Supplementary Materials

Effects of Hydrocarbons and Ionic Impurities on Foaming and Purification of UDS Desulfurization Solvent

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Figures

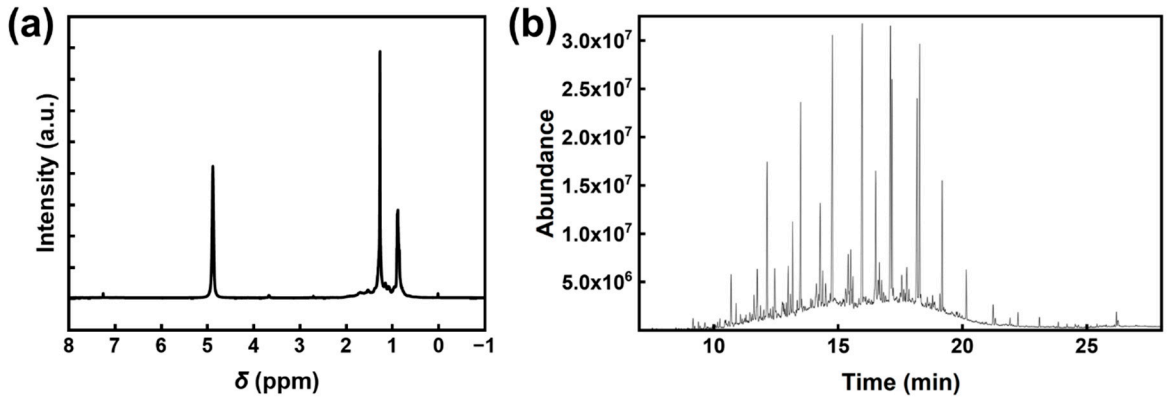


Figure S1. (a) ^{1}H NMR spectrum of the concentrated extract from produced water, (b) GC-MS of the concentrated extract from produced water.

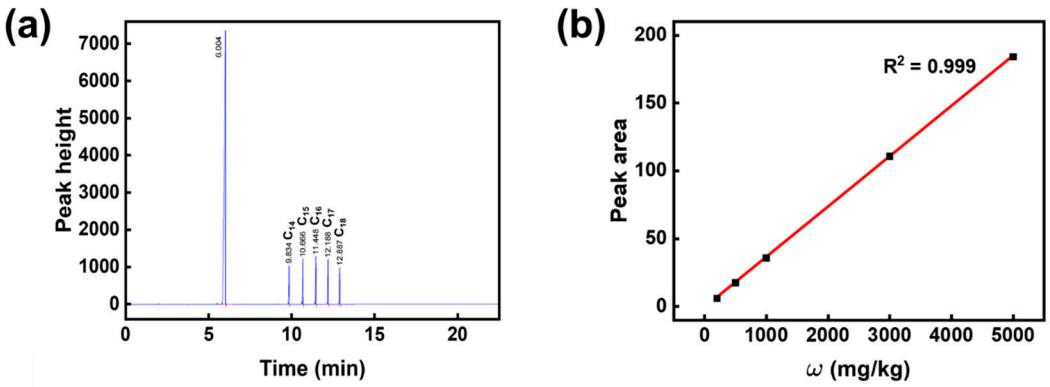


Figure S2. (a) GC chromatogram of the standard oil, (b) external calibration curve for total hydrocarbon quantification.

