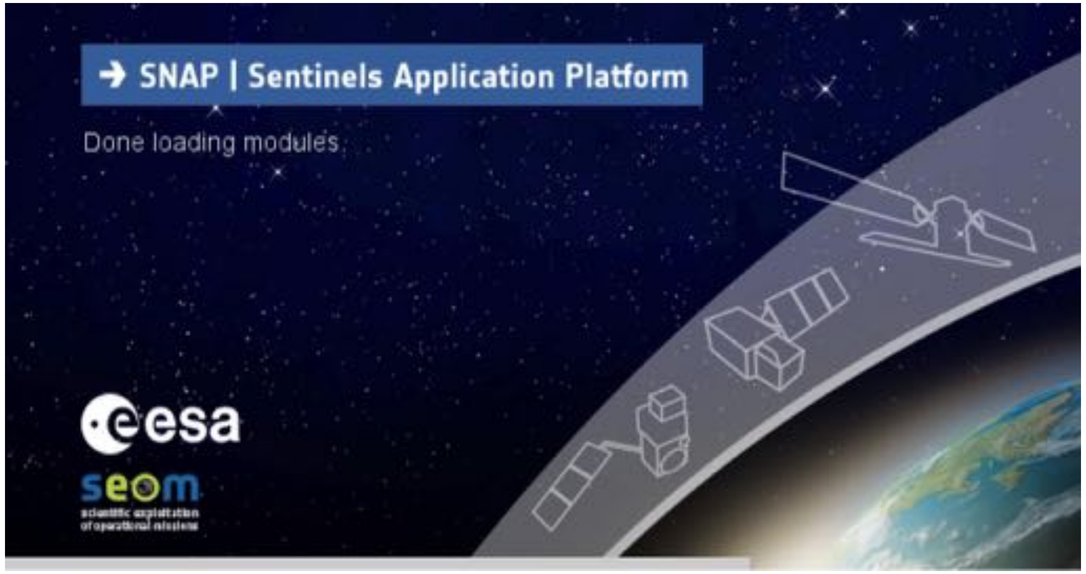
C2RCC Heritage

- Neural Network inversion of large database of simulated TOA radiances
  - Case2Regional, C2R
  - Doerffer & Schiller 2007 & 2008
  - Used in MERIS 3rd reprocessing for Case2 water branch

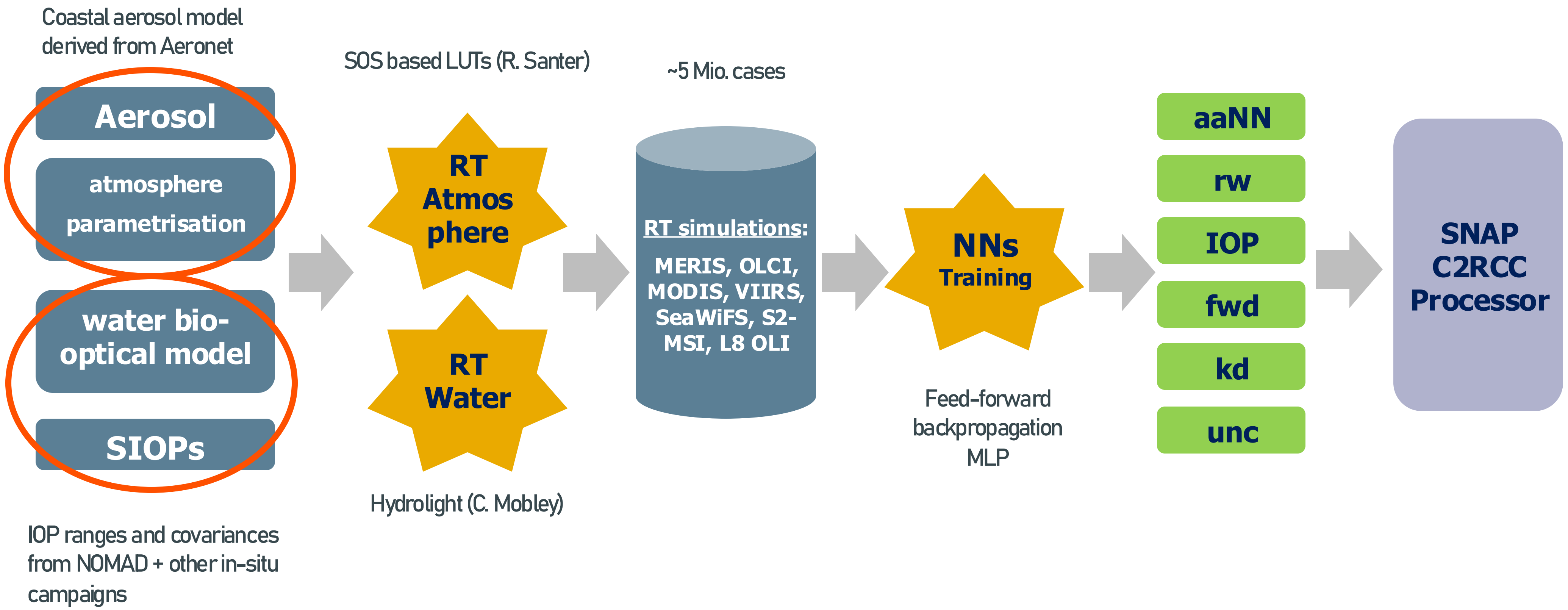
- Significant update through ESA CoastColour
  - C2RCC

Today

- Available through SNAP Sentinels Application Platform since 2016
- Open source within Optical Toolbox Kit
- Used in OLCI processing for Case2 water branch
- C2RCC community project



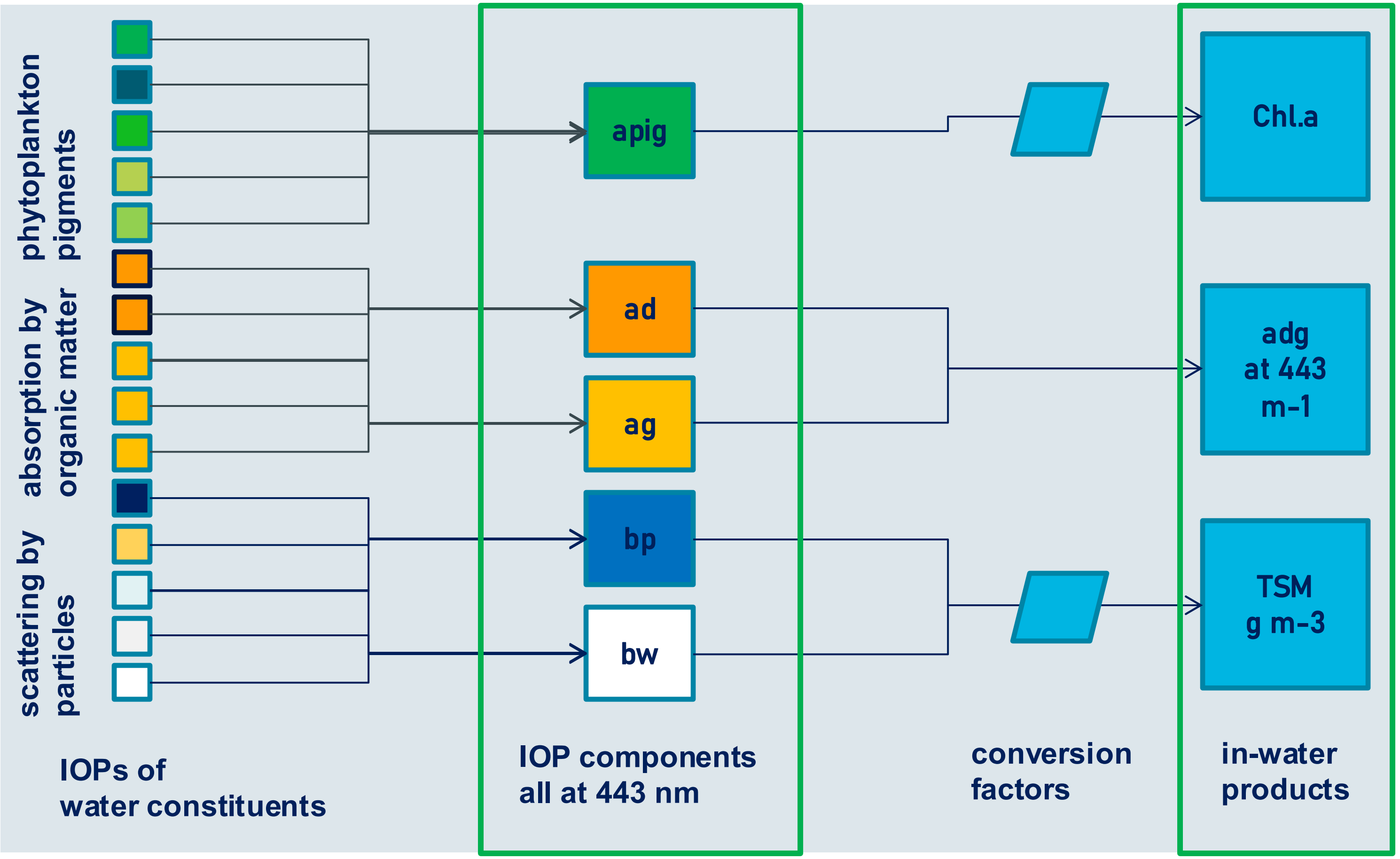
C2RCC Development



Source: Brockmann et al 2016 Evolution of the C2RCC Neural Network

Target: 5 IOP components

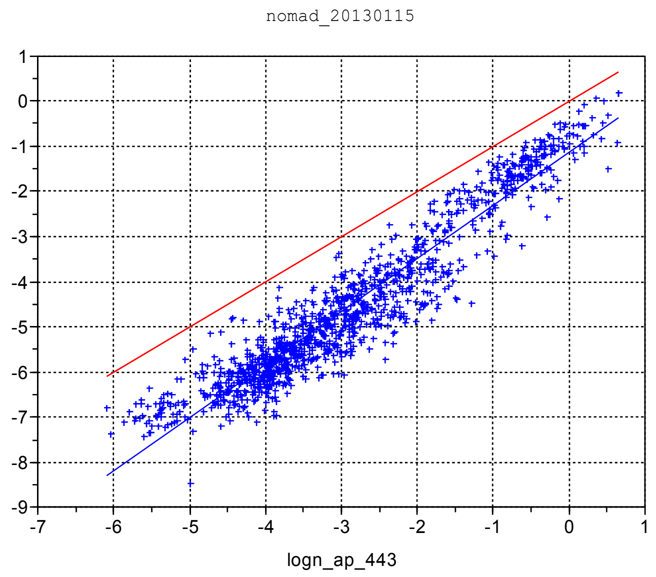
Bio-optical Model

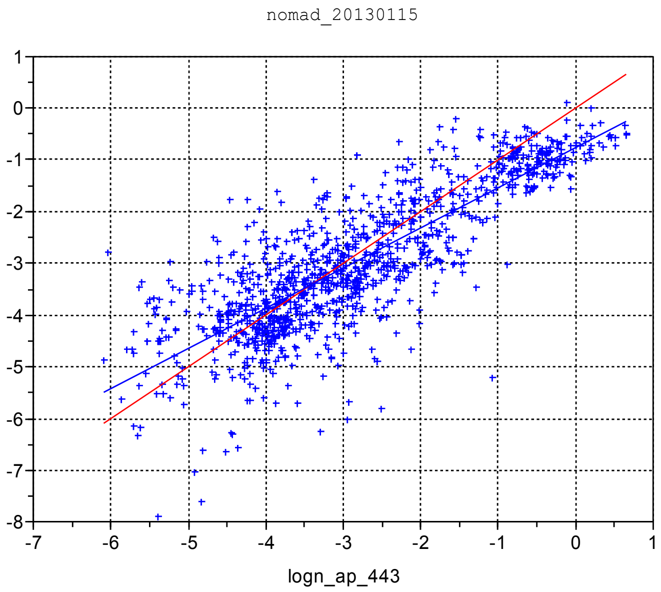


C2RCC product

OLCI L2 WFR product

Ranges and covariances are based on NOMAD analysis Example: a_det, a_pig and a_gelb, a_pig





Select **a_pig** randomly. Calculate **a_det** and **a_gelb** including random term for natural variability.

logn_ad_443 = logn_ap_443 * 1.172 - 1.152 +- 0.5
ad_443 =exp(logn_ap_443*1.172 -1.152 - 1 + rand*2.0)

logn_ag_443=logn_ap_443 * 0.775 – 0.77 +- 0.751
ag_443=exp(logn_ap_443*0.775 - 0.77 - 1.5 + rand*3.0)

Ranges are based on Aeronet analysis

Sun zenith angle	θ_s	[deg]	0 - 79.6
View zenith angle	θ_v	[deg]	0 - 45
View azimuth angle	ϕ_v	[deg]	0-180
Optical thickness at 550 nm of:	$\tau(550)$	[-]	
- maritime aerosols (99% relative humidity) in 0-2 km height			0 - 0.2
- urban aerosols (45% relative humidity) in 0-2 km height			0-0.5
- continental aerosols in 2-12 km height			0-0.165
- cirrus clouds in 8-11 km height			0.-0.3
- stratospheric aerosols in 12-50 km height:			0-0.5
Angstrom exponent of aerosols determined with τ_a:	$\alpha(490-870)$	[-]	0 - 2.4
Wind speed at 10 m	U_{10}	$[ms^{-1}]$	0-10
Air pressure at sea level	P	[hPa]	800-1040

Creating the atmosphere training data with *SOS* based LUTs (R. Santer):

- Create combinations of aerosols following natural distributions (combined to maximum τ550=0.8)
- Select water leaving reflectance spectrum as boundary condition (from HydroLight training data)
- Run simulations for different angles (sun and observation direction, including nadir view for normalisation), surface conditions (wind) at OLCI band wavelengths -> $5*10^6$ cases
  - *rTOSA*
  - *upwelling and downwelling transmittance*
  - *path radiance*

