Optimization of Solid State Urea Clathrate Formation as a Chemical Separation Method Coupled to Compound Specific Stable Carbon Isotope Analysis

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Supporting Information

Characterization of the water samples

Table S1. Basic water quality parameters of the tested water samples: DW: Distilled Water; TW: Tap Water; RW: River Water; IWW 1-3: Industrial Wastewater 1-3; CF: Confined Water; GW 1-2: Groundwater 1-2. The concentration of NH_4^+ was not determined in samples IWW 1-3 because of the disturbance of hydrogen sulfide. The Electrical Conductivity (EC) was referred to 20°C. The dissolved O_2 and the O_2 saturation was not determined for samples GW 1, GW 2 and CW samples.

	DW	TW	RW	IWW 1	IWW 2	IWW 3	CW	GW 1	GW 2
pH	5.45	7.66	7.62	7.25	6.92	6.73	6.65	6.52	6.72
EC / $\mu\text{S cm}^{-1}$	3	448	375	553	1054	1285	1325	916	1157
O_2 / mg L^{-1}	6.3	5.3	6.4	3.4	1.6	2.0	-	-	-
Oxygen saturation / %	93	73	84	49	23	29	-	-	-
COD_{Cr} / $\text{mg L}^{-1} \text{O}_2$	blank	<1	23	75	144	181	2	5	5
NH_4^+ / mg L^{-1}	blank	<0.01	0.1	n.d.*	n.d.*	n.d.*	<0.01	<0.01	<0.01
NO_3^- / mg L^{-1}	blank	15.1	20.3	11.5	10.2	9.0	4.3	62.8	83.4
NO_2^- / mg L^{-1}	blank	<0.02	0.029	0.021	<0.02	<0.02	<0.02	0.22	0.39
PO_4^{3-} / mg L^{-1}	blank	<0.1	0.6	1.4	5.8	10.6	0.1	0.3	0.5

Water quality parameters were determined using the following instruments. pH was measured with WTW ProfiLine pH 3110 portable pH meter with SenTix 41 pH electrodes. Electrical conductivity was determined with HANNA HI 98303 DiST3 EC-tester with automated temperature compensation (20°C). Dissolved oxygen and oxygen saturation was measured with WTW ProfiLine Oxi 3205 portable dissolved oxygen meter with DurOx 325 membrane covered galvanic dissolved oxygen sensor. Ammonium ion, nitrite ion, nitrate ion and reactive orthophosphate ion concentration were measured with an MN PF-11 filter photometer.

The pH, electrical conductivity, dissolved oxygen and oxygen saturation were determined by electroanalytical methods on the spot of sampling. The concentration of ammonium ion was measured by photometric phenate method at 720 nm. The concentration of nitrite ion was determined photometrically. Nitrite produces diazonium salt with sulphanilamide. This product reacts with N-(1-naphtyl)-ethylenediamine to form an intensive red-violet azo dye. The intensity of developed colour was measured at 520 nm. The concentration of nitrate ion was determined photometrically with 2,6-dimethylphenol in sulphuric-phosphoric acid mixture. In acidic solution nitrate ions react with 2,6-dimethylphenol to form 4-nitro-2,6-dimethylphenol. Measurements were performed at 470 nm. Reactive orthophosphate was determined by photometric molybdenum blue method at 720 nm. Chemical oxygen demand (COD) was determined in a strong acidic solution of potassium dichromate in the presence of silver sulphate and mercury(II) sulphate. At a temperature of 148°C, after two hours, the dichromate ion was reduced to chromium(III) ion. After this digestion the amount of residual dichromate ion was determined photometrically at 380 nm.

The m/z 44 chromatograms of the purified n -alkane solutions from the different water samples and the contaminating diesel fuel

Figure S1. m/z 44 chromatogram of the purified n -alkane solution from distilled water sample.

Figure S2. m/z 44 chromatogram of the purified n -alkane solution from the tap water sample.

Figure S3. m/z 44 chromatogram of the purified n -alkane solution from river water sample.

Figure S4. m/z 44 chromatogram of the purified n -alkane solution from industrial wastewater sample 1.

Figure S5. m/z 44 chromatogram of the purified n -alkane solution from industrial wastewater sample 2.

Figure S6. m/z 44 chromatogram of the purified n -alkane solution from industrial wastewater sample 3.

Figure S7. m/z 44 chromatogram of the purified n -alkane solution from confined water sample.

Figure S8. m/z 44 chromatogram of the purified n -alkane solution from groundwater sample 1.

Figure S9. m/z 44 chromatogram of the purified n -alkane solution from groundwater sample 2.

Figure S10. m/z 44 chromatogram of the purified n -alkane solution from contaminating diesel fuel.