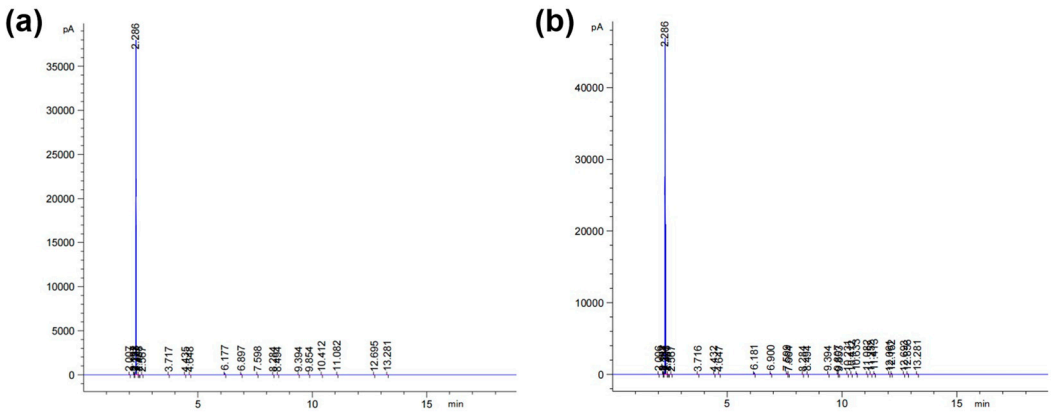


Figure S3. Representative GC-FID chromatograms of (a) fresh-UDS blank extract and (b) 1000 mg/kg matrix-spiked UDS extract.

Tables

Table S1. Basic properties of the 50 wt% fresh UDS working solution at 40°C

Property	Unit	Value
Appearance	—	Clear light-yellow liquid
Density	g/cm^3	1.0298
Dynamic viscosity	mPa·s	2.81
Surface tension	mN/m	29.1
Foam height	mm	20.0
Defoaming time	s	4.13

* Foam height and defoaming time were measured at 40°C and an N_2 flow rate of 250 mL/min.

Table S2. Basic properties of activated carbon samples

Code	Product description	Appearance	Particle size / specification	Moisture / %	Strength / %	pH	Ash / %	Iodine adsorption value / (mg/g)	Methylene blue adsorption value / (mL/0.1 g)
AC-01	Water-treatment activated carbon, 4–8 mesh	Brown to black solid	4–8 mesh	6.3	95	9.2	12.5	—	—
AC-02	Water-treatment activated carbon, 8–30 mesh	Brown to black solid	8–30 mesh	7	97.5	—	11.5	152	<2.0
AC-03	Solvent-recovery activated carbon, 4–8 mesh	Brown to black solid	4–8 mesh	6.3	95	9.2	12.5	—	—

AC-04	Solvent-recovery activated carbon, 6–12 mesh	Brown to black solid	6–12 mesh	6.3	96.5	9.8	3	900	5
AC-05	Cylindrical activated carbon for desulfurization and denitrification, 1.5 mm	Brown to black solid	1.5 mm	4.7	96	7–11	—	618	—
AC-06	Cylindrical activated carbon for desulfurization and denitrification, 6.0 mm	Brown to black solid	6.0 mm	7.5	96.5	7–12	—	—	—
AC-07	Activated carbon/coke, 2–5 mm	Brown to black solid	2–5 mm	3.5	90	10.2	14.5	535	<2.0

AC-08	Activated carbon for pressure swing adsorption, 2.0 mm	Black solid	2.0 mm	2.8	95	—	30.5	600	<2.0
AC-09	Wood-based powdered activated carbon, 325 mesh	Brown to black powder	325 mesh	9.3	—	7 – 12	10	900	10 mL
AC-10	Coconut-shell activated carbon for gold refining, 4–8 mesh	Brown to black solid	4–8 mesh	5.1	96	9.5	—	950	—
AC-11	Coconut-shell activated carbon for gold refining, 6–12 mesh	Brown to black solid	6–12 mesh	4.3	98.4	—	5.5	1140	13

AC-12	Gas-purification activated carbon, 10–24 mesh	Brown to black solid	10–24 mesh	3.6	97.9	—	5.9	800	4
AC-13	Rod-shaped gas-purification activated carbon	Brown to black solid	1.5 mm	7.5	89.2	—	10.3	1058	10.5

Table S3. Detailed ion chromatography conditions

Item	Anions	Cations
Eluent	20 mmol/L NaOH	20 mmol/L methanesulfonic acid
Separation column	IonPac AS-11	IonPac CS-12A
Suppressor	ASRS-ULTRA anion suppressor	DIS-5C
Detection method	Conductivity detector / ICS-1100	Conductivity detector / ICS-1100
Separation mode	High-performance ion-exchange chromatography	High-performance ion-exchange chromatography