IOP Training Ranges

Ranges and covariances are based on NOMAD analysis

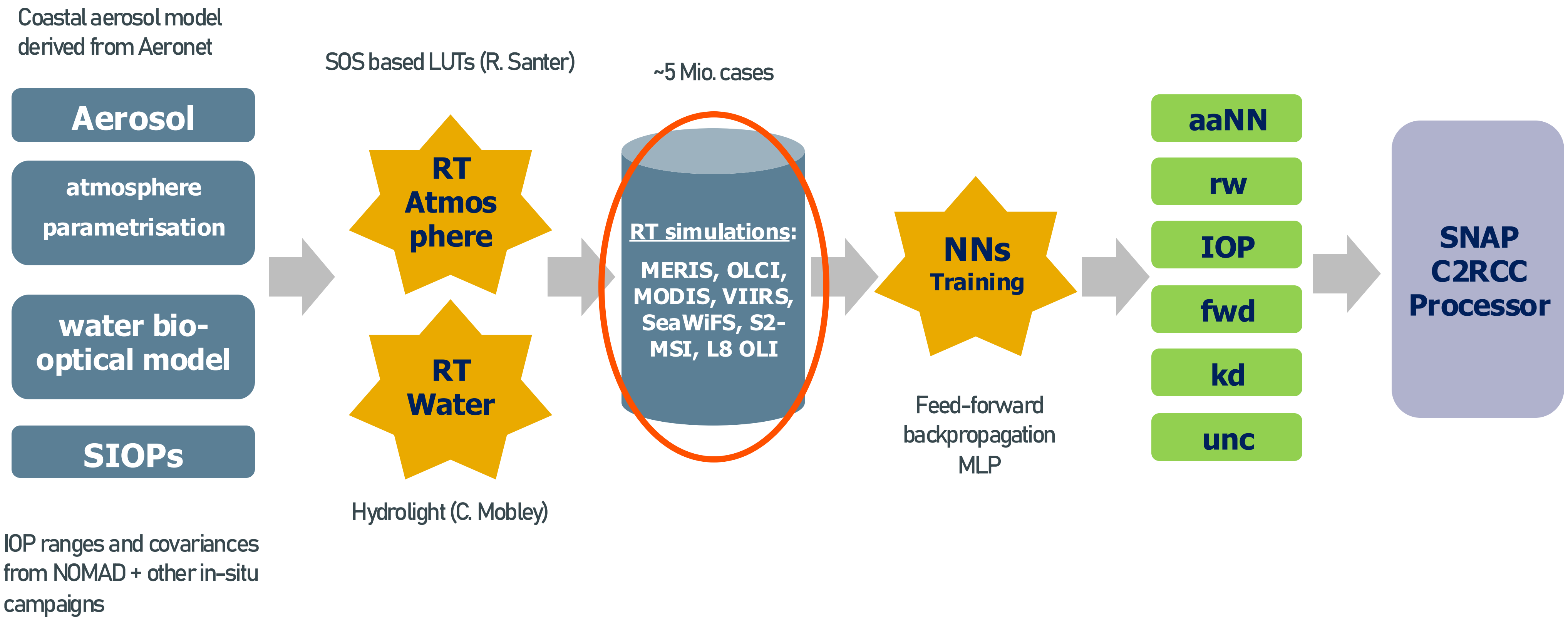
IOPs
- a_pig
- b_part
- a_det
- b_wit
- a_gelb

Wind speed at 10 m	U_{10}	$[ms^{-1}]$	0-10
Air pressure at sea level	P	[hPa]	800-1040
Sea Surface Temperature	SST	[deg C]	0-36
Sea Surface Salinity	SSS	[PSU]	0-43
Phytoplankton pigment absorption coefficient	$a_d 442$	$[m_1]$	0 -53.5
Particle scattering coefficient	$b_p 442$	$[m_1]$	0 - 589
Detritus (bleached particle) absorption coefficient	$a_d 442$	$[m_1]$	0 - 60
Detritus absorption wavelength exponent	S_d	$[m_1]$	0.008±0.005
White* particle scattering coefficient (* slope=0)	$b_w 442$	$[m_1]$	0 - 577
Gelbstoff (CDOM) absorption coefficient	$a_g 442$	$[m_1]$	0-60.0
Gelbstoff absorption wavelength exponent	S_g	$[m_1]$	0.014±0.002

Creating the in-water training data with *HydroLight* (C. Mobley):

- Create combinations IOPs following the natural distributions
- Select random specific phytoplankton absorption (mixture of 2 of 6 types)
- White scatterer (bwit) accounts for air bubbles, coccolithophores and sun glint.
- Run simulations of **rho_w** for different angles (sun and observation direction including nadir view for normalization), surface conditions (wind) at OLCI band wavelengths

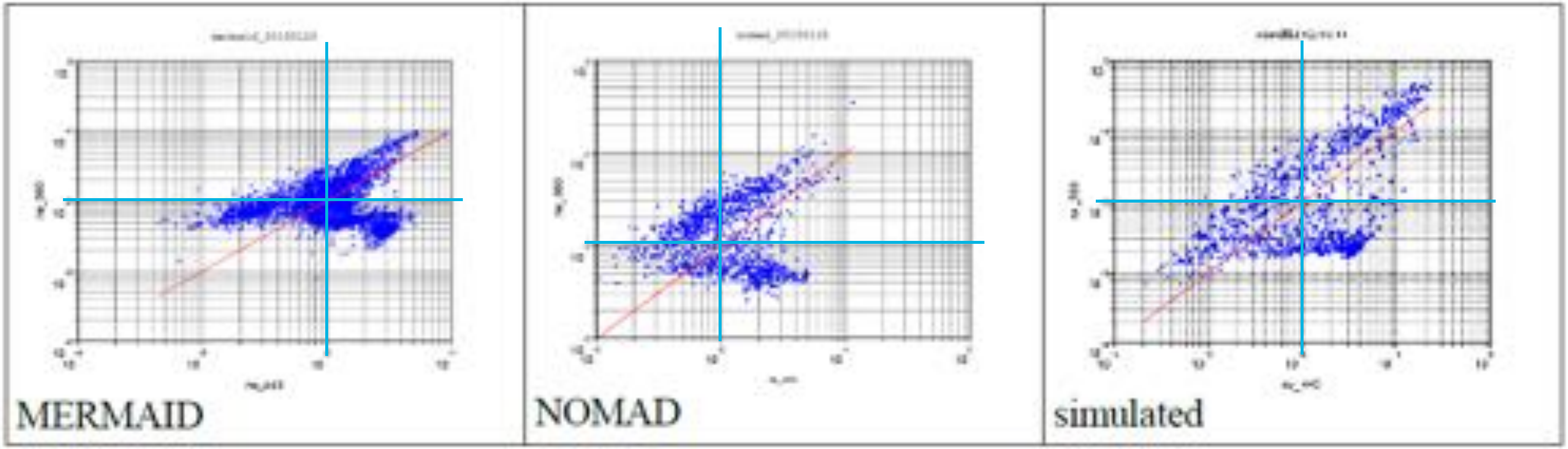
C2RCC Development



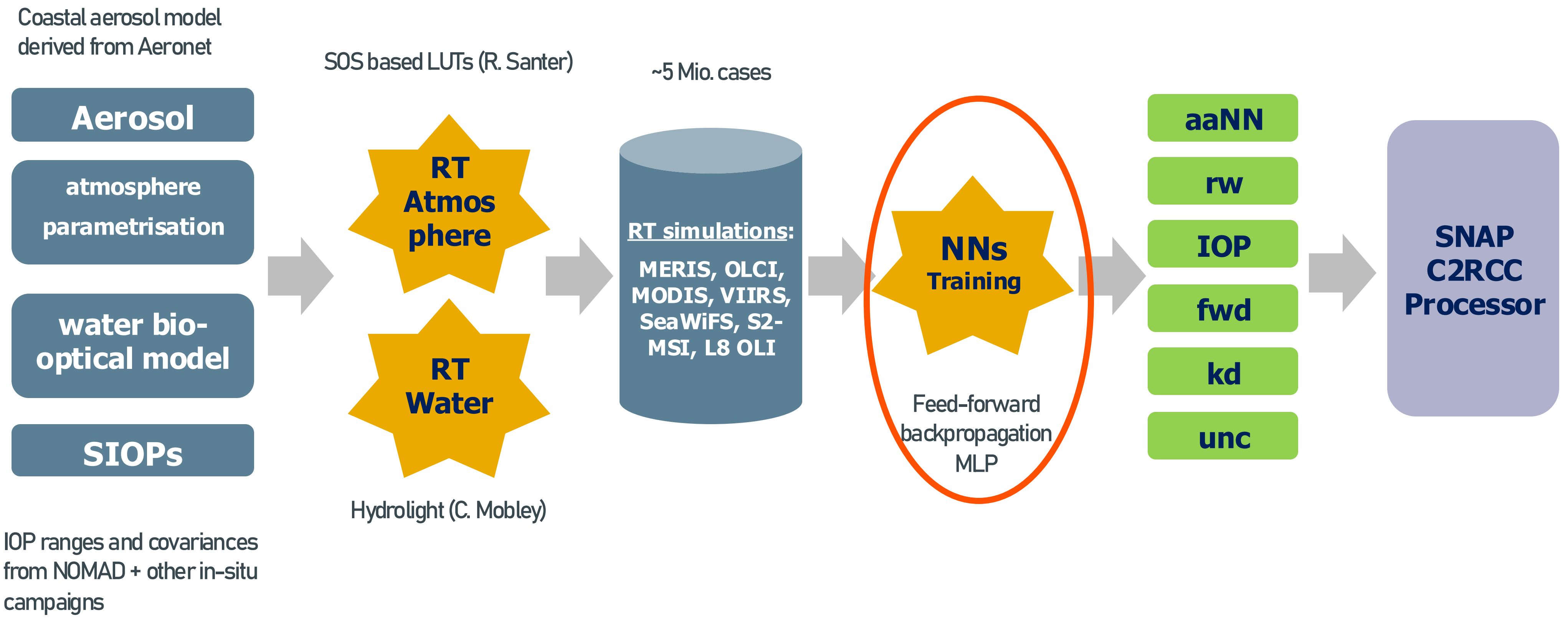
Source: Brockmann et al 2016 Evolution of the C2RCC Neural Network

Verification of in-water training data set

rho_w_560 vs rho_w_443, measured and simulated

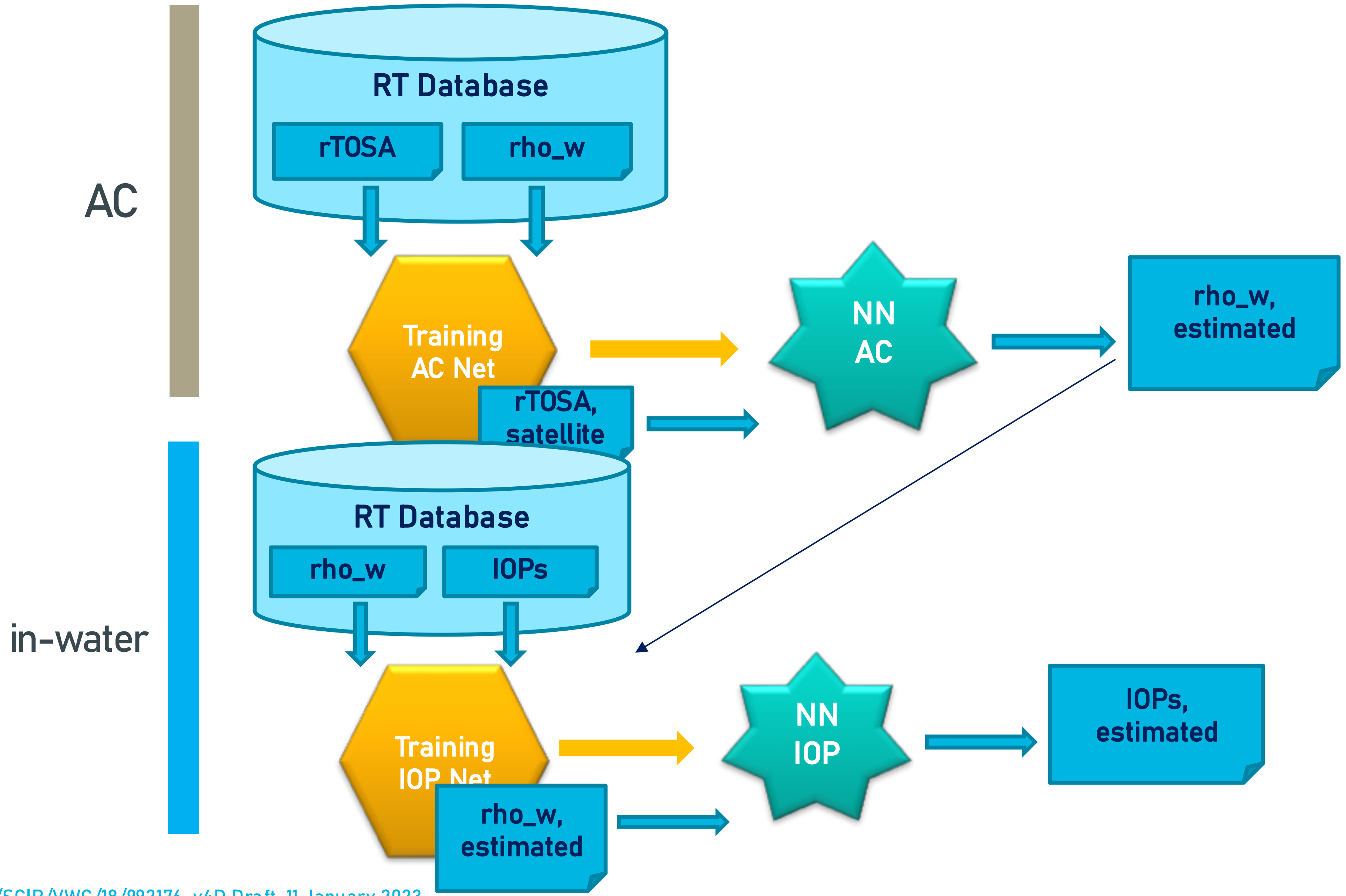


C2RCC Development



Source: Brockmann et al 2016 Evolution of the C2RCC Neural Network

NN training – Atmospheric correction AC + in-water



Inputs:
- rhow simulated with SOS
- rTosa from satellite
- rTosa simulated with SOS

Outputs:
- rhow_w estimated

Inputs:
- rhow simulated
- rhow_estimaded
- IOPs simulated

Outputs:
- IOPs_estimated

C2RCC Design - Overview

C2RCC processor is built as a combination of several Neural Networks trained for specific tasks.

