# Supplementary Information for: Sustainable and scalable development of PVDF-OH Ag/TiO<sub>x</sub> nanocomposites for simultaneous oil/water separation and pollutant degradation

Ondřej Havelka,<sup>*a,b*</sup> Fatma Yalcinkaya,<sup>*a*</sup> Stanislaw Waclawek,<sup>*a*</sup> Vinod V.T. Padil,<sup>*c*</sup> Vincenzo Amendola,<sup>*d*</sup> Miroslav Černík <sup>*a*</sup> and Rafael Torres-Mendieta <sup>*a,\**</sup>

<sup>a</sup>Institute for Nanomaterials, Advanced Technologies and Innovation, Technical University of Liberec, Liberec, Studentská 1402/2, 461 17, Czech Republic.

<sup>b</sup>Faculty of Mechatronics, Informatics and Interdisciplinary Studies, Technical University of Liberec, Liberec, Studentská 1402/2, 461 17, Czech Republic.

<sup>c</sup>Amrita School for Sustainable Development (AST), Amrita Vishwa Vidyapeetham, Amrita University, Amritapuri, Clappana P. O. Kollam, Kerala, India, PIN-690525

<sup>d</sup>Department of Chemical Sciences, University of Padova, Padova, I-35131, Italy.

## 1. Permeate flux



Figure S1: Set of graphs displaying the fitted permeate fluxes of the nanocomposites prepared at the pH 2 (A), original pH (B), and pH 11 (C).

Sample	Cycle	Permeate flux fit	Estimated permeate after 1 month
pH 2	1	4932+127848 · exp(-0.51184 · x)	4932
	2	$4522 + 46256 \cdot \exp(-0.22075 \cdot x)$	4522
	3	$5670 + 56482 \cdot \exp(-0.2673 \cdot x)$	5670
	4	$1641 + 40887 \cdot \exp(-0.15555 \cdot x)$	1641
	5	$887 + 39190 \cdot \exp(-0.1644 \cdot x)$	887
	6	$4044 + 50908 \cdot \exp(-0.19875 \cdot x)$	4044
	7	$-604+40835 \cdot \exp(-0.13084 \cdot x)$	0
	8	$305+38729 \cdot \exp(-0.11574 \cdot x)$	305