Table S4. Composition analysis of major hydrocarbon impurities in produced water

Component No.	Compound name	Mass fraction (%)	CAS No.
1	Decane	0.050	124-18-5
2	Undecane	0.306	1120-21-4
3	4-Methyldecane	0.099	2847-72-5
4	Dodecane	1.467	112-40-3
5	2,6-Dimethylundecane	0.727	17301-23-4
6	5-Butyl-4-nonene	1.129	7367-38-6
7	7-Methyltridecane	1.665	26730-14-3
8	Tridecane	4.530	629-50-5
9	2-Methyltridecane	3.538	1560-96-9
10	2,6,10-Trimethyldodecane	2.036	3891-98-3
11	Tetradecane	6.521	629-59-4
12	2,7,10-Trimethyldodecane	5.336	74645-98-0
13	n-Pentadecane	8.469	629-62-9
14	2-Methylpentadecane	6.756	1560-93-6
15	n-Hexadecane	9.063	544-76-3
16	2,6,10-Trimethyltetradecane	8.490	14905-56-7
17	n-Heptadecane	8.656	629-78-7
18	n-Octadecane	6.519	593-45-3
19	Phytane	8.621	638-36-8
20	n-Heneicosane	3.232	629-94-7

21	n-Eicosane	1.208	112-95-8
22	n-Heptacosane	0.360	593-49-7

Table S5. Composition of the standard oil

Compound	CAS No.	Content in produced water (%)	Content in standard oil (%)
n-Tetradecane (n-C_{14})	629-59-4	6.521	16.62
n-Pentadecane (n-C_{15})	629-62-9	8.469	21.59
n-Hexadecane (n-C_{16})	544-76-3	9.063	23.10
n-Heptadecane (n-C_{17})	629-78-7	8.656	22.07
n-Octadecane (n-C_{18})	593-45-3	6.519	16.62

Table S6. Replicate determination results and method validation metrics

Item		1	2	3
Replicate	1	481.89	1052.48	2989.81
	2	472.17	1024.24	3051.03
	3	481.35	1056.42	3059.46
Mean(mg/kg)		478.47	1044.38	3033.43
Relative standard deviation, *RSD*(%)		1.14	1.68	1.25
Theoretical concentration,μ(mg/kg)		500.00	1000.00	3000.00
Relative error,*RE*(%)		−4.31%	4.44%	1.11%

Table S7. Ion concentrations of UDS solvent before and after adsorbent treatment

ion	sample	XRK207	A-98FM	IRA-900	A-654	Activated Carbon
$Formate^-$(mg/L)	900	96.7	9	481.4	570.33	899.28
$Acetate^-$(mg/L)	2381	647.7	151.9	1334.4	1681.4622	2165.106218
$Oxalate^{2-}$(mg/L)	509	66.2	29.4	29.6	444.0007	508.11
Cl^-(mg/L)	75	12.7375	3.29	28.8375	51.165	71.1525
SO_4^{2-}(mg/L)	60.8	0	0	0	0	11

Table S8. Packed masses of activated carbons used for q_{0-12} calculation

Sample	m_{ads} (g)
AC-02	27.4890
AC-11	20.0277
AC-12	22.7766
AC-04	21.9912
AC-13	20.0277
AC-08	24.3474
AC-07	27.8817

* The packed-bed volume was 39.27 mL. The initial total hydrocarbon content C_0 was 200 mg/kg. The volumetric flow rate was 5 mL/min, and the density of the 50 wt% UDS working solution was 1.0298 kg/L. Thus, the feed mass flow rate F_m was 0.30894 kg/h.

Table S9. Concentrations of individual anions in field-aged UDS lean solvent before and after A-98FM treatment

Sample	Formate (mg/L)	Acetate (mg/L)	Chloride (mg/L)	Sulfate (mg/L)	Oxalate (mg/L)	Total anionic impurities (mg/L)
Field-aged lean solvent	2466	1158	117	60.8	490	4288.8
After A-98FM treatment	24.7	73.9	38.4	3.77	28.3	165.07