Main parts

- Atmospheric correction AC:
  L1b TOA reflectance Rtoa to water leaving reflectance Rw
- Inversion in-water properties: water leaving reflectance to Inherent Optical Properties IOPs

Outputs

- AC
  - TOA reflectance Rtoa
  - water leaving reflectance Rw
  - normalised water leaving reflectance Rwn
  - *optional* path radiance, downwelling and upwelling transmittance Rpath, td, tu
  - Flags: Rtosa_oos, Rpath_oor
- in-water
  - IOPs
    - pigment, detritus and gelbstoff absorption at 443nm apig, adet, agelb
    - scattering coefficient of marine particles at 443nm bpart
    - scattering coefficient of white particles at 443nm bwit
    - and combinations detritus + gelbstoff adg, total absorption atot, total scattering btot
  - Uncertainties per IOP
  - Concentrations
    - Total suspended matter TSM as function of btot
    - Chlorophyll concentration as function of apig
  - Attenuation
    - Irradiance attenuation coefficient at 489nm kd489
    - kdmin
    - kd_z90max
  - Flags

AC

in-water

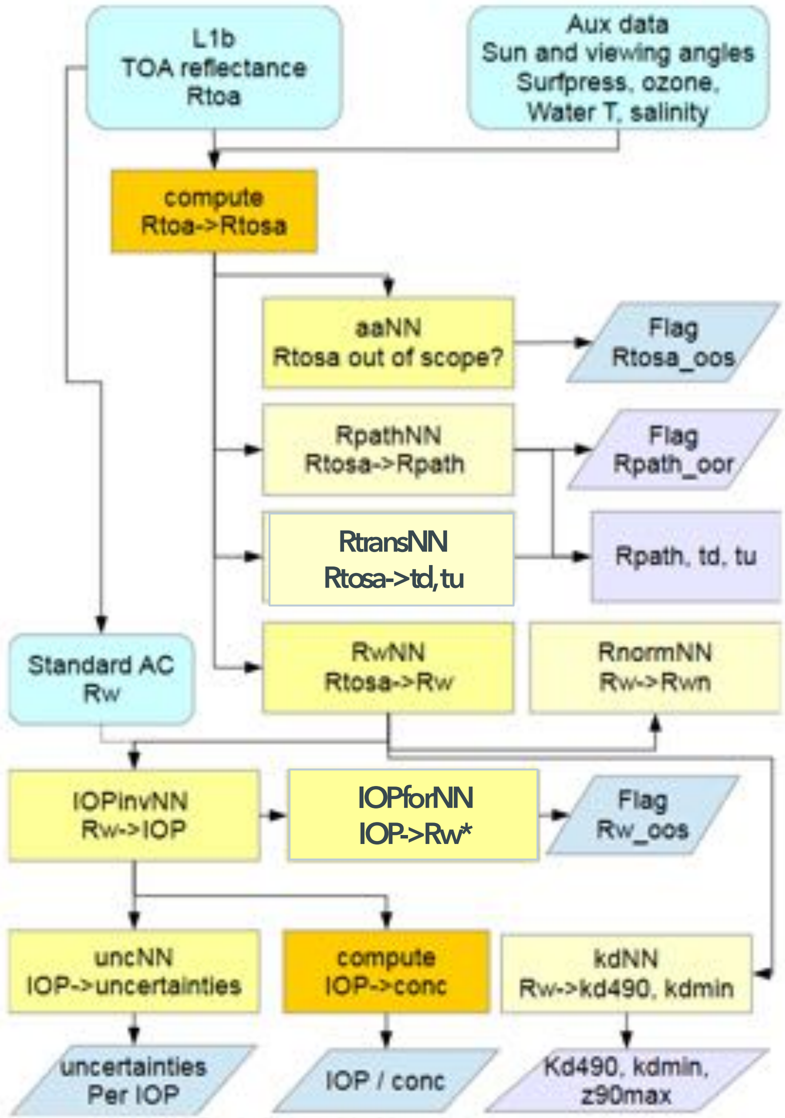
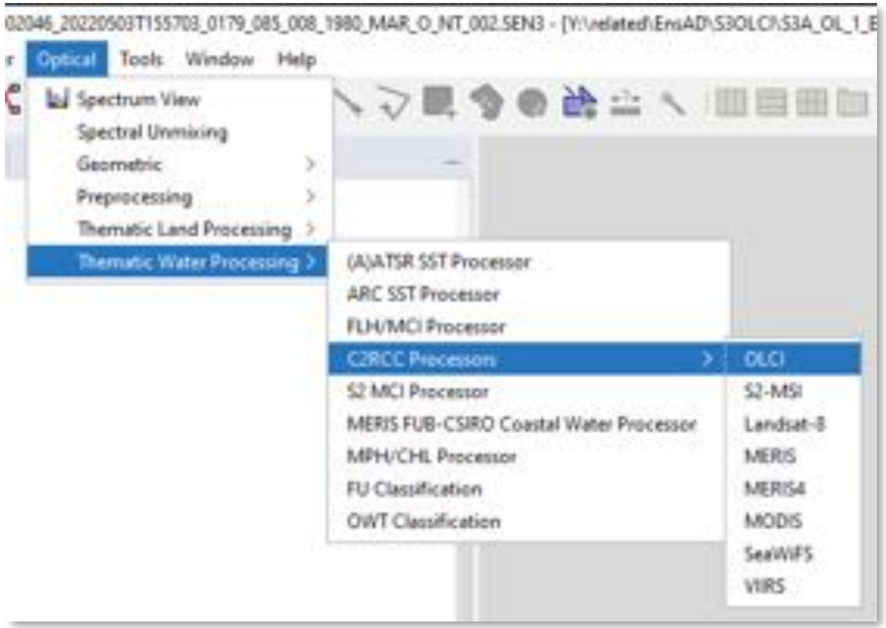
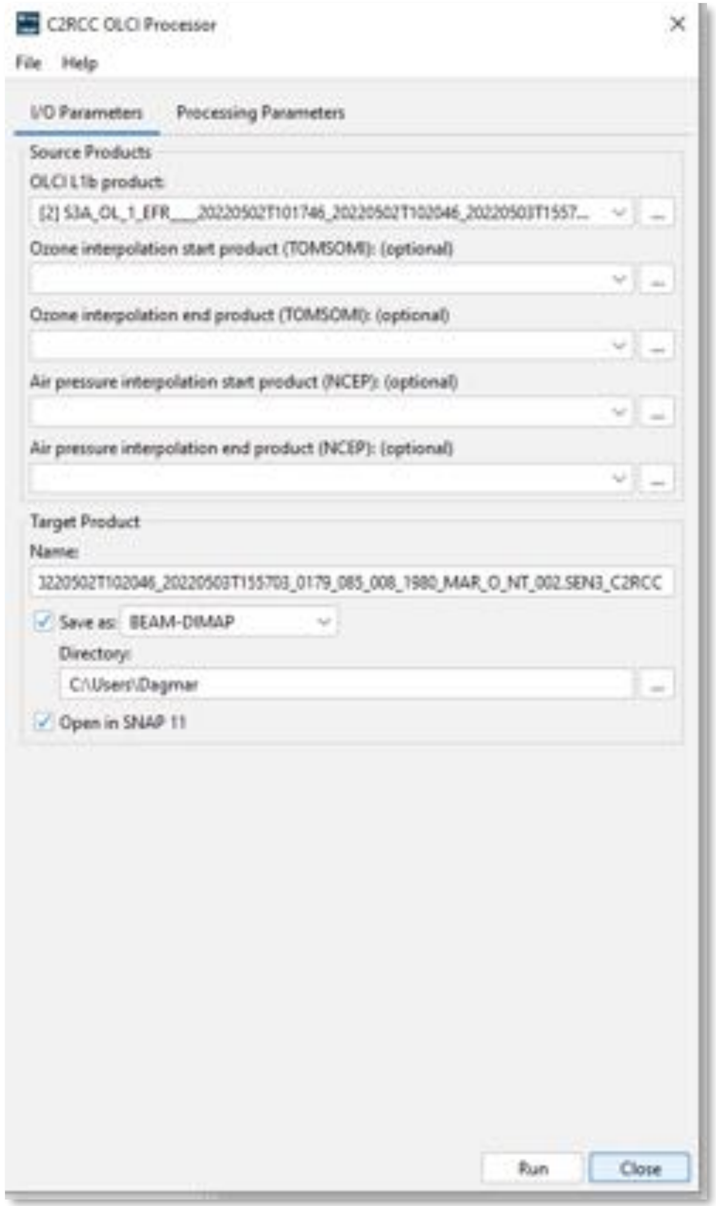


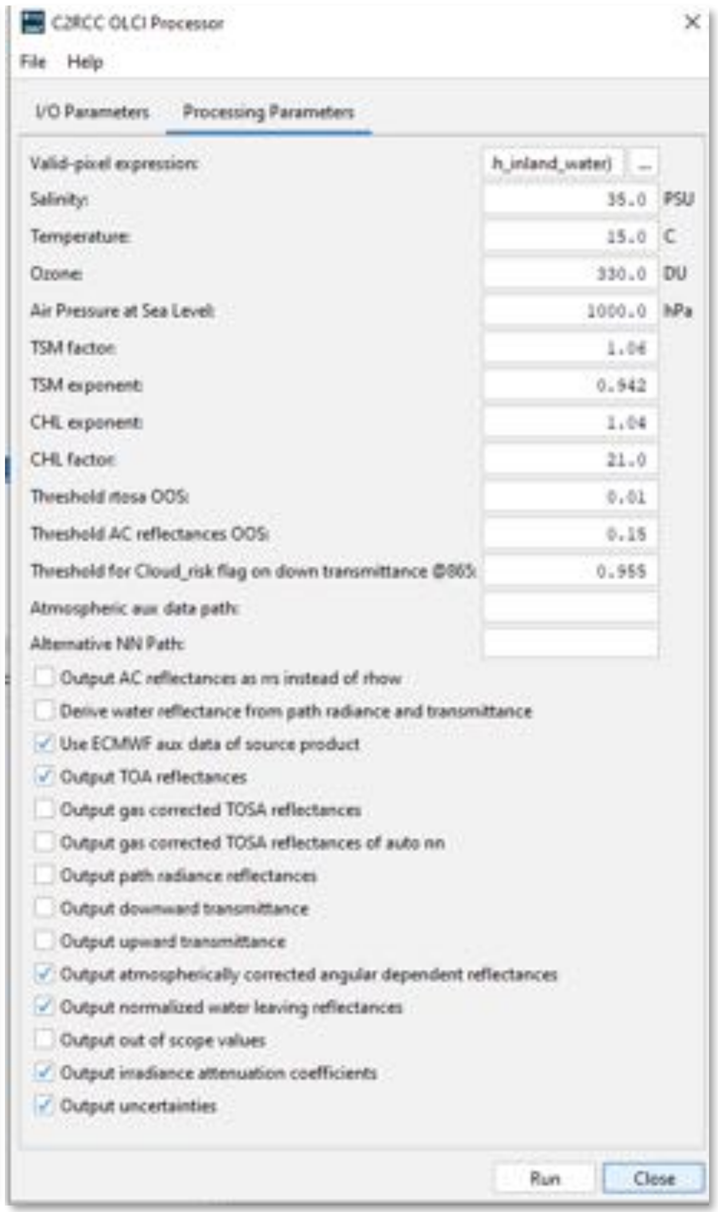
Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc.

C2RCC – Processing with SNAP







SNAP includes an implementation of the C2RCC Processor for sensors

- Sentinel 3 OLCI
- Sentinel 2 MSI
- Landsat-8
- MERIS (3rd reprocessing)
- MERIS (4th reprocessing)
- MODIS
- SeaWiFS
- VIIRS

Atmospheric Correction – RwNN

Atmospheric correction starts with the translation of TOA radiance into reflectance Rtoa.

Rtoa undergoes **gas correction** to standard atmosphere **Rtosa**:

- Water vapour correction at 709nm
- Ozone correction all bands

Water leaving reflectance Rw is calculated with a dedicated NN from Rtosa.

Water leaving reflectance NN RwNN

- OLCI: 23 inputs, 3 fully connected hidden layers (33x23x13), 16 outputs
- **Input**: Rtosa (16 bands) + Pressure corrected to sea level + geometry, T, S
- **Output**: Rw (16 bands)

Radiative Transfer Simulations are used as training data. A wide range of sun and observations angles, aerosol properties and boundary conditions.

Aerosol optical thickness can have a maximum of τ(550nm)=0.8, combining maritime, urban, continental aerosols with cirrus clouds and stratospheric aerosols.

