Accessory publication

Photodegradation of nonylphenol polyethoxylates in aqueous solution

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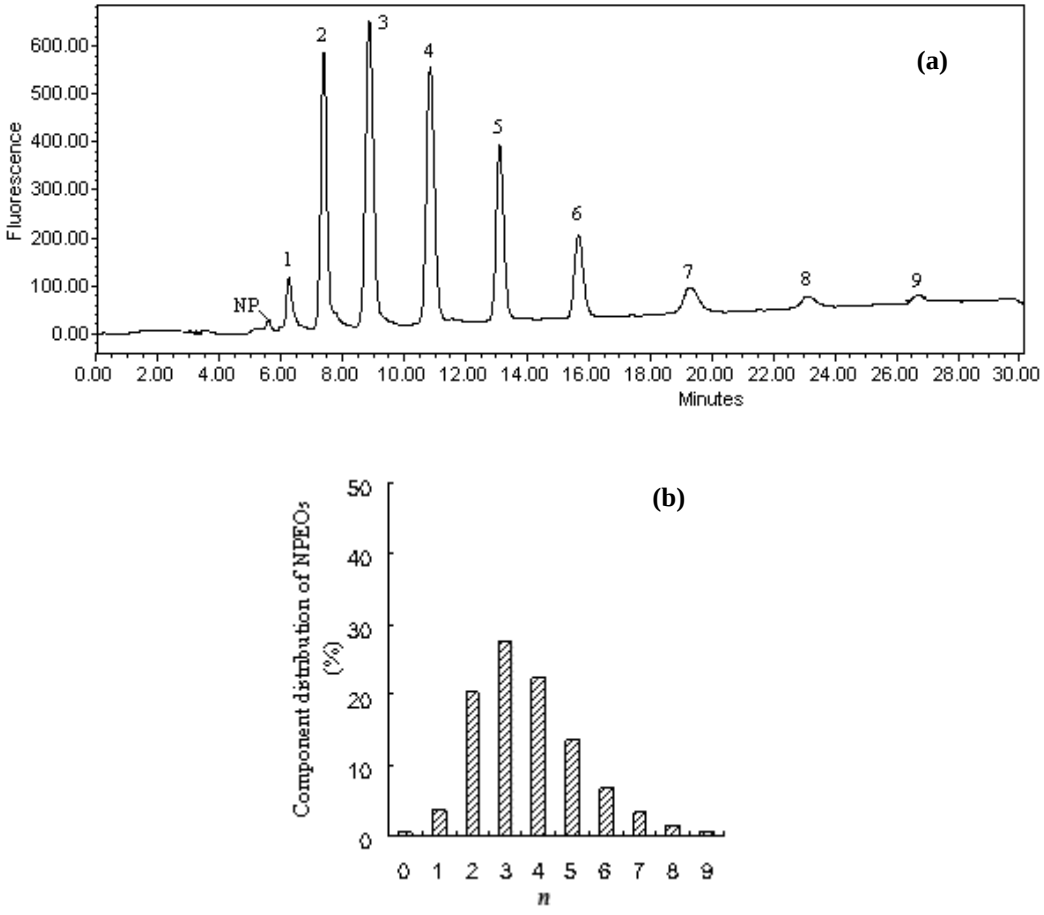

Fig. A1. Sample chromatogram (a) and component distribution (b) of $NPEO_{0–9}$ in the NPEO (nonylphenol polyethoxylates) mixture used in experiment. Peaks and columns from left to right represent $NPEO_n$ with n = 0–9, respectively.

