

DOC characterisation of Raw water and UPW

Your proj.-ID/ our proj.-ID: /
Project Partner/ contact: /
and type of samples: 2 (water)
Measuring conditions: column: 5036 / 006 flows: 1.0 / Ø / Ø buffer: STD
column: 5036 / 006 flows: 1.0 / Ø / Ø buffer: STD x 0.2
Sampling date: 2010-Jul- STD MC
Incoming date: 2010-Jul-19 report: Y N
Measuring date: 2010-Jul-19+20 data processing: Dr. M. Abert
Date of Report: 2010-Jul-20 report: Dr. M. Abert

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Technical note: LC-OCD stands for "Liquid Chromatography – Organic Carbon Detection". Separation is based on size-exclusion chromatography (SEC) followed by multidetection with organic carbon (OCD), UV-absorbance at 254 nm (UVD) and organic bound nitrogen (OND). All concentration values refer to mass of organic bound carbon (OC). As a „rule-of-thumb“ compound mass is about twice (for acids threefold) the value of OC. Chromatograms are processed on the basis of area integration using the program ChromCALC. In many samples the acid fraction contains low-molecular mass humic acids which are subtracted by ChromRES on the basis of SAC/OC ratio for HS. Thus, despite the visible presence of an acid peak there may no LMW acids be present.

SUMMARIC PARAMETERS:

DOC (Dissolved OC): Determined in the column bypass after in-line 0.45 µm filtration.

HOC (Hydrophobic OC): Difference DOC minus CDOC, thus all OC retained on the column is defined as „hydrophobic“. This could be natural hydrocarbons or sparingly soluble "humins" of the humic substances family.

INORGANIC COLLOIDS (respond only in UV-Chromatograms): Negatively charged inorganic polyelectrolytes, polyhydroxides and oxidhydrates of Fe, Al, S or Si are detected by UV light-scattering (Raleigh-effect).

CDOC (Chromatographic DOC): This is the OC value obtained by area integration of the total chromatogram. Chromatographic subfractions of CDOC are:

ROM = Refractory Organic Matter:

A: Humics (HS): In LC-OCD measurements there is a tight definition for HS based on retention time, peak shape and SAC. Calibration on the basis of „Suwannee River“ Standard IHSS-FA and IHSS-HA. In addition, statistical data are given, like number-averaged molecular mass (Mn) and aromaticity (SAC/OC).

B: Building Blocks (BB): The HS-fraction is accompanied by shoulders, shape, concentration and UV-activity varies. This are sub-units of HS with molecular weights of 300-450 g/mol. Building Blocks are considered to be natural breakdown products of humics. They cannot be removed in flocculation processes.

BOM = Biogenic Organic Matter:

C: Biopolymers (BP): This fraction is very high in molecular weight (100.000 - 2 Mio. g/mol), hydrophilic, not UV-absorbing. BP are typically polysaccharides but may also contain proteinic matter (this is quantified on basis of OND). BP exist only in surface waters.

D: LMW Organic Acids (OA): In this fraction all aliphatic, low-molecular weight (LMW) organic acids co-elute due to an ion chromatographic effect. A small amount of HS may fall into this fraction and is subtracted on the basis of SAC/OC ratios.

E: LMW Neutrals (NEU): Low-molecular weight (LMW) weakly or uncharged hydrophilic or slightly hydrophobic ("amphiphilic") compounds appear in this fraction. This includes alcohols, aldehydes, ketones and amino acids. The hydrophobic character increases with retention time, e. g. pentanol appears at 120 min, octanol at 240 min. NEU may be in part refractory.

SOM = Synthetic Organic Matter

With LC-OCD all water-soluble synthetic organic compounds can be quantified and identified (after comparison with model compound) down to the low ppb-range. However, chromatographic resolution in SEC is moderate (about 15000 theoretical plates/metre). Typical examples for SOM are flocculant polymers, antiscalants, org. additives like amines, resin leaching products like polysulfonic acids (PSS) or trimethyl amine (TMA).

Inorganic Colloids (only visible in UV-detection): Inorganic colloidal or particulate matter eluting slightly before the biopolymer fraction becomes visible by Raleigh light scattering. This material could be iron oxid hydrates or colloidal sulfur.

SUVA (SAC/DOC): Additional parameter derived from the ratio of DOC and SAC.

Results

Table 1 –for raw water only

Project:	DOC			Approx. Molecular Weights in g/mol:										Inorg. Colloid. SAC (m ⁻¹)	SUVA (SAC/DOC) L/(mg*m)						
	Dissolved	Hydrophob.	Hydrophil.	>>20.000			~1000 (see separate HS-Diagram)					300-500	<350			<350					
				BIO-polymers	DON (Norg)	N/C	% Proteins in BIOpol.**	Humic Subst. (HS)	DON (Norg)	N/C	Aromaticity (SUVA-HS)	Mol-Weight (Mn)	Position in HS diagram			Building Blocks	LMW Neutrals	LMW Acids			
ppb-C	ppb-C	ppb-C	ppb-C	ppb-N	µg/µg	% BIOpol.	ppb-C	ppb-N	µg/µg	L/(mg*m)	g/mol	--	ppb-C	ppb-C	ppb-C	% DOC	% DOC	% DOC	--	--	
Raw water	1719	156	1563	73	8	0,10	31	794	41	0,05	1,85	444	A	401	285	10	4,3%	--	--	n.q.	2,01
	100%	9,1%	90,9%	4,3%	--	--	--	46,2%	--	--	--	--	--	23,3%	16,6%	0,6%				--	--