AC

in-water

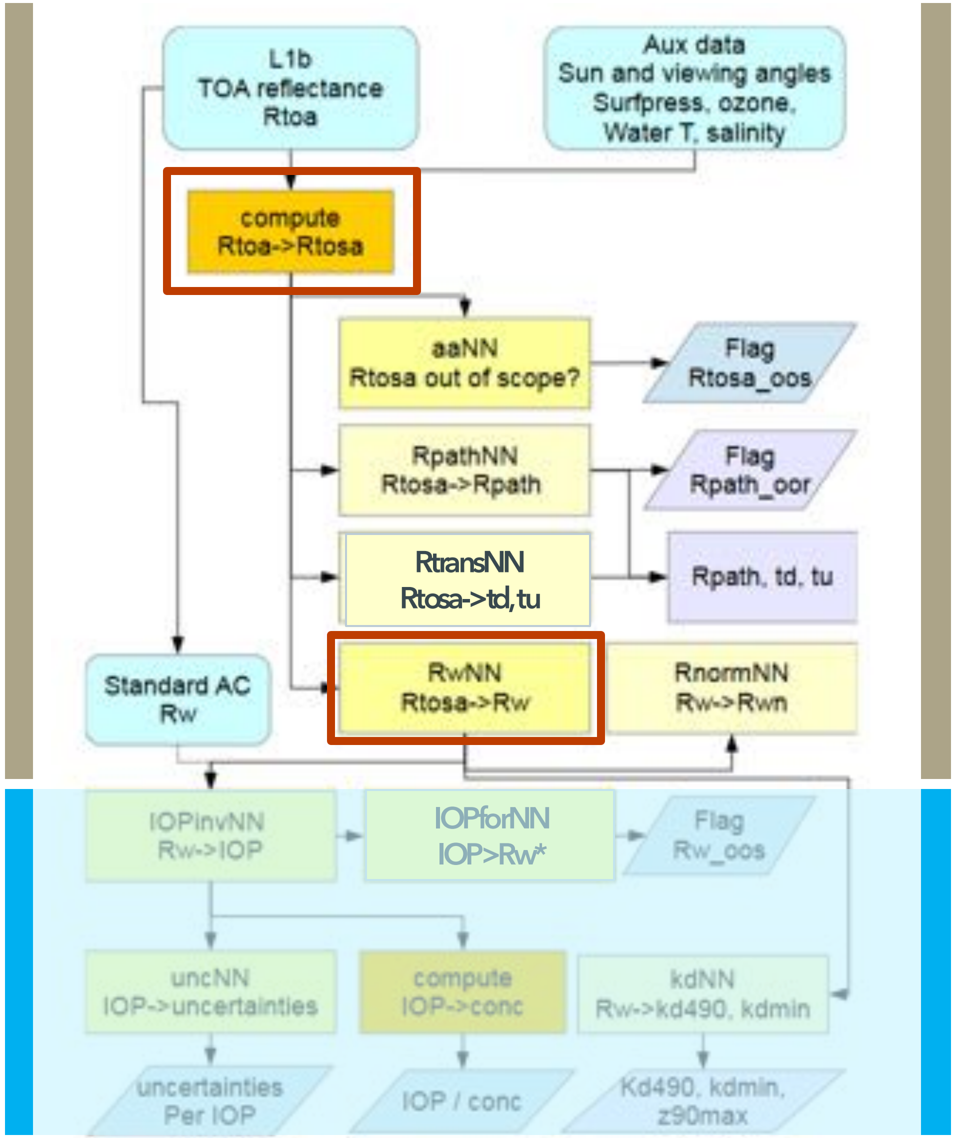


Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

Atmospheric Correction – RnormNN

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Aerosol optical thickness can have a maximum of τ(550nm)=0.8, combining maritime, urban, continental aerosols with cirrus clouds and stratospheric aerosols.

Normalised Water leaving reflectance NN RnormNN

- OLCI: 17 inputs, 3 fully connected hidden layers (77x77x77), 12 outputs
- **Input**: Rw (12 bands) + geometry, T, S
- **Output**: Rwn (12 bands)

All reflectances are trained in log-transform, both in input and output.
Therefore, C2RCC always generates non-negative reflectance values.

AC

in-water

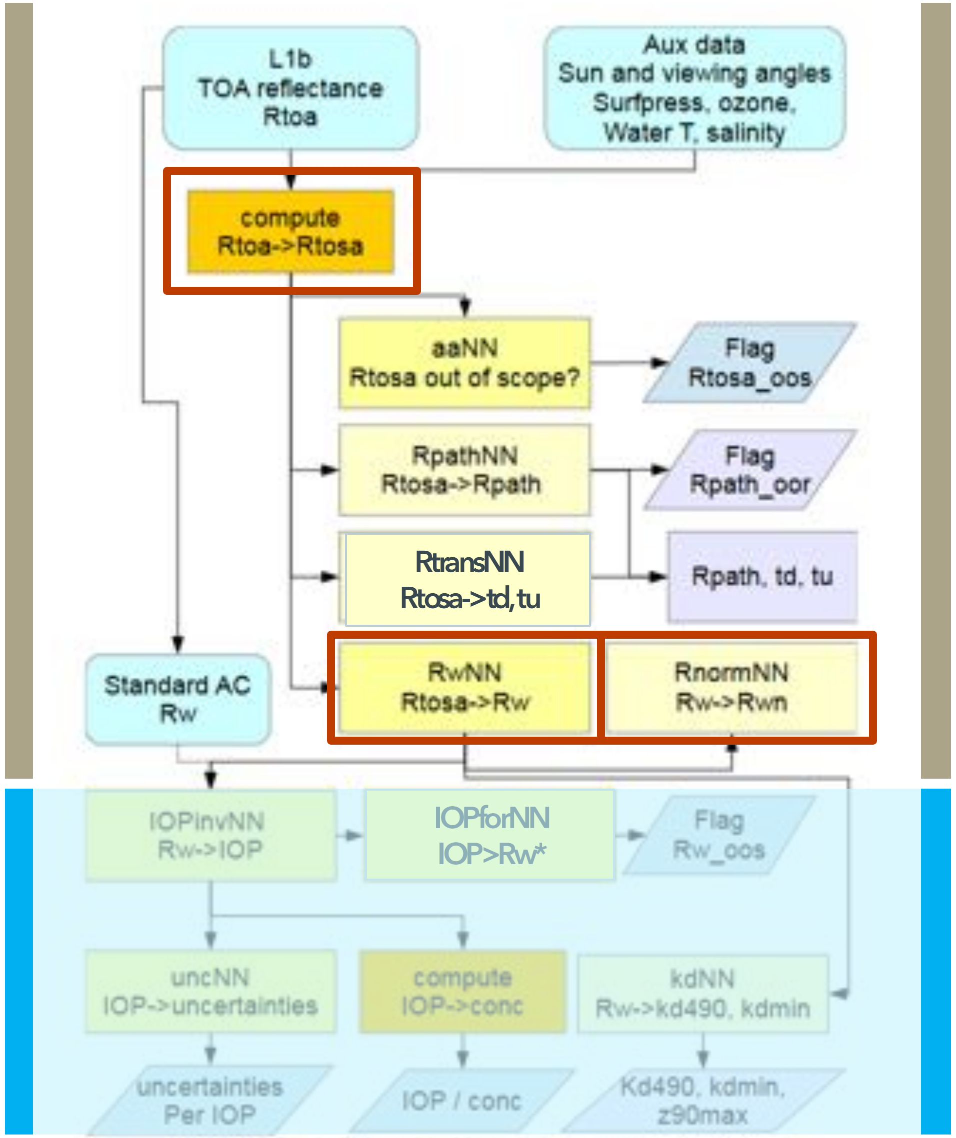


Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

Atmospheric Correction – Flag Rtosa_oos

Auto-associative Neural Network aaNN

- Bottleneck architecture
- OLCI: 23 inputs, 3 fully connected hidden layers (31x7x31), 16 outputs
- **Input**: Rtosa (16 bands) + Pressure corrected to sea level + geometry, T, S
- **Output**: Rtosa (16 bands)

The flag out of scope Rtosa_oos is raised, if the output spectrum is not similar to the input spectrum. The aaNN learns amplitudes and shapes of the spectra in the training data and reproduces them accurately.

If deviation is large, the input spectrum has not been part of the training dataset and therefore the following NNs will not be able to provide reasonable answers to the task of atmospheric correction.

AC

in-water

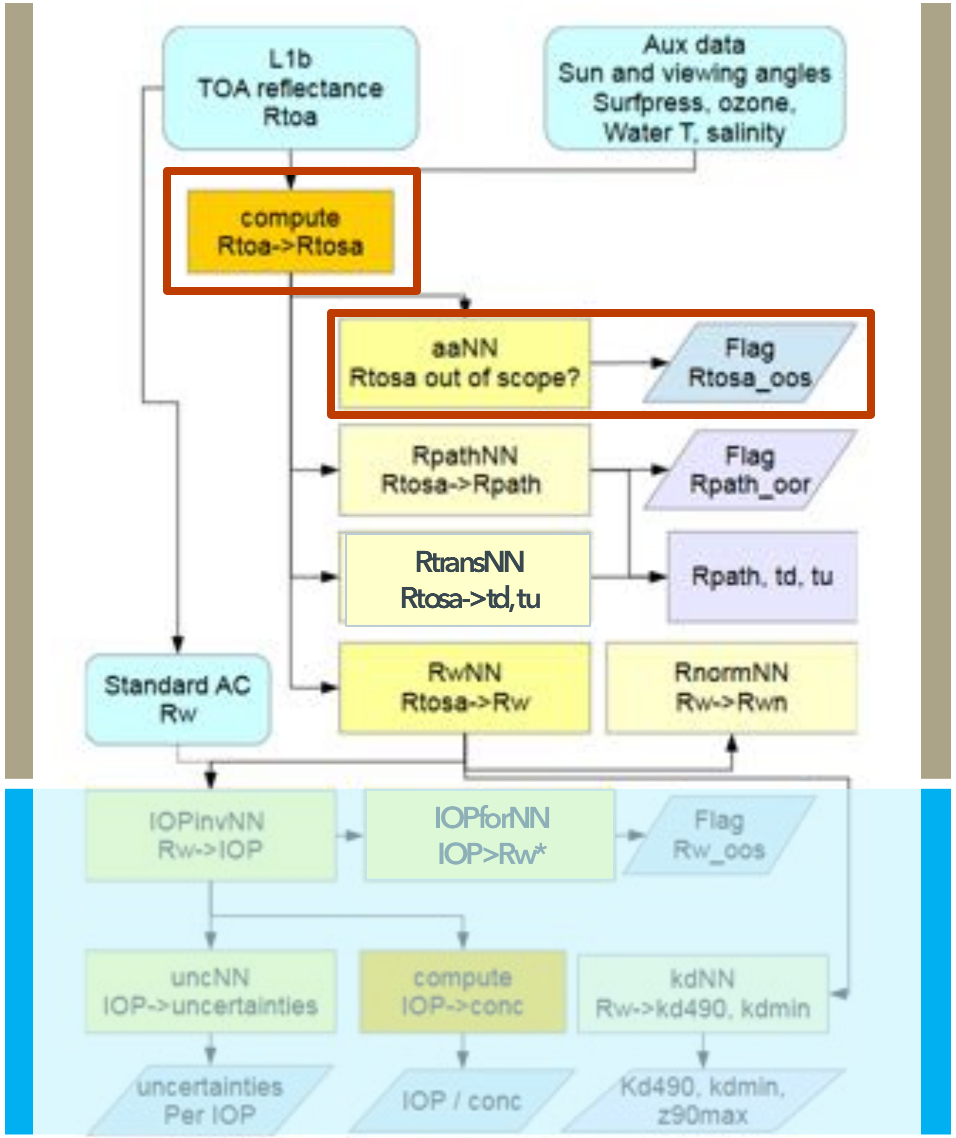


Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

Path radiance and atmospheric downwelling and upwelling transmittance is calculated by two NNs from Rtosa. (*Optional*)

Path Radiance NN RpathNN

- OLCI: 23 inputs, 3 fully connected hidden layers (31x37x37), 16 outputs
- **Input**: Rtosa (16 bands) + Pressure corrected to sea level + geometry, T, S
- **Output**: Rpath (16 bands)

Transmittance NN RtransNN

- OLCI: 23 inputs, 3 fully connected hidden layers (31x37x37), 16 outputs
- **Input**: Rtosa (16 bands) + Pressure corrected to sea level + geometry, T, S
- **Output**: transd (16 bands) + transu (16 bands)