**Table S1.** Fitting of permeate flux in each cycle

	9	$2811 + 42907 \cdot \exp(-0.17186 \cdot x)$	2811
	10	$-44+40914 \cdot \exp(-0.13024 \cdot x)$	0
pH 7.1	1	11115+78943 · exp(-0.47383 · x)	11115
	2	9650+44919 · exp(-0.26282 · x)	9650
	3	$11042 + 61360 \cdot \exp(-0.35609 \cdot x)$	11042
	4	$8754 + 36420 \cdot \exp(-0.15094 \cdot x)$	8754
	5	9915+35917 · exp(-0.2914 · x)	9915
	6	9260+46570 · exp(-0.21775 · x)	9260
	7	8485+36210 · exp(-0.1458 · x)	8485
	8	11000+81971 · exp(-0.60588 · x)	11000
	9	$10994 + 39650 \cdot \exp(-0.22358 \cdot x)$	10994
	10	$9050+36071 \cdot exp(-0.20097 \cdot x)$	9050
pH 11	10 1	9050+36071 · exp(-0.20097 · x) 10325+41971 · exp(-0.09362 · x)	9050 10325
pH 11	10 1 2	9050+36071 · exp(-0.20097 · x) 10325+41971 · exp(-0.09362 · x) 9209+41255 · exp(-0.08432 · x)	9050 10325 9209
pH 11	10 1 2 3	9050+36071 · exp(-0.20097 · x) 10325+41971 · exp(-0.09362 · x) 9209+41255 · exp(-0.08432 · x) 6861+37369 · exp(-0.39876 · x)	9050 10325 9209 6861
pH 11	10 1 2 3 4	9050+36071 · exp(-0.20097 · x) 10325+41971 · exp(-0.09362 · x) 9209+41255 · exp(-0.08432 · x) 6861+37369 · exp(-0.39876 · x) 3676+35050 · exp(-0.26109 · x)	9050 10325 9209 6861 3676
pH 11	10 1 2 3 4 5	$9050+36071 \cdot exp(-0.20097 \cdot x)$ $10325+41971 \cdot exp(-0.09362 \cdot x)$ $9209+41255 \cdot exp(-0.08432 \cdot x)$ $6861+37369 \cdot exp(-0.39876 \cdot x)$ $3676+35050 \cdot exp(-0.26109 \cdot x)$ $245+30314 \cdot exp(-0.0923 \cdot x)$	9050 10325 9209 6861 3676 245
pH 11	10 1 2 3 4 5 6	$9050+36071 \cdot \exp(-0.20097 \cdot x)$ $10325+41971 \cdot \exp(-0.09362 \cdot x)$ $9209+41255 \cdot \exp(-0.08432 \cdot x)$ $6861+37369 \cdot \exp(-0.39876 \cdot x)$ $3676+35050 \cdot \exp(-0.26109 \cdot x)$ $245+30314 \cdot \exp(-0.0923 \cdot x)$ $3773+33858 \cdot \exp(-0.12639 \cdot x)$	9050 10325 9209 6861 3676 245 3773
pH 11	10 1 2 3 4 5 6 7	$9050+36071 \cdot \exp(-0.20097 \cdot x)$ $10325+41971 \cdot \exp(-0.09362 \cdot x)$ $9209+41255 \cdot \exp(-0.08432 \cdot x)$ $6861+37369 \cdot \exp(-0.39876 \cdot x)$ $3676+35050 \cdot \exp(-0.26109 \cdot x)$ $245+30314 \cdot \exp(-0.0923 \cdot x)$ $3773+33858 \cdot \exp(-0.12639 \cdot x)$ $3466+31820 \cdot \exp(-0.10741 \cdot x)$	9050 10325 9209 6861 3676 245 3773 3466
pH 11	10 1 2 3 4 5 6 7 8	$9050+36071 \cdot \exp(-0.20097 \cdot x)$ $10325+41971 \cdot \exp(-0.09362 \cdot x)$ $9209+41255 \cdot \exp(-0.08432 \cdot x)$ $6861+37369 \cdot \exp(-0.39876 \cdot x)$ $3676+35050 \cdot \exp(-0.26109 \cdot x)$ $245+30314 \cdot \exp(-0.0923 \cdot x)$ $3773+33858 \cdot \exp(-0.12639 \cdot x)$ $3466+31820 \cdot \exp(-0.10741 \cdot x)$ $4374+39204 \cdot \exp(-0.30942 \cdot x)$	9050 10325 9209 6861 3676 245 3773 3466 4374
pH 11	10 1 2 3 4 5 6 7 8 9	$\begin{array}{c} 9050+36071\cdot \exp(-0.20097\cdot x)\\ 10325+41971\cdot \exp(-0.09362\cdot x)\\ 9209+41255\cdot \exp(-0.08432\cdot x)\\ 6861+37369\cdot \exp(-0.39876\cdot x)\\ 3676+35050\cdot \exp(-0.26109\cdot x)\\ 245+30314\cdot \exp(-0.0923\cdot x)\\ 3773+33858\cdot \exp(-0.12639\cdot x)\\ 3466+31820\cdot \exp(-0.10741\cdot x)\\ 4374+39204\cdot \exp(-0.30942\cdot x)\\ 4025+39178\cdot \exp(-0.18341\cdot x)\end{array}$	9050 10325 9209 6861 3676 245 3773 3466 4374 4025

### 2. Rejection rates details



Figure S2: Set of graphs displaying the rejection rates of the nanocomposites prepared at the pH 2 (A), original pH (B), and pH 11 (C) over a period of first and second 10 minutes in 20 min cycles.

### 3. Catalytic contact time

The calculation of the catalytic contact time is determined according to the following set of formulas, where the volumetric flux can be described as the rate of volume flow across a unit area *S*, which is, in our case, the effective membrane area.

$$volumetric flux = \frac{rate of volume flow}{s}$$
(S1)  
$$t = \frac{h}{volumetrix flux}$$
(S2)

The catalytic contact time is the ratio between the decorated membrane thickness h and the calculated volumetric flux. The values for each cycle are displayed in Fig.S3.



Figure S3: Catalytic contact time

## 4. Economic sustainable footprint analysis

Material	Amount	Price (€)	Supplier
AgNO <sub>3</sub>	per 1 g	3.3	SigmaAldrich
Ti foil	per 1 g	1.1	SigmaAldrich
$dH_2O$	per 1 L	0.11	Envichem
Isopropanol	per 1 L	9.4	Penta s.r.o.
КОН	per 1 g	2.5	Fluka
PET support	per 10 m <sup>2</sup>	3.75	Mogul
Adhesive web	per 10 m <sup>2</sup>	0.98	-
Glass bathtub	1 piece	10.9	P-Lab
Laser batch	1 piece	8.8	Thermofisher

Table S2. Material cost

 Table S3. Instruments cost

Instrument	Price (€)	Supplier
Laser and optical system	112 558	NKT Photonics
Magnetic stirrer	162	Vevor

# Table S4. Instruments' lifetime

Instrument	Time (h)
Laser and optical system	100 000
Magnetic stirrer	10 000
Laser batch	2 600
Glass bathtub	2 600

 Table S5. Energy consumption of different parts of the setup, while the cost of 1 kWh in Czechia was 0.11599

 EUR during 2022 (www.kurzy.cz/komodity/cena-elektriny-graf-vyvoje-ceny/).