LMW = low-molecular weight

DON = Dissolved organic nitrogen

n.q. = not quantifiable (< 1ppb; signal-to-noise ratio)

n.m. = not measured

*:Grey colour in HOC: Significance unclear

**:under the presumption that all org. N in the BIOpolymer fraction originates from proteins

**:pale green: cross sensitivity inferred

Sample	Sample 1
<i>Treatment Scheme</i>	<i>Raw Water</i>
Humics (HS) quantitative	794 ppb C or 46 % of DOC. Absolute concentration is in medium range. Percentage is relative high for a water which was presumably treated by a flocculation step before. This might be due to aquagenic fulvic acid character of HS before assumed flocculation: This type of HS can hardly be reduced by flocculation.
Humics (HS) qualitative	(Remaining) HS are of aquagenic fulvic acid type.
Building Blocks (BB)	Proportion compared to HS indicates a flocculation step.
Biopolymers (BP)	73 ppb C or 4 % of DOC. Relative concentration is in lower range for surface water. Presumably BP are not affected by pre-treatment of Raw water. 31 % of BP can be assigned to proteins.
Neutrals (NEU)	
LMW Acids	Found in traces only. Nearly all LMW Acids can be assigned to LMW HS.
Other Compounds	Sample contains nitrate but no ammonium.
Comments	

(Void boxes = no peculiarities)

Discussion

Raw Water

DOC in Raw Water is 1719 ppb.

Urea in Raw water was quantified to 2.4 ppb Urea-C.

UPW

DOC in UPW is 0.92 ppb. All DOC can be related to urea (0.52 ppb urea-C) and LMW acids (0.40 ppb C).

End of Report

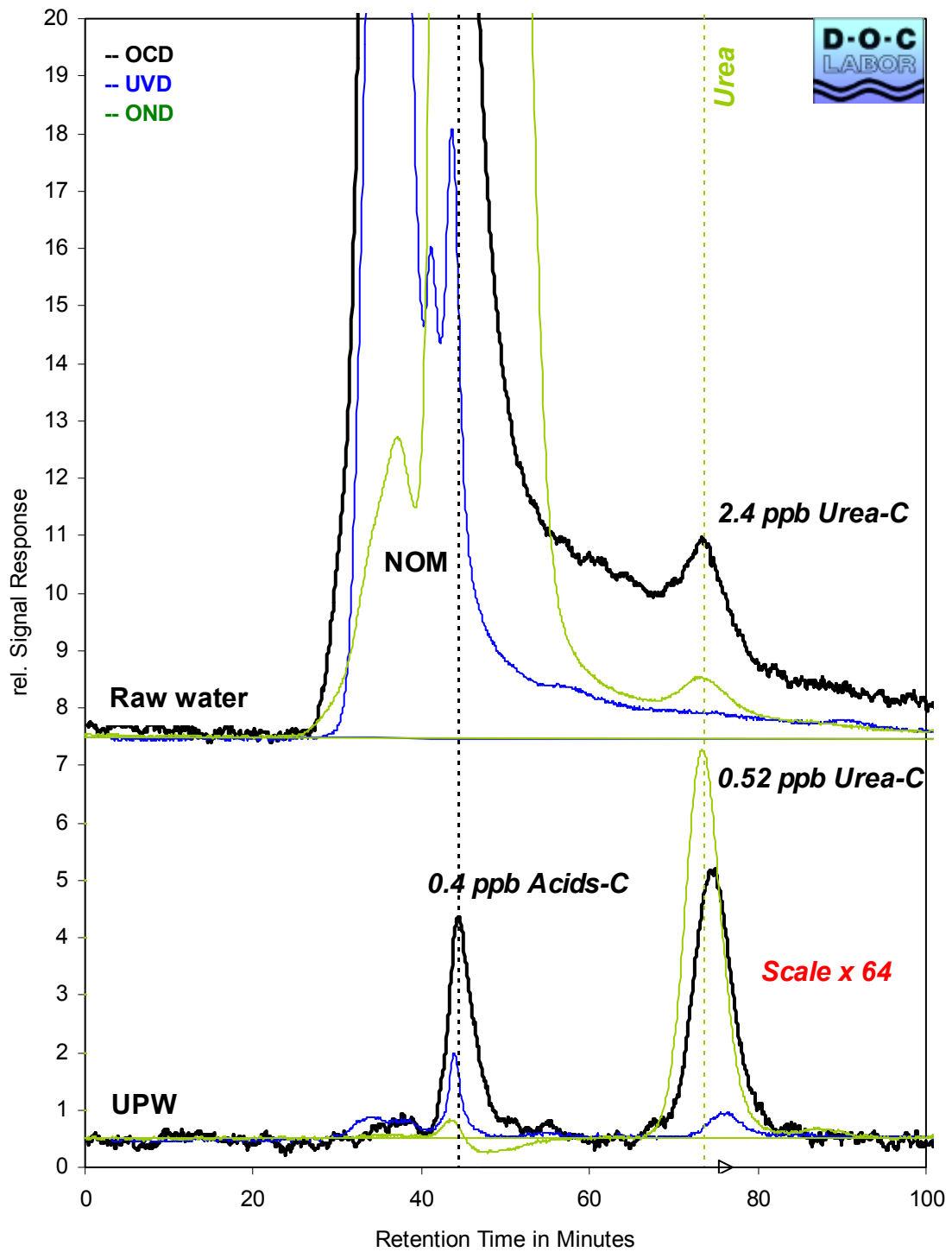


Fig. 1: LC-OCD chromatograms (Urea quantification in raw water and UPW)