Cloud_risk flag: trans_d(865nm) < 0.955

Optional output: Water leaving reflectance from path radiance and transmittance

AC

in-water

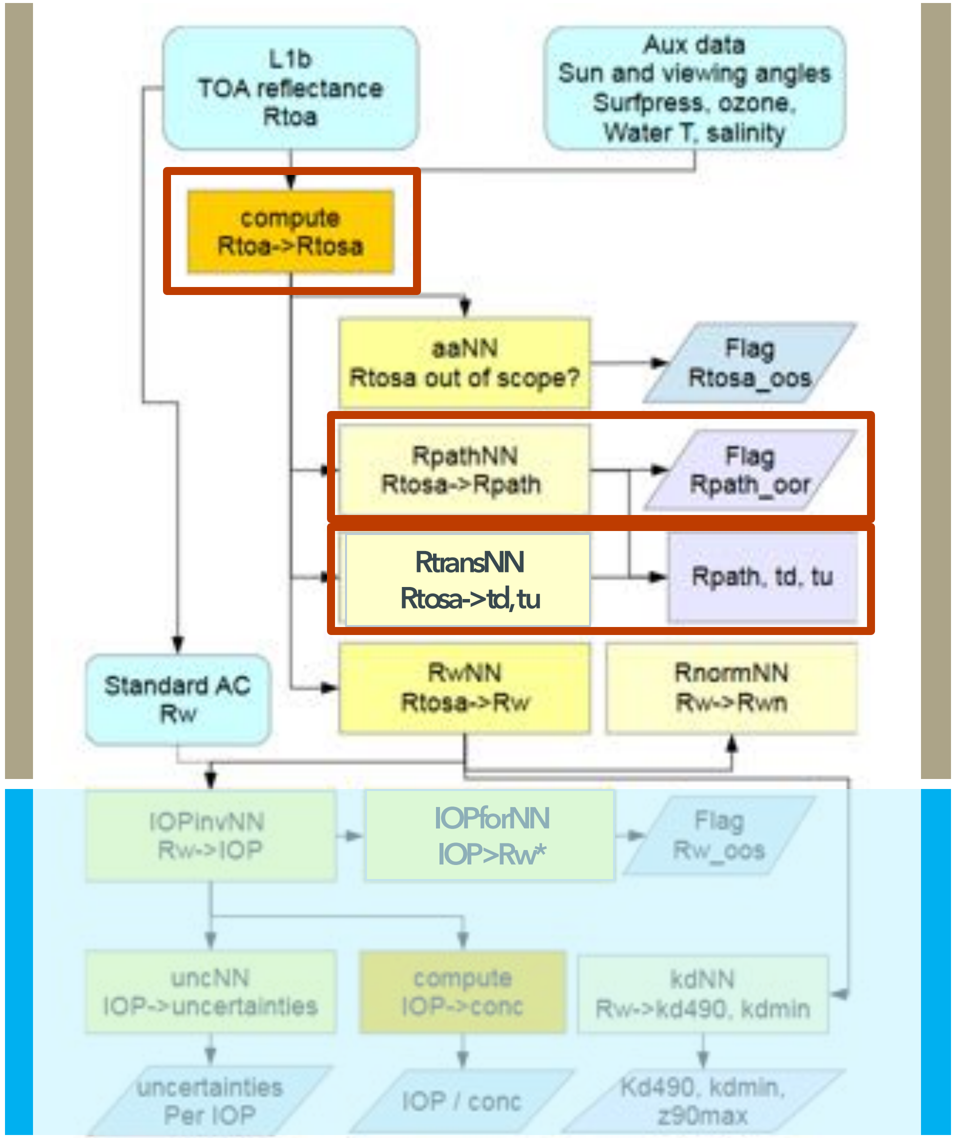
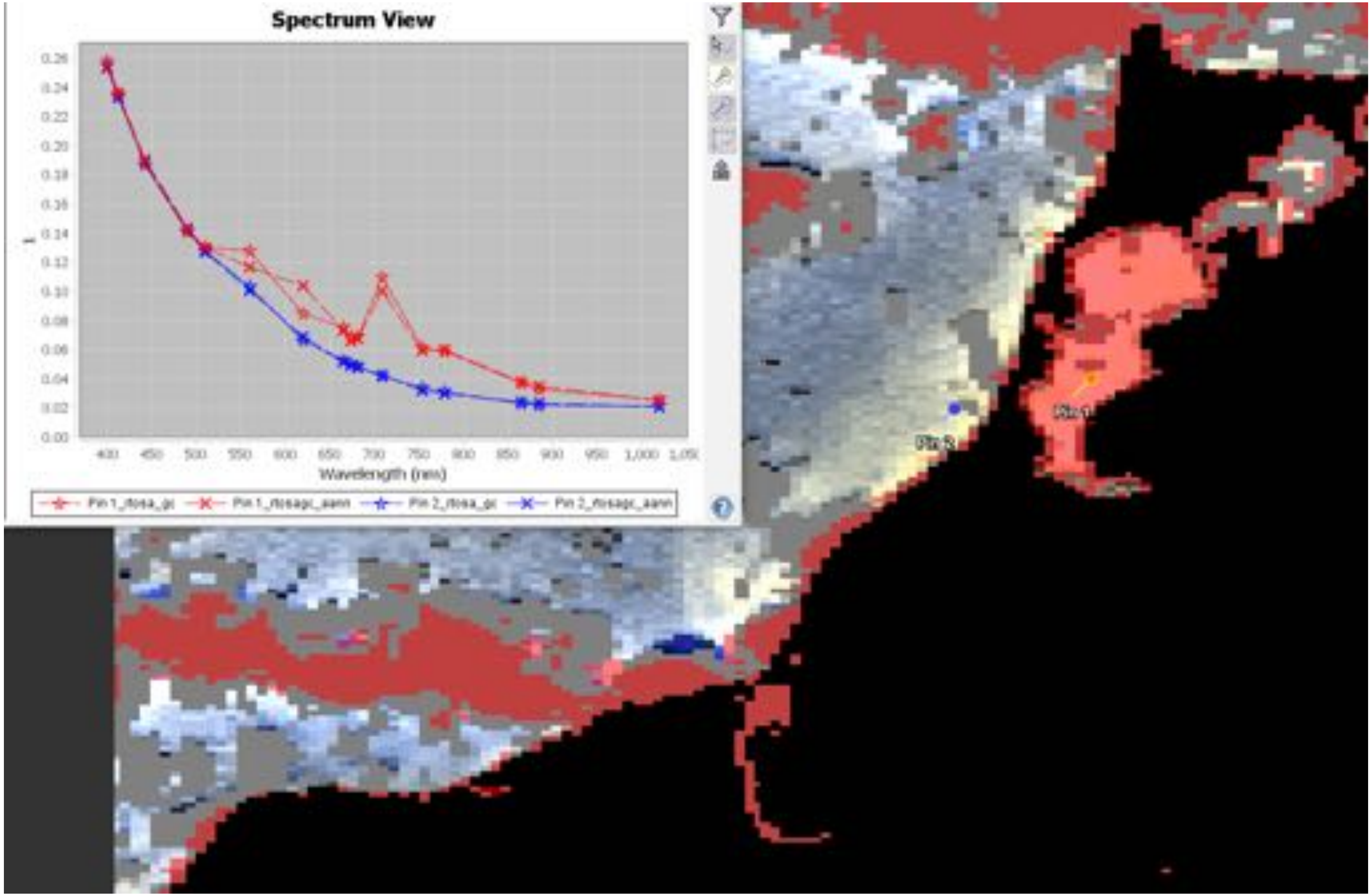


Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

Atmospheric Correction – Example C2RCC Flags



Example:

- **rtosa_oos flag (red)**
- **cloud_risk flag (grey)**

Gas corrected TOA spectrum compared to aaNN result of this spectrum.

Spectrum in the Saaler Bodden (**Pin 1**) with strong cyanobacteria bloom cannot be reconstructed sufficiently by the aaNN.

Spectrum in the Baltic Sea (**Pin 2**) shows good agreement between TOAgc and its counterpart from the aaNN. These kind of spectra have been part of the training dataset and AC can be applied here and is expected to be successful.

In-water Processing - IOPinvNN

Inverting the water leaving reflectance into inherent optical properties is the main task in the in-water processing.

Inherent Optical Properties Inversion NN IOPinvNN

- OLCI: 17 inputs, 3 fully connected hidden layers (37x37x37), 5 outputs
- **Input**: Rw (12 bands, 400-754nm) + geometry, T, S
- **Output**: apig, adet, agelb, bpart, bwit at 443nm

Radiative Transfer Simulations with HydroLight built the training dataset.

Reflectances and IOPs are trained in log-transformed state to avoid negative values and emphasize small values.

Mixtures of different specific phytoplankton absorption functions have been used to accommodate a large variety of algae groups.

The white scatterer (bwit) accounts for air bubbles, coccolithophores and sun glint.

water (surface) parameters

Wind speed at 10 m	U_{10}	$[ms^{-1}]$	0-10
Air pressure at sea level	P	[hPa]	800-1040
Sea Surface Temperature	SST	[deg C]	0-36
Sea Surface Salinity	SSS	[PSU]	0-43
Phytoplankton pigment absorption coefficient	a_d442	$[m_1]$	0 -53.5
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Detritus absorption wavelength exponent	S_d	$[m_1]$	0.008±0.005
White* particle scattering coefficient (* slope=0)	b_w442	$[m_1]$	0 - 577
Gelbstoff (CDOM) absorption coefficient	a_g442	$[m_1]$	0-60.0
Gelbstoff absorption wavelength exponent	S_g	$[m_1]$	0.014±0.002

in-water

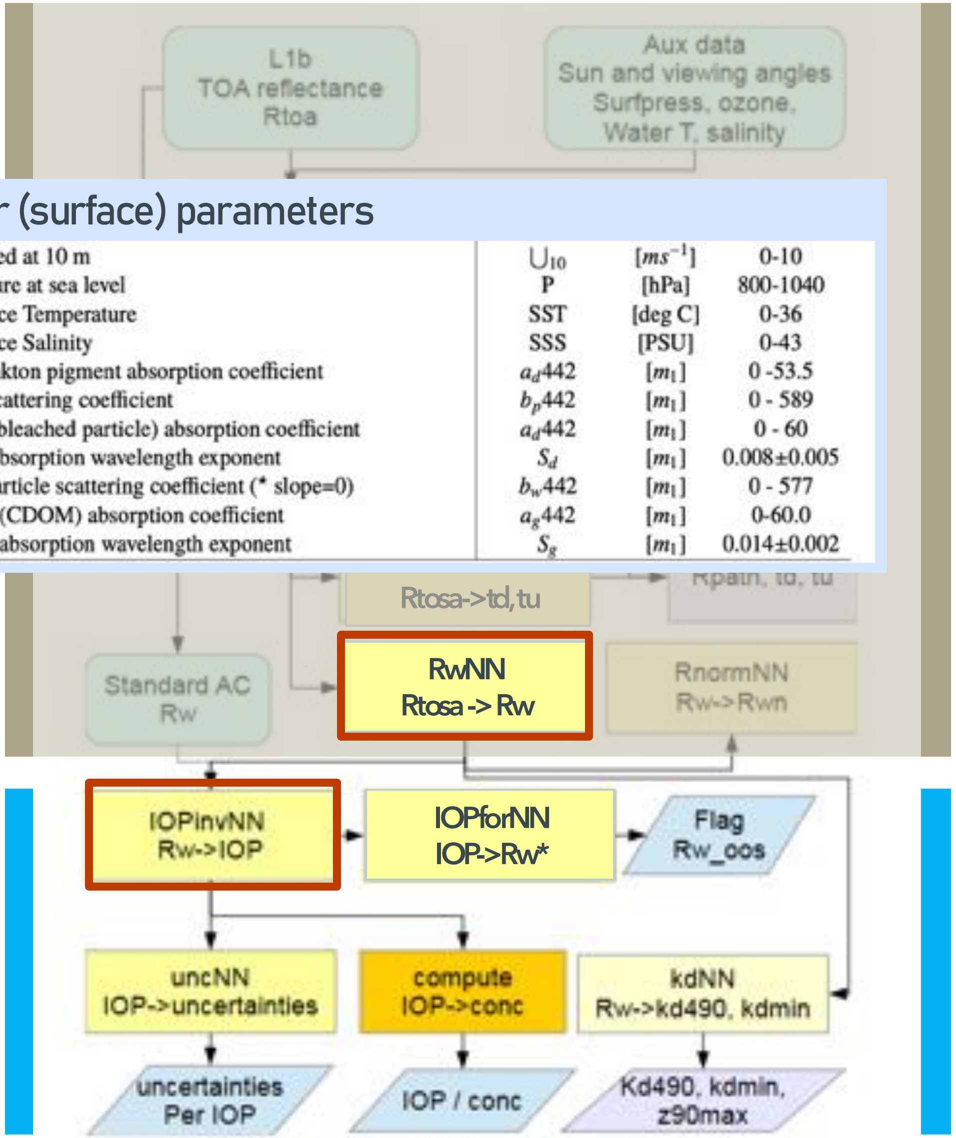


Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

In-water Processing – IOP conversion

TSM and **chlorophyll concentrations** are calculated by empirical relationships of **apig** and **btot**. Derived from NOMAD database and measurements in the North Sea.

$$TSM[\frac{g}{m^3}] = 1.06 * b_{tot}^{0.942}$$

$$Chl\left[\frac{\mu g}{l}\right] = 21.0 * a_{pig}^{1.04}$$

TSM and Chl can easily be adapted to regional conditions, if in-situ data is available and new relationships with apig and btot can be derived.

Non-phytoplankton absorption at 443nm (from dissolved constituents and detritus):

$$a_{dg}(443nm)[m^{-1}] = a_{gelb}(443nm) + a_{det}(443nm)$$

AC

in-water

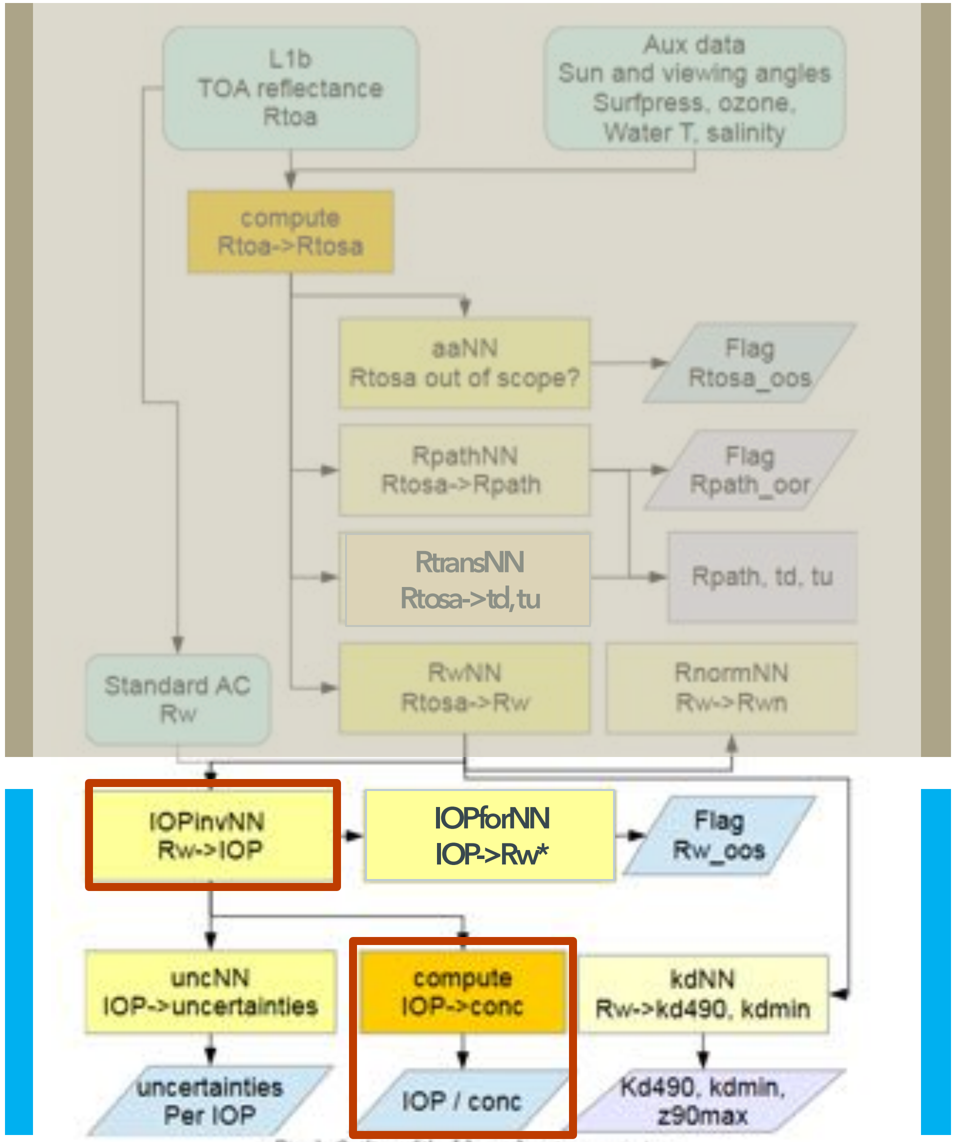


Fig. 1: Outline of the L2 case2 water processing

Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

In-water Processing – Flag Rw_oos

C2RCC contains a forward NN, which emulates the bio-optical simulations of the physical model.