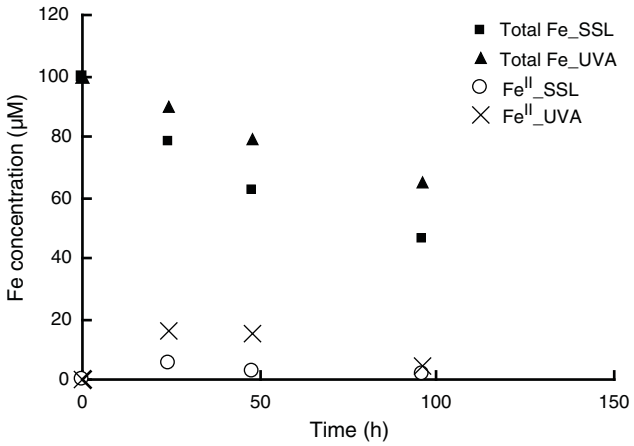

Fig. A2. Concentrations of Fe^{II} and total Fe in Fe^{III} solution as a function of irradiation time. Note: Fe^{II} in solution was determined spectrophotometrically at 510 nm as the Fe^{II}-*o*-phenanthroline complex. SSL, simulated sunlight. For analysis of total Fe, Fe^{III} in solution was converted to its ferrous state by reaction with acidified hydroxylamine. (W. B. Fortune, M. G. Mellon, Determination of iron with *o*-phenanthroline: a spectrophotometric study. *Ind. Eng. Chem. Anal. Ed.* **1938**, *10*, 60.)

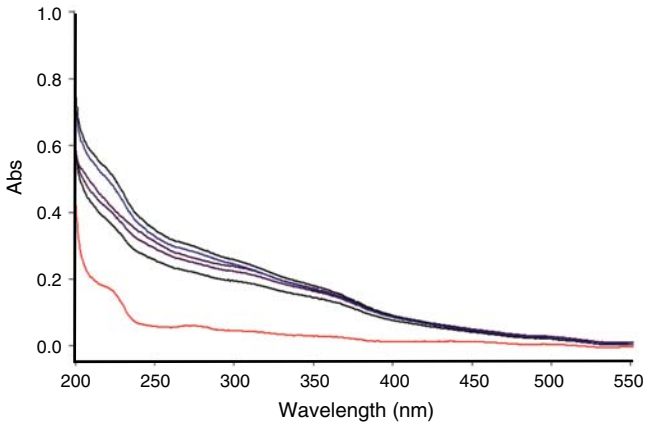

Fig. A3. UV-visible absorption spectra of different aquatic solutions containing (from lower to upper curve): 100 μM $NPEO_3$ at 0 h; 100 μM $NPEO_3$ and 100 μM Fe^{III} under SSL (simulated sunlight) irradiation at 1 h; 100 μM Fe^{III} at 0 h; 100 μM $NPEO_3$ and 100 μM Fe^{III} under UVA irradiation at 1 h; 100 μM $NPEO_3$ and 100 μM Fe^{III} in the dark at 1 h; 100 μM $NPEO_3$ and 100 μM Fe^{III} at 0 h. NPEO, nonylphenol polyethoxylate.

Table A1. Parameters of full-scan mass spectrometry for electrospray ionisation (ESI–/ESI+)

RF, radio frequency; LM, low mass; HM, high mass

Ion model	ESI–	ESI+
Capillary (kV)	3.00	3.20
Cone (V)	25.00	25.00
Extractor (V)	3.00	3.00
RF lens (V)	0.5	0.5
Source temperature (°C)	110	110
Desolvation temperature (°C)	450	450
Cone gas flow (L h^{-1})	20	20
Desolvation gas flow (L h^{-1})	500	500
LM 1 resolution	13.0	14.0
HM 1 resolution	13.0	14.0
Ion energy 1 (eV)	0.8	0.8
Entrance (V)	30	30
Collision energy (eV)	1	1
Exit (V)	30	30
LM 2 resolution	13.0	14.0
HM 2 resolution	13.0	14.0
Ion energy 2 (eV)	1.5	0.5
Multiplier (V)	650	650
Syringe pump flow (μL min^{-1})	10.0	10.0
Gas cell Pirani pressure (hecto-Pa)	<1e–4	<1e–4