EVOLUTION OF THE C2RCC NEURAL NETWORK FOR SENTINEL 2 AND 3 FOR THE RETRIEVAL OF OCEAN COLOUR PRODUCTS IN NORMAL AND EXTREME OPTICALLY COMPLEX WATERS

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ABSTRACT

Retrieval of water constituents, or its optical properties, requires inversion of the water leaving reflectance spectrum, measured at top of atmosphere by ocean colour satellites. The Case 2 Regional processor, originally developed by Doerffer and Schiller [6], uses a large database of radiative transfer simulations inverted by neural networks as basic technology. Through the CoastColour project major improvements were introduced. It has been amended by a set of additional neural networks performing specific tasks and special neural networks have been trained to cover extreme ranges of scattering and absorption. The processor has been renamed into C2RCC (Case 2 Regional CoastColour) and is applicable to all past and current ocean colour sensors as well as Sentinel 2. It has been validated in various studies and is available through ESA's Sentinel toolbox SNAP. It is also used in the Sentinel 3 OLCI ground segment processor of ESA for the generation of the Case 2 water products, as well as in the processor for the upcoming MERIS 4th reprocessing.

1. INTRODUCTION

While in the open ocean the light field emerging from the water surface and measured by a satellite is determined by the concentration of the phytoplankton pigment chlorophyll-a, in coastal waters, estuaries, rivers and inland waters, other substances contribute to the optical signature of the water body, i.e. the reflected light spectrum. Conventionally, the manifold of constituents is reduced to three components [8]: phytoplankton pigments, inorganic suspended sediments, and yellow substances. Retrieval of concentrations of these constituents requires a bio-optical model, which includes the inherent optical properties (absorption and scattering coefficients) of these components as well as the concentration ranges and co-variations and a procedure for the inversion of the of the water leaving reflectance spectrum. Satellites measure the light field emerging at top-of-atmosphere, and thus an atmospheric correction needs to be performed as part of the processing of ocean colour data. Due to the generally low reflectances at water surface, the signal measured at the satellite is determined to more than 90% by the atmospheric path radiance. Consequently, the requirements for the atmospheric correction is very demanding.

The Case 2 Regional processor, originally developed by Doerffer and Schiller [6], [7] uses a large database of radiative transfer simulations of water leaving radiances ("water signal") as well as top-of-atmosphere radiances ("satellite signal"). The inversion of the satellite signal as well as the water signal is performed by neural networks as basic technology. This concept was first introduced in the late 1990's in the MERIS ground segment, and then further developed and made publicly available as open source processor in the BEAM EO data processing Toolbox (Case 2 Regional Processor). Using dedicated bio-optical models for inland waters, special versions for lakes were also made available (MERIS Lakes processors). Thanks to the open source distribution these processors were used by many other scientists [12], [1], [13], [11]. These helped to understand the strengths and weaknesses of the method, to characterise its scope and limitations and to constantly improve it. The Case 2 Regional algorithm was then used in the MERIS 3rd Reprocessing which is the current version of ESA's distributed products [3]. A major upgrade of the algorithm was developed in the ESA DUE CoastColour project [5] when a 5-component bio-optical model and a coastal aerosol model [15], [2] were introduced. This processor version is available through the CoastColour processing on-demand service. The current version, called C2RCC (Case 2 Regional CoastColour) version is further developed and is described in the following sections. It is made available through ESA's Sentinel Toolbox SNAP, and it is used to generate the Case 2 water products in Sentinel 3 OLCI standard ESA products as well as in the upcoming MERIS 4th Reprocessing.

2. PROCESSOR OVERVIEW

The C2RCC processor relies on a large database of simulated water leaving reflectances, and related top-of-atmosphere radiances. Neural networks are trained in order to perform the inversion of spectrum for the atmospheric correction, i.e. the determination of the water leaving radiance from the top of atmosphere radiances, as well as the retrieval of inherent optical properties of the water body. A schematic overview is given in *Figure 1*.