Forward NN IOPforNN

- OLCI: 10 inputs, 3 fully connected hidden layers (77x77x77), 12 outputs
- **Input**: apig, adet, agelb, bpart, bwit at 443nm + geometry, T, S
- **Output**: Rw* (12 bands) -> *Flag Rw_oos*

Training is done with log-transformed IOPs as input and Rws as output. Only non-negative values will be derived.

Definition: Rw out of scope flag

Band ratios Rw $s1 = \frac{Rw560}{Rw420}, s2 = \frac{Rw620}{Rw560}$

Band ratios Rw* $s1^* = \frac{Rw^*560}{Rw^*420}, s2^* = \frac{Rw^*620}{Rw^*560}$

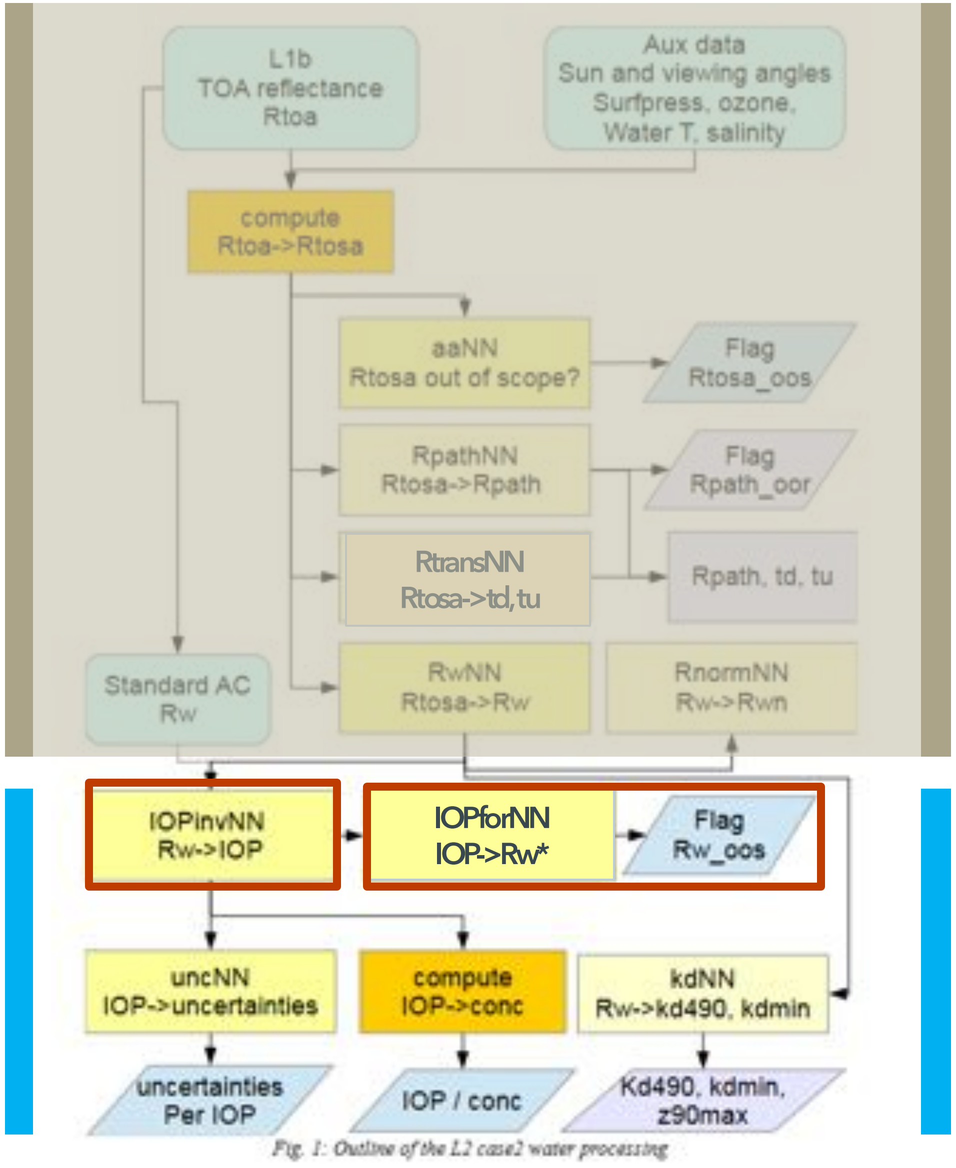
$$\text{test} = \max(|s1 - s1^*|, |s2 - s2^*|)$$

if test > 0.15 : Rw_oos raised

slopes of spectra are compared!

AC

in-water



Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

C2RCC Design – In-water Processing IV

C2RCC derives a set of "uncertainties" per IOP.

IOP Uncertainty NN uncNN

- OLCI: 5 inputs, 3 fully connected hidden layers (77x77x77), 5 outputs
- **Input**: apig, adet, agelb, bpart, bwit at 443nm
- **Output**: uncertainty for apig, adet, agelb, bpart, bwit at 443nm

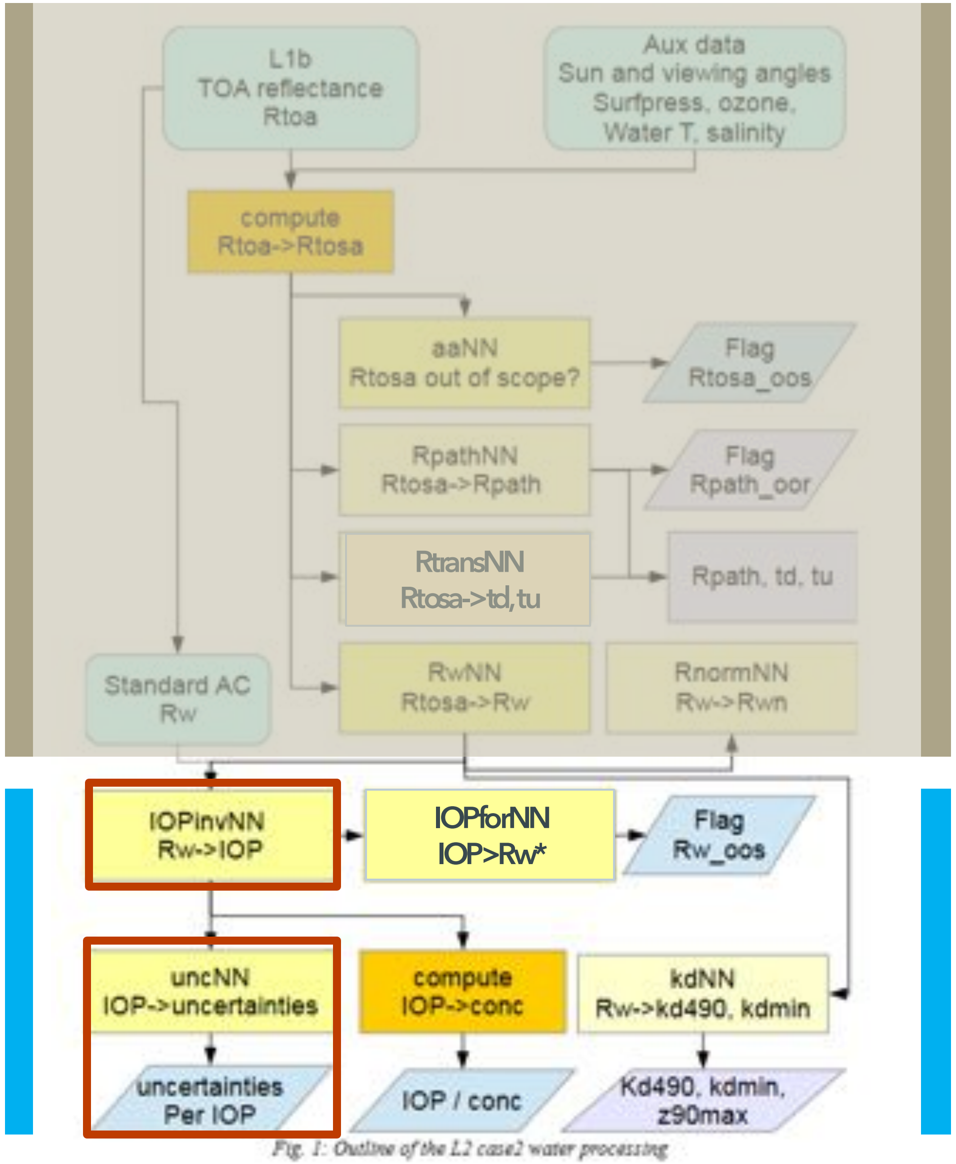
Definition:

$$Error = \|\log IOP_{train} - \log IOP_{NN}\|$$

The uncNN is trained with the absolute differences of log-transformed IOPs based on the simulated data set. IOP_train are the inputs of the simulated data, the simulated spectrum is inverted by the IOPinvNN and the IOP_NN are derived.

AC

in-water



Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

C2RCC Design – Uncertainties IOPs

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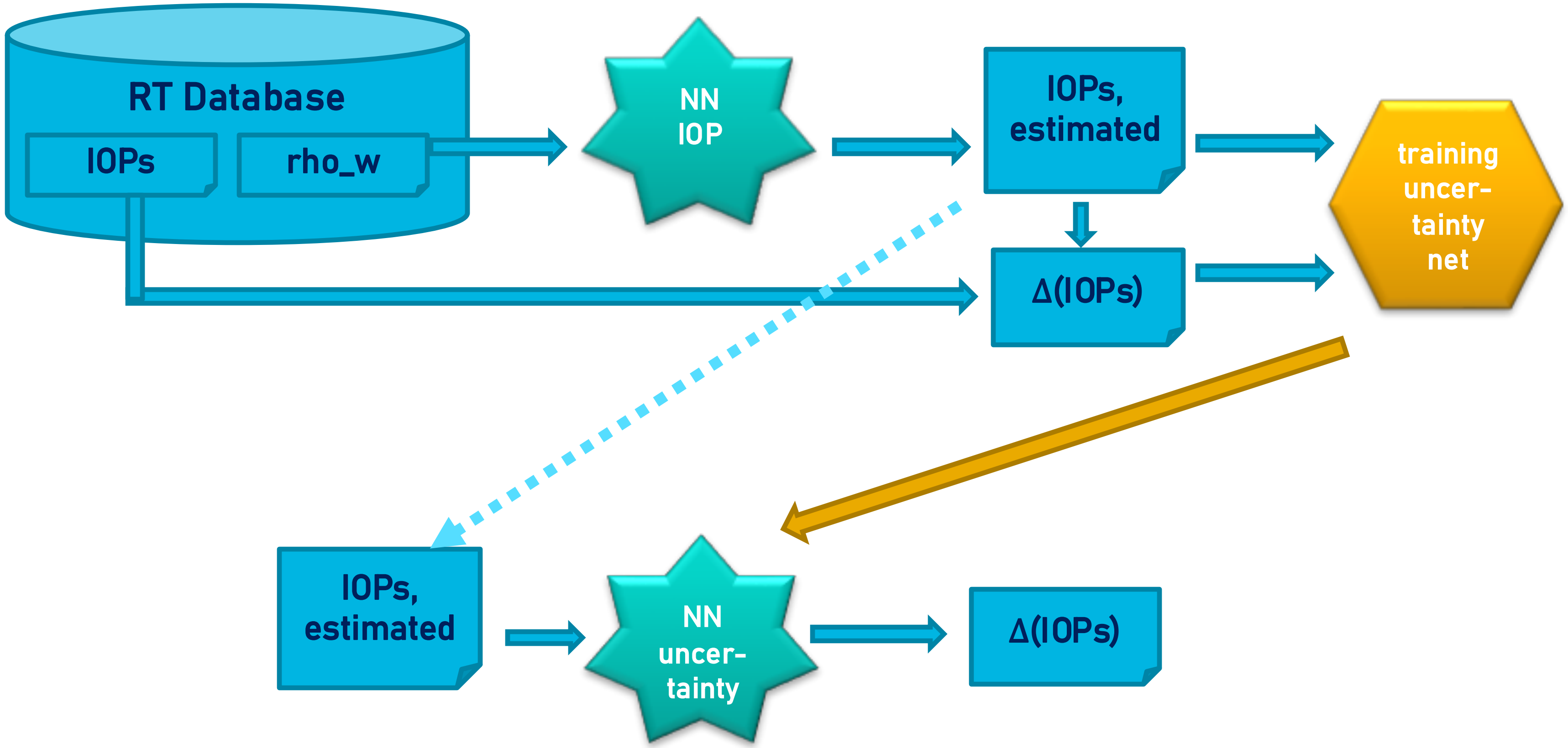


