Supplementary Information

Ozone compatibility with polymer nanofiltration membranes

Sara Ouali^{1, 2}, Patrick Loulergue¹, Pierre-François Biard¹, Noureddine Nasrallah², Anthony Szymczyk^{1*}.

¹Univ Rennes 1, Ecole Nationale Supérieure de Chimie de Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) – UMR 6226, F-35000 Rennes, France.

²Faculté de Génie Mécanique et Génie des Procédés, Université des Sciences et de la Technologie Houari Boumediene, Algiers, Algeria.

*Corresponding author: anthony.szymczyk@univ-rennes1.fr

Degradation of ozone in pure water according to the SBH (Staehelin, Bader and Hoigné) model [1]

Initiation reactions:

$0_3 + 0H^- \rightarrow HO_2^- + 0_2$	k=70 M ⁻¹ s ⁻¹	(1)
$O_3 + HO_2^- \to HO' + O_2^{-1} + O_2$	$k=2.8 \times 10^6 \mathrm{M}^{-1} \mathrm{s}^{-1}$	(2)

According to these reactions, the ozone decomposition initiation can be enhanced by increasing the pH or adding hydrogen peroxide.

Propagation reactions:

$0^3 + 0^5 \rightarrow 0^3 + 0^5$	$k=1.6 \times 10^9 \mathrm{M}^{-1} \mathrm{s}^{-1}$	(3)
<i>HO</i> ; → HO'+O ₂	$k=1.4 \times 10^5 \mathrm{M}^{-1} \mathrm{s}^{-1}$	(4)
$H0^{\bullet}+O_3 \longrightarrow H0^{\bullet}_2+O_2$	$2 \times 10^{8} \mathrm{M}^{-1} \mathrm{s}^{-1} < \mathrm{k} < 2 \times 10^{9} \mathrm{M}^{-1} \mathrm{s}^{-1}$	(5)
HO_4 \rightarrow HO_2 $+O_2$	$k = 2.8 \times 10^4 \mathrm{M}^{-1} \mathrm{s}^{-1}$	(6)

Ending reactions:

HO_4 + HO_4 $\to H_2O_2 + 2O_3$	$k = 5 \times 10^9 \mathrm{M}^{-1} \mathrm{s}^{-1}$	(7)
HO_4 + HO_3 $\to H_2O_2 + O_3 + O_2$	$k = 5 \times 10^9 \mathrm{M}^{-1} \mathrm{s}^{-1}$	(8)

The reaction rate constant of the reaction (5) is controversial in the literature [2].

Ozonation of PES powder

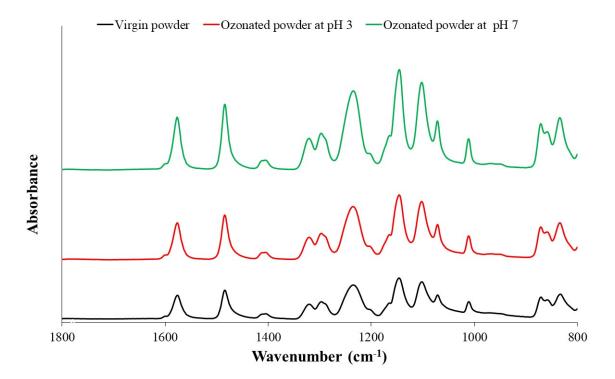


Figure S1. ATR-FTIR spectra of a PES powder (virgin and ozonated at pH 3 and 7).

The ozonation experimentation on the PES powder was performed with the same device and protocol than for the membranes (part 2.3). The flask containing the membrane sample was just replaced by a glass tube filled with 0.3 g of PES powder. Two filters were introduced at the inlet and outlet of the tube to avoid powder leaching in the apparatus.

References

[1] R.E. Buehler, J. Staehelin, J. Hoigne, Ozone decomposition in water studied by pulse radiolysis. 1. Perhydroxyl (HO2)/hyperoxide (O2-) and HO3/O3- as intermediates, The Journal of Physical Chemistry. 88 (1984) 2560–2564. https://doi.org/10.1021/j150656a026.

[2] U. von Gunten, Ozonation of drinking water: Part I. Oxidation kinetics and product formation, Water Research. 37 (2003) 1443–1467. https://doi.org/10.1016/S0043-1354(02)00457-8.