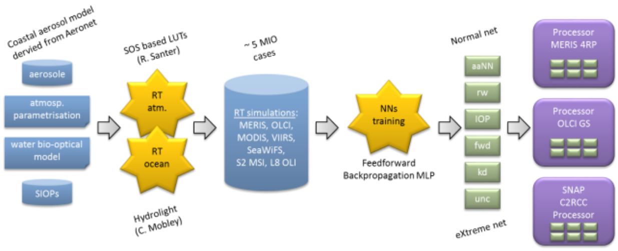

Figure 1. Schematic of the C2RCC development process

A careful characterisation of optically complex waters through its inherent optical properties (IOP) as well as of coastal atmospheres is used to parameterise radiative transfer models for the water body and the atmosphere. Covariances between the water constituents are taken into account and a large database of reflectances at the water surface is calculated. These reflectances are further used as lower boundary condition for the radiative transfer calculation in the atmosphere and finally a database of ~5 million cases is generated. This is the basis for training neural nets. For example, the top-of-atmosphere full spectrum is input to a neural net, and the water leaving reflectance in the VIS and NIR bands is the output. The training can be understood as a nonlinear multiple regression, as described in [6]. The different neural nets will be described in detail later in this paper. These nets are combined in a certain logic which eventually comprises the C2RCC processor. This processor is used in various instances: In the SNAP toolbox it is fully accessible with all possible outputs available to the user. In the MERIS 4th reprocessing and the ESA OLCI ground segment the Case 2 water constituents are derived with the C2RCC neural nets.

3. RADIATIVE TRANSFER MODELLING

The in-water modelling is performed using the Hydrolight model [10]. The bio-optical model used to parameterise the model uses 5 components for scattering and absorption:

The total absorption is composed of pigment absorption (a_{pig}) and two components for detritus (a_{det}) and gelbstoff (a_{gelb}). These two components differ by their spectral slopes. The total scattering is composed of two components, namely a white scatterer (b_{whit}) and a typical sediment scatterer (b_{tsm}). The white scatterer represents calcareous sediments. These are larger particles which is reflected in a corresponding phase function. All IOPs are defined at 443nm wavelengths.

These 5 components are an abstraction of the large variety of IOPs in natural waters. From a user perspective, IOPs are a proxy for concentration of the three optically active constituents mentioned before, and *Figure 2* shows the relationship between these. The conversion from IOPs to concentration is done using scaling factors. These can be regionally variable, and thus the main output of the C2RCC processor are the 5 IOPs.

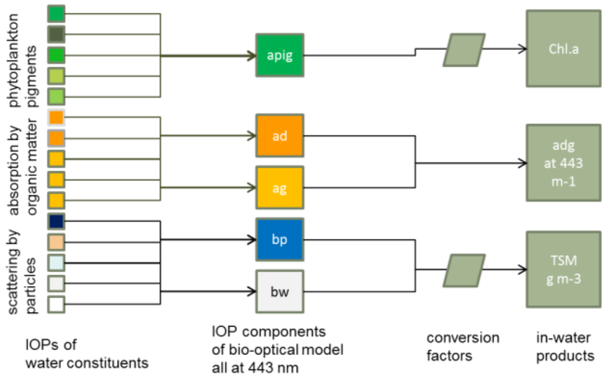

Figure 2: Bio-optical model

The IOPs found in the NOMAD database [14] and complemented by the CoastColour data set to extend the range for coastal waters including extreme cases, were analysed in order to create a realistic bio-optical model. In particular the correlation between the scattering and absorbing components was modelled using a probability approach and thus to allow for a partial correlation as found in the NOMAD database.

The value ranges of the concentrations was also determined from the NOMAD database. The neural nets trained with these ranges are called the “normal nets” and used as defaults in the SNAP version of the processors, as well as in the ESA OLCI and MERIS 4th processing. A special set of nets for extreme ranges of absorption and scattering have also been trained. This is only available through the SNAP version of the processor. The ranges are summarized in table 1.

Table 1: Training ranges of the neural nets

IOP	Normal min	Normal max	extreme min	extreme max
a_pig	~ 0	5.3	~ 0	51
a_det	~ 0	5.9	~ 0	60
a_gelb	~ 0	1.0	~ 0	60
b_part	~ 0	60	~ 0	590
b_wit	~ 0	60	~ 0	590

The atmospheric radiative transfer is based on the SOS model [4], [9] with aerosol optical properties derived from analysis of Aeronet measurements. For computational efficiency the full model has been approximated by several look-up tables.