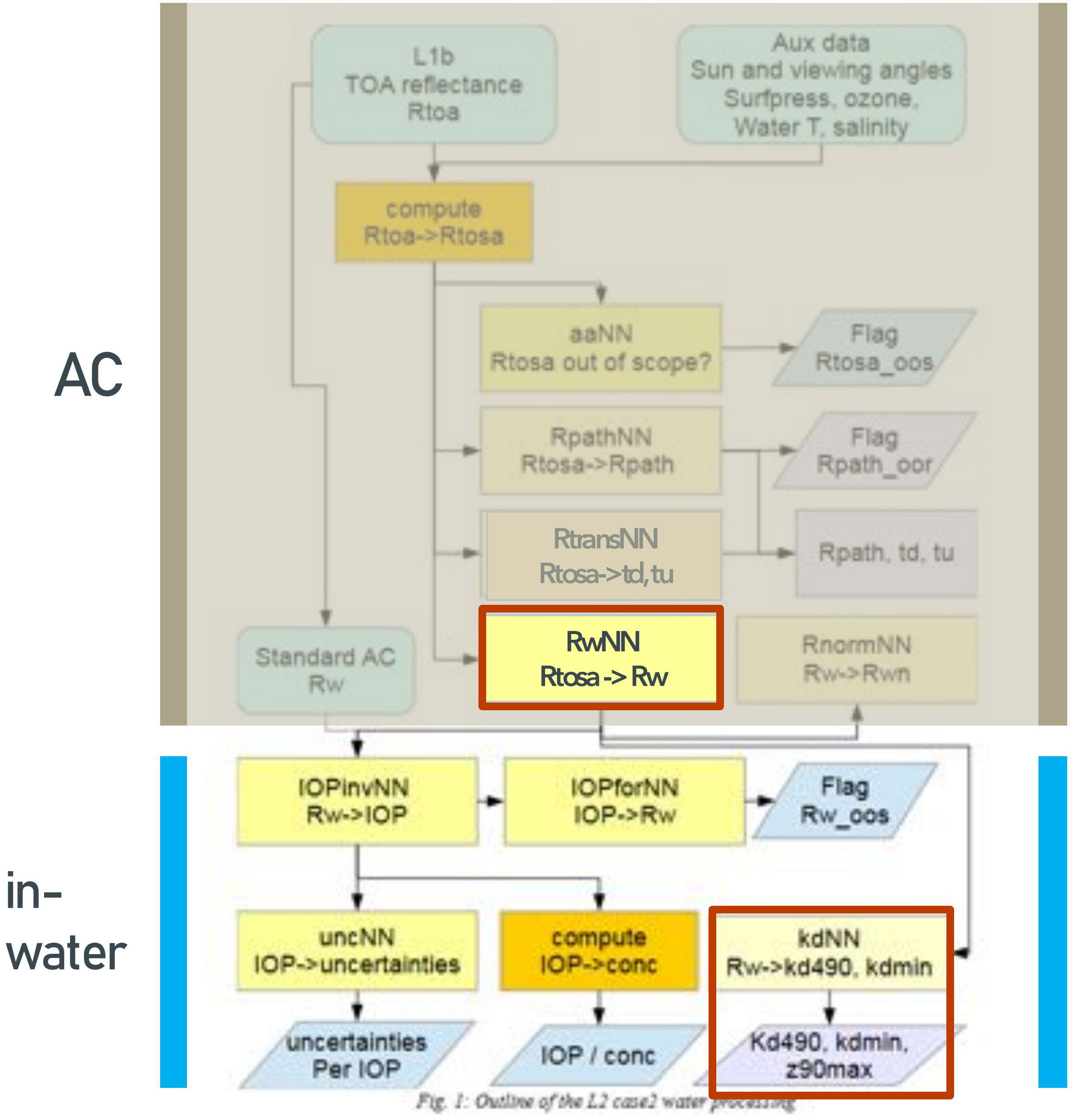
In-water Processing - Attenuation

Attenuation NN kdNN

- OLCI: 17 inputs, 3 fully connected hidden layers (97x77x77), 2 outputs
- **Input**: Rw (12 bands, 400-754nm) + geometry, T, S
- **Output**: kdmin, kd498

Depth of light penetration maximum with 90% intensity

z90max = 1/kdmin

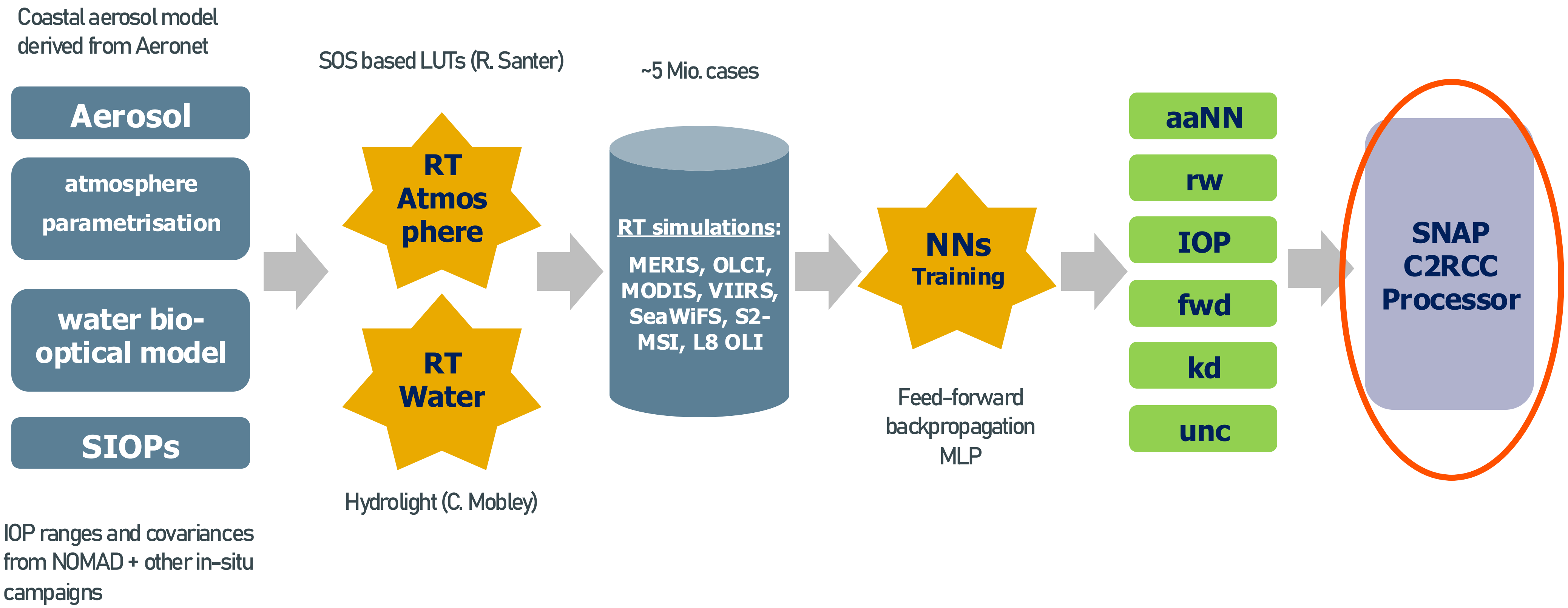


Source: Doerffer 2015. MERIS Case 2 water ATBD 4th reproc

C2RCC- Flags Overview

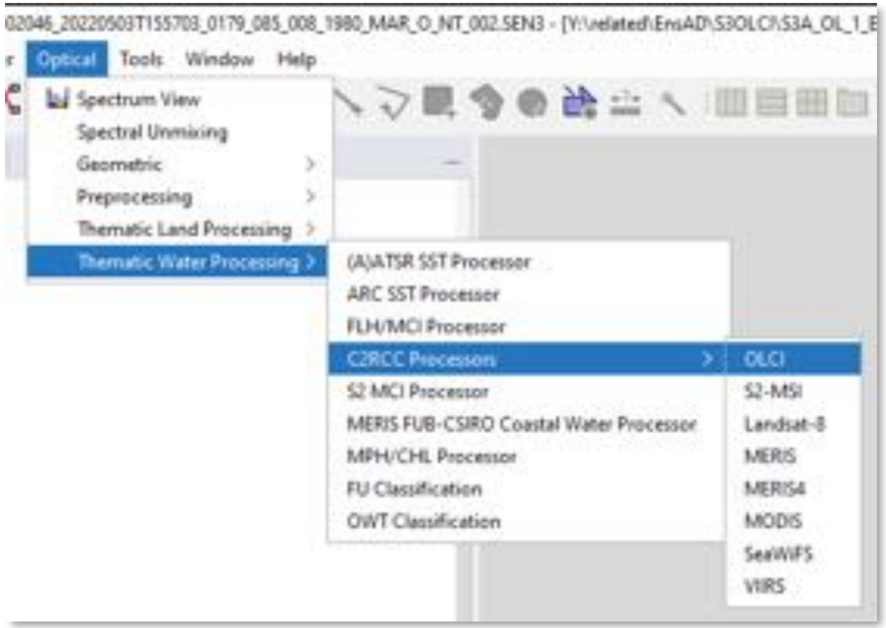
Name	Value (Bit)	Description
Rtosa_OOS	0	The input spectrum to the atmospheric correction neural net was out of the scope of the training range and the inversion is likely to be wrong
Rtosa_OOR	1	The input spectrum to the atmospheric correction neural net out of training range
Rhow_OOR	2	One of the inputs to the IOP retrieval neural net is out of training range
Cloud_risk	3	High downwelling transmission is indicating cloudy conditions
IOP_OOR	4	One of the IOPs is out of range
Apig, Adet, Agelb, Bpart, Bwit **at_max**	5, 6, 7, 8, 9	Output of the IOP retrieval neural net is at its maximum. The true value is this value or higher.
Apig, Adet, Agelb, Bpart, Bwit **at_min**	10, 11, 12, 13, 14	Output of the IOP retrieval neural net is at its minimum. The true value is this value or lower.
Rhow_OOS	15	The Rhow input spectrum to IOP neural net is probably not within the training range of the neural net, and the inversion is likely to be wrong.
Kd489_OOR	16	Kd489 is out of training range
Kdmin_OOR	17	Kdmin is out of training range
Kd489_at_max	18	Kd489 is at maximum of training range
Kdmin_at_max	19	Kdmin is at maximum of training range
Valid_PE	20	Default: !quality_flags.invalid && (!quality_flags.land || quality_flags.fresh_inland_water)