Item	Power (kWh)
Laser	0.5
Computer	0.2
Scanning head	0.3
Magnetic stirrer	0.02
Heating (Heat-press process)	1.0
Pressing (Heat-press process)	7.2

# Table S6. Non-industrially-optimized laser production

Material	Production (mg/h)
NPs	5.8
Ag	2.0
Ti	3.8

**Table S7.** Non-industrially-optimized laser irradiation times, which are necessary for the preparation of 1 m<sup>2</sup> nanocomposite. Since the element distributions on the nanocomposites vary depending on the employed pH, different irradiation times are necessary for producing the required amount of material.

Modification pH	Time (h)
2	24.4
original	3.6
11	36.9

**Table S8.** Additional parameters associated with the preparation of 1 m<sup>2</sup> membrane. The PVDF nanofibers are prepared by electrospinning, then integrated into a PET nonwoven support by a heat-press process, and finally dehydrofluorinated to allow the addition of NPs.

Item	Cost (€)	Preparation time (h)	Amount of material	Supplier
PVDF nanofibers	8.54	-	-	Elmarco
Heat-press	0.95	1	-	Pracovní stroje Teplice s.r.o.
Adhesive web	0.98	-	per 10 m <sup>2</sup>	Sigma Aldrich
PET support	3.75	-	per 10 m <sup>2</sup>	Mogul
Consumed KOH	0.09	1	0.04 g	Fluka
Consumed isopropanol	0.11	1	30 mL	Penta s.r.o.

**Table S9.** PVDF microfilter membranes available on the market.

Product	Dimensions	Supplier	Price
PVDF membrane, pore size 0.45 µm	diameter 4.7 cm, 200 pcs	Membrane Solutions	115€
PVDF membrane, pore size 0.3 µm	30.5 x 30.5 cm	Synder filtration	102€
PVDF membrane, pore size 0.45 µm	diameter 14.2 cm, 50 pcs	Durapore	656€
PVDF membrane, pore size 0.45 µm	26.5 cm x 375 cm	Thermo Scientific	452€

#### a. RLAL OPEX and CAPEX calculations

Note that IRT represents irradiation time.

$$IRT = MAX \left(\frac{amount of element (Ag,Ti) on the membrane}{production of element (Ag,Ti) per hour}\right)$$
(S3)

 $Energy \ cost \ of \ RLAL = \ cost \ per \ kWh \ x \ laser \ setup \ power \ x \ IRT$ (S4)

$$Ag \ cost = AgNO3 \ price \ x \ \frac{M(AgNO3)}{M(Ag)} \ x \ silver \ production \ x \ IRT$$
(S5)

Ti cost = titanium foil price x titanium production x IRT (S6)

dH20 cost = dH20 price x volume of dH20 consumed during IRT (S7)

RLAL OPEX = Energy cost of RLAL + Ag cost + Ti cost + dH20 cost (S8)

$$Laser usage cost = \frac{Laser setup \ cost}{Laser \ setup \ lifetime} \ x \ IRT$$
(S9)

 $Other RLAL CAPEX = \left(\frac{Magnetic \ stirrer \ cost}{Magnetic \ stirrer \ lifetime} + \frac{Laser \ batch \ cost}{Batch \ lifetime}\right) x \ IRT$ (S10)

RLAL CAPEX = Laser usage cost + Other CAPEX (S11)

#### b. Heat-press process and alkalizations process cost calculations

Note that HP is an abbreviation for heat-press process and AT represents alkalization time.

$$Energy \ cost \ of \ HP = \ HP \ time \ x \ cost \ per \ kWh \ x \ HP \ power$$
(S12)

 $HP \ cost = Energy \ cost \ of \ HP + Adhesive \ web \ price + \ PET \ price$  (S13)

KOH cost = KOH price x amount of KOH on the membrane (S14)

 $Isopropanol \ cost = \ Isopropanol \ price \ x \ consumed \ isopropanol \ (S15)$ 

 $\left(\frac{Glass \ bathtub}{Bathtub \ lifetime}\right) + \frac{Alkalization \ cost}{Magnetic \ stirrer \ cost} = KOH \ cost \ + \ Isopropanol \ cost \ + \\ + \ Magnetic \ stirrer \ cost} + magnetic \ stirrer \ power \ x \ cost \ per \ kWh\right) \ x \ AT \ (S16)$ 

## 5. Table of Content



Figure S4: Freshwater scarcity remains a global challenge, often exacerbated by oil contamination. The current study tackles this issue by cleaning oily wastewater while removing its dissolved organic pollutants with PVDF-OH Ag/TiO<sub>x</sub> sustainable nanocomposites.