4. QUALITY CHECKS

Two types of quality checks are performed: out of range checks compare the top-of-atmosphere radiances, as well as the water leaving reflectances, at each wavelength individually, and the derived IOPs with the ranges used in the radiative transfer calculations and the training of the neural nets. If any input value is outside the training range, the method is out of its definition range and a warning flag is raised.

However, this out-of-range is not sufficient for the spectral quantities. Even if the reflectance at each spectral wavelength is within the limits of the training, a spectrum of a shape that did not occur during training is outside the definition range of the algorithm. Thus, a second type of test compares the spectrum as a whole against the training range in order to verify that such a spectrum is "known" to the algorithm. We call this the out-of-scope test (OOS)

The OOS test on the top-of-atmosphere spectrum is performed by auto-associative neural net technique (aaNN). With only 7 bottle-neck neurons the aaNN can only reproduce such spectra which are contained in the training dataset. Unknown spectra cannot be reproduced and a difference between the input spectrum and the aaNN result will be large.

The OOS test on the water leaving spectrum is performed by testing optical closure. The derived IOPs are fed into a forward neural net, trained on the same database of radiative transfer simulations as the inverse model. If the input spectrum was within the training range, and the optical characteristics of the measured water body can be model with the bio-optical model used for the simulations, the forward neural net will produce a water leaving reflectance spectrum very similar to the input spectrum. Large deviations indicate either a spectrum not within the training database, or different optical conditions in the water body, i.e. the spectrum is out-of-scope of the algorithm definition.

5. UNCERTAINTIES

The uncertainty of determination of the IOPs has always to take into account all IOPs, i.e. the uncertainty of pigment absorption depends on the pigment absorption itself but also on the value of the other absorbing and scattering components. This is also known as the masking effect. For example, low chlorophyll concentrations (low a_{pig}) are determined with a large error if the TSM concentration (b_{TSM}) is high but less error under low TSM conditions. Using the database of radiative transfer simulations as "truth", and the trained IOP inversion net as estimator for all IOP components, it is possible to construct a table with "truth" and "estimates" for all combination of the IOP components. This table is used to train neural nets that output the uncertainty per IOP (difference between "truth" and "estimate") with the estimated IOP as input. Thus these nets model the masking effect properly.

6. C2RCC PROCESSOR LOGIC

The C2RCC processor breaks down into two major parts: the atmospheric correction part, and the in-water part. *Figure 3* presents the architecture of the C2RCC processor.

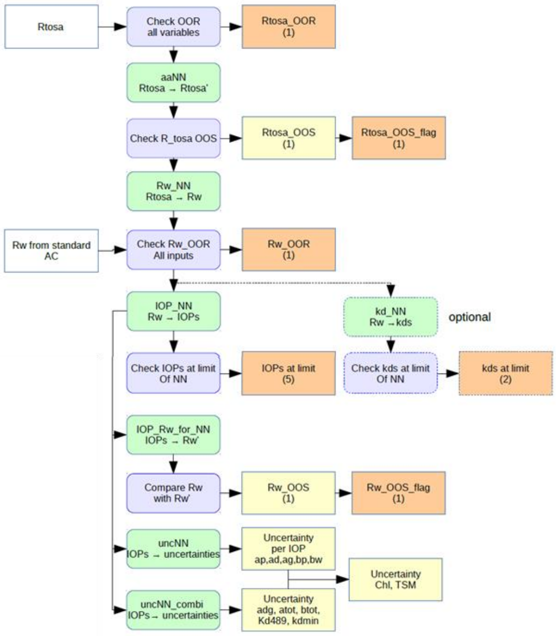

Figure 3: C2RCC processor architecture. Neural nets are shown as green boxes, and quality tests as blue boxes

The main input to the atmospheric part are the top-of-atmosphere radiances/reflectances of the sensor. Currently these instruments are supported as input: MERIS, OLCI, MODIS, VIIRS, SeaWiFS and Sentinel 2 MSI. The input spectra are corrected for gaseous absorption (white box Rtosa in *Figure 3*). Air pressure, and thus a proper altitude correction, is inherent part of the neural network processing. The main output of the atmosphere part are directional water leaving reflectances produced by the atmospheric correction neural net (green box Rw_NN). The atmosphere part contains out-of-range tests (blue box check OOR) and out-of-scope tests (green box "aaNN" and blue box "check R_tosa") of the TOA reflectances, resulting in corresponding quality flags. Optionally the output of the auto-associative neural net used of the out-of-scope test can be written to the output file in the SNAP version of the processor. The output from the transmittance NN is also used to raise a cloud-risk flag.