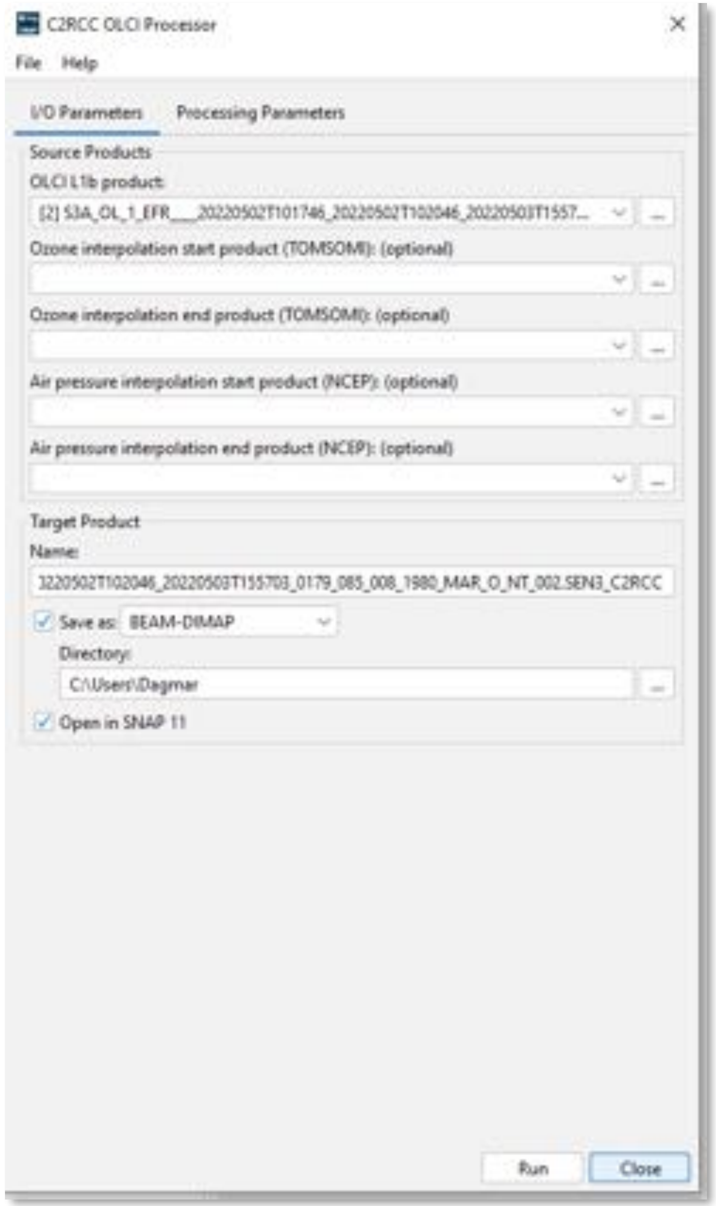
C2RCC Development

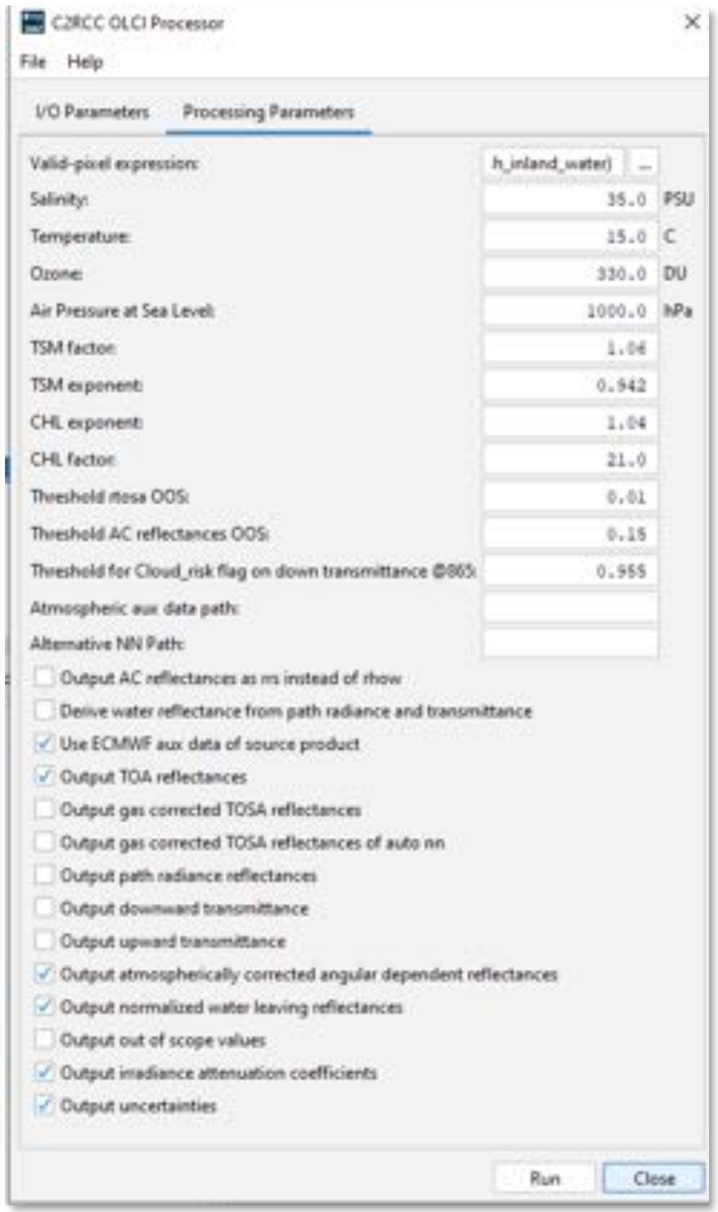


Source: Brockmann et al 2016 Evolution of the C2RCC Neural Network

C2RCC – Processing with SNAP





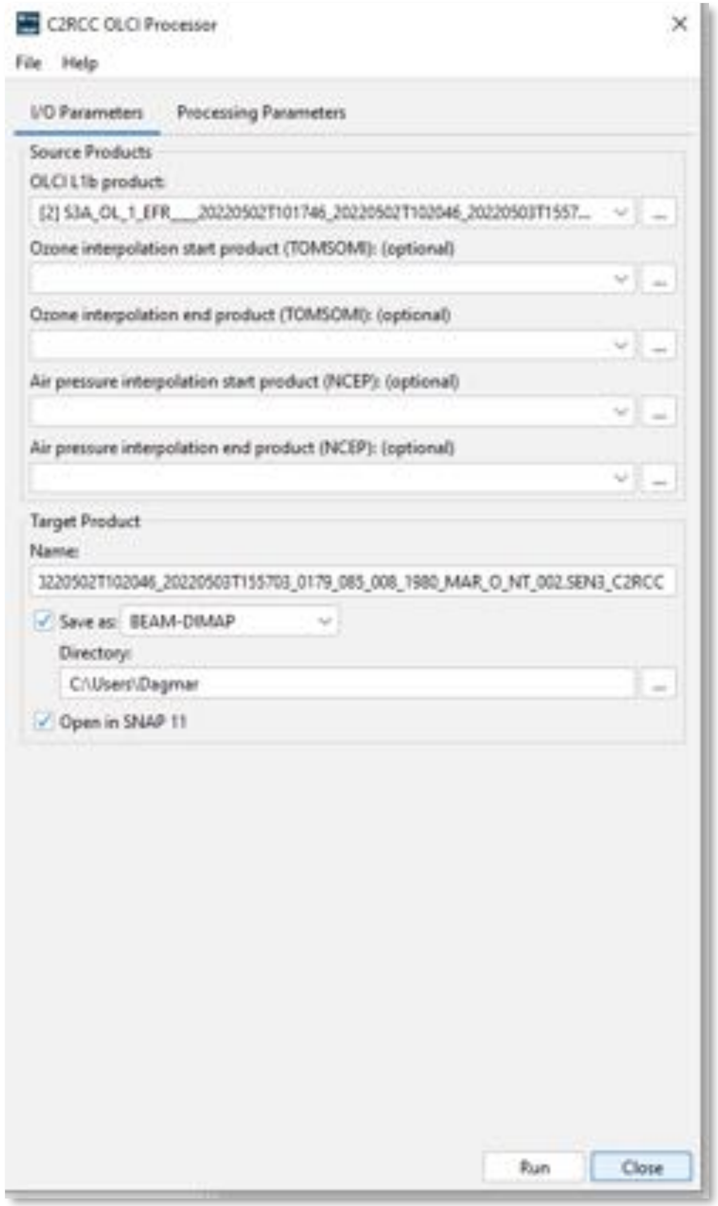


SNAP includes an implementation of the C2RCC Processor for sensors

- Sentinel 3 OLCI
- Sentinel 2 MSI
- Landsat-8
- MERIS (3rd reprocessing)
- MERIS (4th reprocessing)
- MODIS
- SeaWiFS
- VIIRS

Example C2RCC OLCI Processor

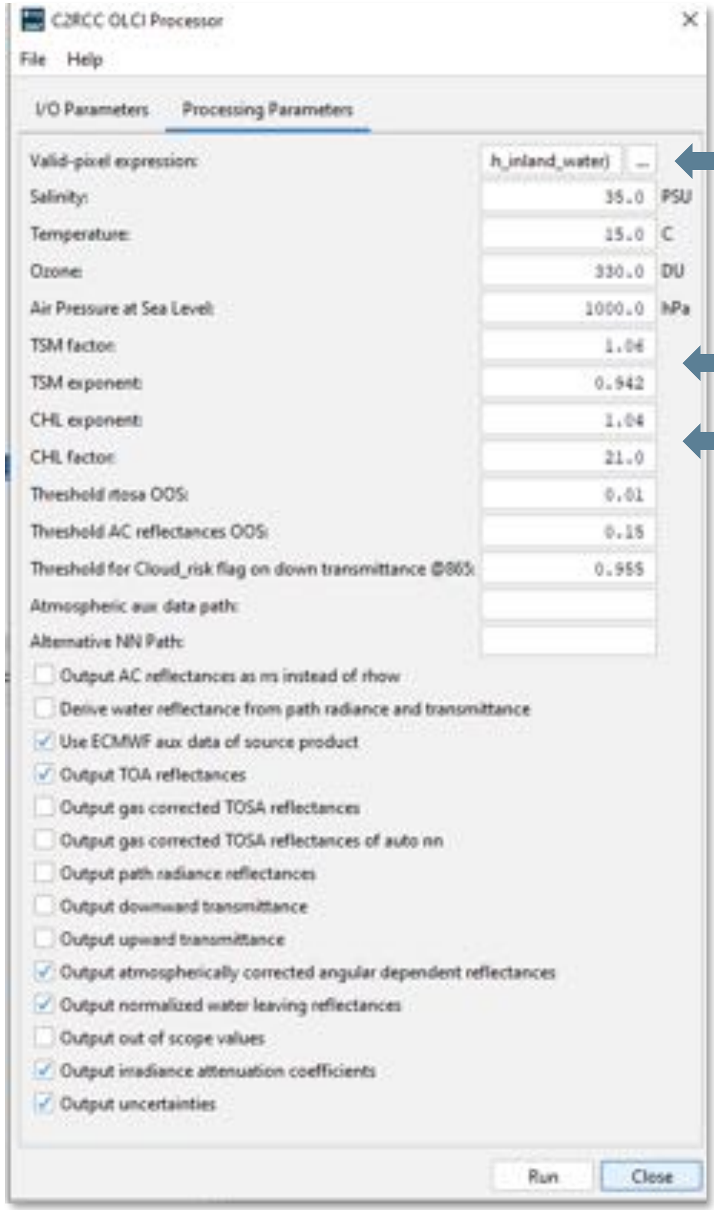
- Select OLCI L1b product as source product
- Target product automatically named original filename + C2RCC
- Select an output format
- Select an output directory
- "Open in SNAP" opens the processed product automatically in SNAP.
- Optional: Provide Ozone data from TOMSOM and air pressure data from NCEP. Data needs to be downloaded from respective sites before.
  OLCI L1b data comes with ozone and air pressure values, which is used by default.



C2RCC – Processing with SNAP

Example C2RCC OLCI Processor Processing Parameters

- valid-pixel expression based on OLCI L1b flags selects all water bodies (ocean + inland water bodies): !invalid && (!land || fresh_inland_water)
- Salinity and Temperature are taken as the fixed values for the scene
- Ozone, air pressure at sea level are only considered as constant fields, if the satellite product has no auxilliary data and no optional data source has been provided.
  By default, the box 'use ESMWF aux data of source product' is checked.
- Factor and exponent of empirical functions for TSM and Chl concentrations
- Thresholds for OOS flag tests
- Threshold for cloud risk flag based on downwelling transmittance at 865nm
- Atmospheric aux data path ?
- Alternative NN path -> for development only



valid pixel expression

TSM conversion

CHL conversion

Example C2RCC OLCI Processor Processing Parameters

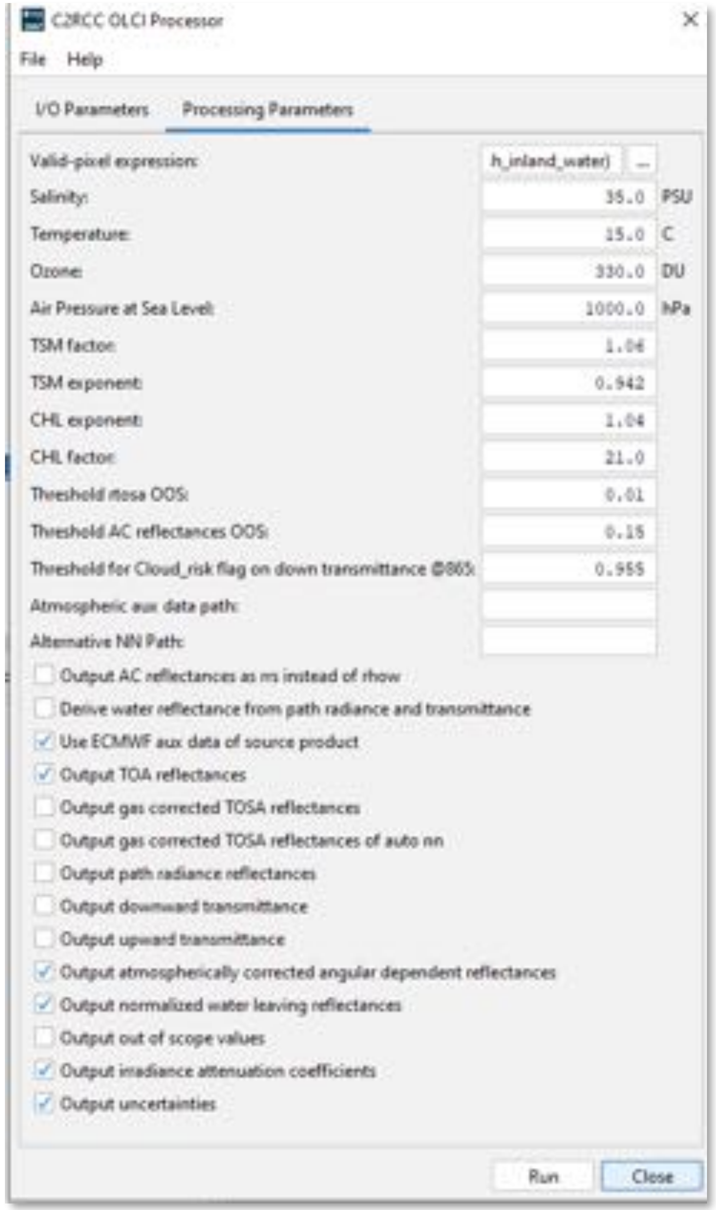
Check boxes control the output primarily

Defaults:

- Use ECMWF aux data of source product
- TOA reflectance
- Rhow (angular dependent)
- normalised Rhow
- kdmin, kd_z90max
- uncertainties of IOPs

Options:

- output rrs instead of rhow
- experimental rhow product from path radiance and transmittance
- Rtosa with gas correction
- Rtosa output from aaNN
- Rpath
- td
- tu
- out of scope values (for Rtosa_OOS)



Summary

- C2RCC is a NN processor based on physical models and their adaptation of in-situ databases
- Atmosphere and water are represented by simulations of SOS and HydroLight
- Multiple NNs are trained to cover the different aspects of the simulations which reflect natural conditions.
- C2RCC is limited by the ranges of the training data and by the relationships the physical models have covered.
- Extension of training data needs a re-training of all NNs.

Please revisit the videos and materials of the Short Course on C2RCC :

https://classroom.eumetsat.int/course/view.php?id=541