The in-water part gets as input the directional water leaving reflectances from the atmosphere part. Alternatively, it will be also possible to use water leaving reflectance from external input so that the in-water part can work with alternative atmospheric correction, too. However, this is currently not implemented in the SNAP processor. After checking for out-of-range values in the spectrum (blue box “check OOR”) the inversion of the spectrum into IOPs is performed (green box “IOP_NN”). These IOPs are then passed to the forward model to calculate back the spectrum (green box “IOP_Rw_for_NN”) and perform the out-of-scope test on the comparison of the input water leaving reflectance and the estimated spectra (blue box “compare Rw”). The result is the OOS flag. An optionally calculation on the input water leaving reflectances derives the diffuse attenuation coefficient by a dedicated neural net from the spectrum (green box “kd_NN”).

Using the derived IOPs as inputs the uncertainties per IOP are calculated by the uncertainty nets (green box “uncNN”) for the 5 components, as well as for the combined 3 components (green box “uncNN_comb”). Finally, the IOPs are converted into chlorophyll-a and TSM concentration using arithmetic conversion factors (not shown in the figure). The conversion coefficients can be modified in the SNAP user interface. The default values of the SNAP processor are used in ESA standard processing for OLCI and MERIS.

The family of processors for the different instruments, and for BEAM and SNAP is shown in *Figure 4*.

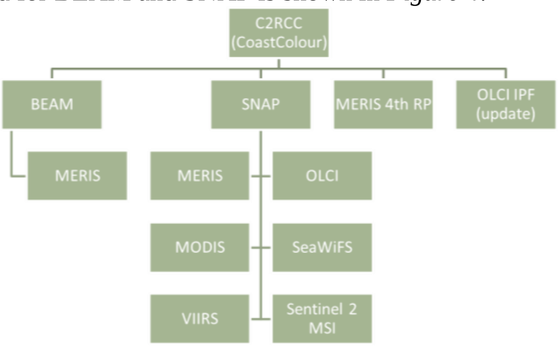

Figure 4: C2RCC processor family tree

7. VALIDATION

The C2RCC processor for MERIS, MODIS and SeaWiFS has been included in the Ocean Colour CCI round robin intercomparison of atmospheric corrections in 2015. This included analysis of match-ups against a large database of in-situ measurements. C2RCC performs very well in Case 2 waters for MERIS, good for MODIS but less good for SeaWiFS. As an example, the match-ups over AAOT are shown in *Figure 5*.

In the framework of the EU Highroc project the TSM concentration derived from MODIS using C2RCC was compared against the Cefas Smartbuoy data (turbidity measurements concerted into TSM concentration). This is shown in *Figure 6*.

During commissioning of Sentinel 3 a first application to OLCI was performed and compared with AAOT data. Only 1 match-up was available so far which shows quite good agreement. However, it should be noted that OLCI data were only preliminary calibrated, and also the Aeronet OC data were Level 1.5 quality only. These results can only be taken as a first indication without allowing any conclusion. Finally, a match-up of C2RCC for Sentinel 2 at AAOT is shown in *Figure 8*. In that figure also the result of the land atmospheric correction, sen2cor, is shown for comparison.

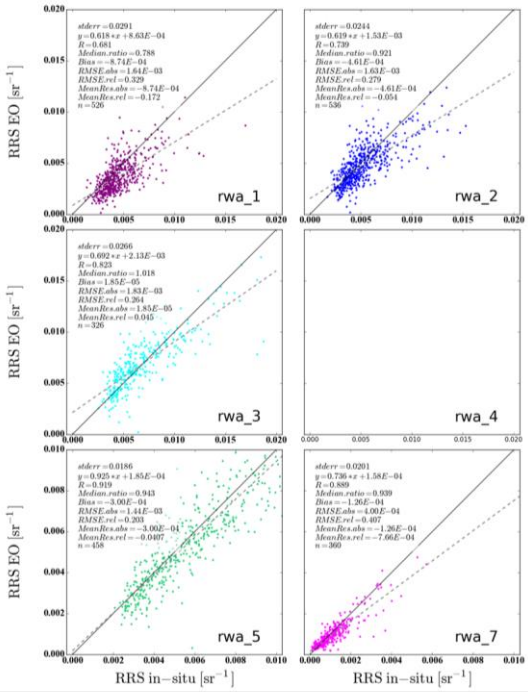

Figure 5: Match-up analysis of C2RCC for MERIS over Aqua Alta Ocean Tower. Rwa_i indicates the MERIS band number.

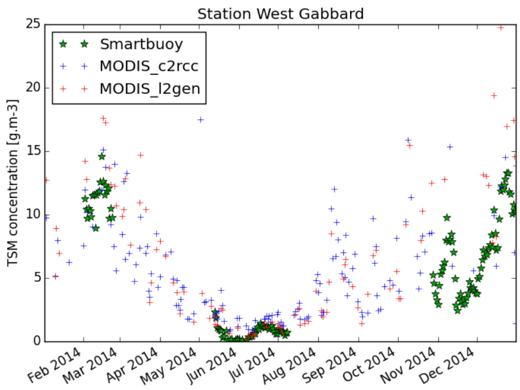

Figure 6: Comparison of TSM concentration at the Cefas Smartbuoy in the North Sea (C2RCC applied to MODIS).

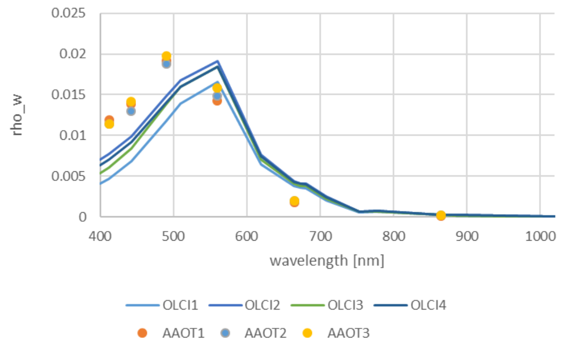

Figure 7: Match-up of C2RCC OLCI at AAOT platform in the Northern Adriatic Sea on 15.04.2016. The three AAOT spectra are from three different times during the day. The 4 OLCI spectra are from 4 full resolution pixels around the AAOT platform. Note: preliminary calibrated OLCI data during commissioning phase and Level 1.5 quality of AAOT only; results should be taken as a preliminary indication of quality.

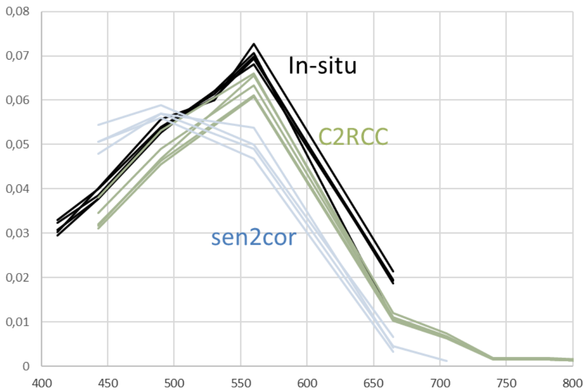

Figure 8: Comparison of C2RCC Sentinel 2 MSI with in-situ measurement at AAOT on 19.02.2016. The different in-situ spectra are taken during the day, and the C2RCC spectra are taken at 6 different pixels around the platform. For comparison the result of the atmospheric correction with sen2cor land atmospheric correction is shown, too.

8. SUMMARY

The Case 2 Regional CoastColour (C2RCC) processor is a multi-mission ocean colour processor, applicable to MERIS, OLCI, MODIS, SeaWiFS and Sentinel 2 MSI. It relies on a large database of radiative transfer simulations, inverted by neural networks. The core is a 5 component IOP model which was derived from NOMAD in-situ measurements. Special neural nets have been trained for extreme IOP ranges. C2RCC has been validated for the different sensors, with good results for Case 2 waters. C2RCC will be used in ESA ground processor for Sentinel 3 OLCI as well as in MERIS 4th Reprocessing to calculate the chlorophyll and TSM concentrations, as well as yellow substance pigment absorption, in Case 2 waters.

The processor with several configuration options and optional outputs such as kd is available as open source software in the ESA SNAP Sentinel Toolbox. With this it is even possible to include user supplied neural networks.

9. ACKNOWLEDGEMENTS

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10. REFERENCES

1. Attila Jenni, Sampsa Koponen, Kari Kallio, Antti Lindfors, Seppo Kaitala, Pasi Ylöstalo (2013): MERIS Case II water processor comparison on coastal sites of the northern Baltic Sea, Remote Sensing of Environment, Volume 128, 21 January 2013, Pages 138-149, ISSN 0034-4257, http://dx.doi.org/10.1016/j.rse.2012.07.009

2. Aznay O. AND R. Santer (2009) MERIS atmospheric correction over coastal waters: Validation of the MERIS aerosol models using AERONET. International Journal of Remote Sensing, 30(18), pp. 4663 - 4684. DOI: 10.1080/01431160802632256

3. Bourg et al (2012): MERIS 3RP validation report. Available from https://earth.esa.int/documents/700255/707222/A879-NT-017-ACR_v1.0.pdf/6fa86bec-9945-4e39-808e-3801f2e3962b

4. Chami M., Santer R., and E. Dilligeard (2001): Radiative transfer model for the computation of radiance and polarization in an ocean-atmopshere system: polarization properties of suspended matter for remote sensing, Applied Optics, 40, 15, 2398-2416, 2001.

5. CoastColour Web www.coastcolour.org

6. Doerffer, R., & Schiller, H. (2007). The MERIS case

2 water algorithm. International Journal of Remote Sensing,28(3), 517−535

7. Doerffer R. and H. Schiller (2008): MERIS Regional Coastal and Lake Case 2 Water Project - Atmospheric Correction ATBD, GKSS Research Center 21502 Geesthacht Version 1.0 18. May 2008

8. IOCCG (2000). Remote Sensing of Ocean Colour in Coastal, and Other Optically-Complex Waters. Sathyendranath, S. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 3, IOCCG, Dartmouth, Canada.

9. Lenoble J., M. Herman, J.L. Deuze,, B. Lafrance, R. Santer, D. Tanre, (2007). A successive order of scattering code for solving the vector equation of transfer in the earths atmosphere with aerosols Journal of Quantitative Spectroscopy & Radiative Transfer 107 (2007) 47950710. Mobley, C. D., L.K. Sundman (2008): Hydrolight 5 Ecolight 5 technical documentation. Sequoia Scientific, Incorporated, Bellevue, WA, 98005 (2008), p. 95

11. Odermatt Daniel, Claudia Giardino, Thomas Heege (2010): Chlorophyll retrieval with MERIS Case-2-Regional in perialpine lakes, Remote Sensing of Environment, Volume 114, Issue 3, 15 March 2010, Pages 607-617, ISSN 0034-4257, http://dx.doi.org/10.1016/j.rse.2009.10.016

12. Palmer Stephanie, Peter D. Hunter, Thomas Lankester, Steven Hubbard, Evangelos Spyrakos, Andrew N. Tyler, Mátyás Présing, Hajnalka H orváth, Alistair Lamb, Heiko Balzter, Viktor R. Tóth (2015): Validation of Envisat MERIS algorithms for chlorophyll retrieval in a large, turbid and optically-complex shallow lake, Remote Sensing of Environment, Volume 157, February 2015, Pages 158-169, ISSN 0034-4257, http://dx.doi.org/10.1016/j.rse.2014.07.024.

13. Vilas Luis Gonzáles, Evangelos Spyrakos, Jesus M. Torres Palenzuela (2011): Neural network estimation of chlorophyll a from MERIS full resolution data for the coastal waters of Galician rias (NW Spain), Remote Sensing of Environment, Volume 115, Issue 2, 15 February 2011, Pages 524-535, ISSN 0034-4257, http://dx.doi.org/10.1016/j.rse.2010.09.021

14. Werdell, P.J. and S.W. Bailey (2005): An improved bio-optical data set for ocean color algorithm development and satellite data product validation. Remote Sensing of Environment , 98(1), 122-140.

15. Zagolski R., Santer R., Aznay O., (2007). A new climatology for atmospheric correction based on the aerosol inherent optical properties. Journal of Geophysical Research, Vol. 112, No. D14, D14208