Electronic Supplementary material

Tailoring the microstructure and properties of PES/SPSf loose nanofiltration membranes using SPES as a hydrophilic polymer for the effective removal of dyes via steric hindrance and charge effect

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MD simulation

First, the conjugate gradient algorithm and energy minimization were performed to obtain a stable structure. Condensed-phased Optimized Molecular Potential for Atomistic Simulation Studies force field was also used to optimize these structures. Each sample was then equilibrated under the NPT ensemble at a constant temperature of 300 K to achieve an equilibrium state with zero pressure for 30 ns. Furthermore, a potential cut-off radius of 2.25 nm is applied in the calculation of the non-bonded interaction. And the PPPM has been used to describe the electrostatic. The Andersen feedback thermostat and Berendsen barostat algorithm are applied in the system with temperature and pressure conversion. Finally, the properties of our structures are

obtained in the last 3000 ps. The radial distribution functions (RDFs), g(r), give the probability of molecules occurring at the distance (r).

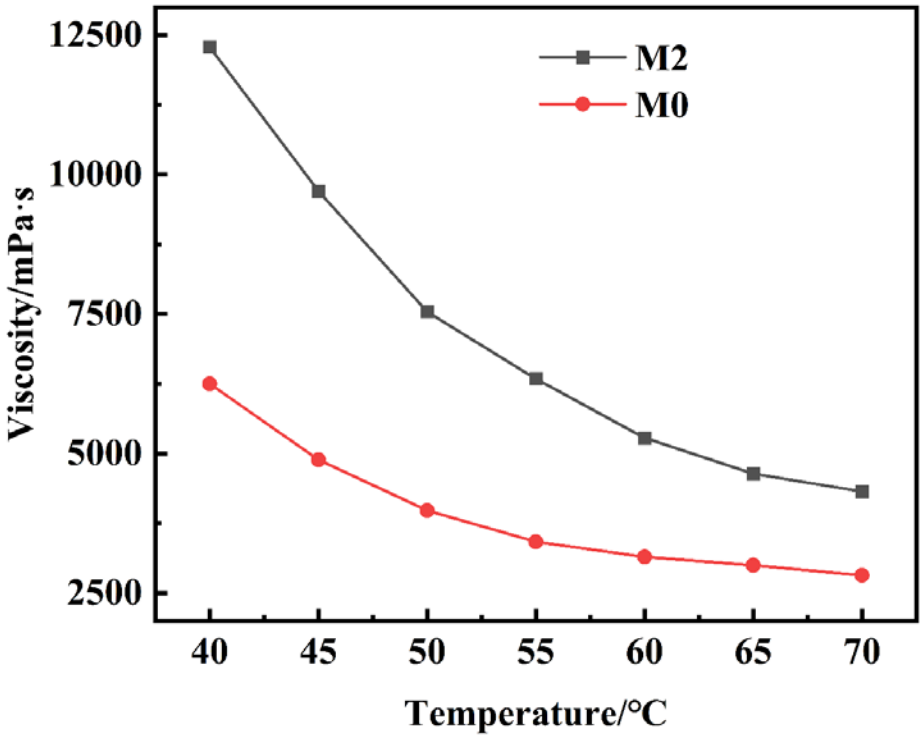

Fig. S1. Viscosity comparison of M2 (with AA) and M0 (without AA).

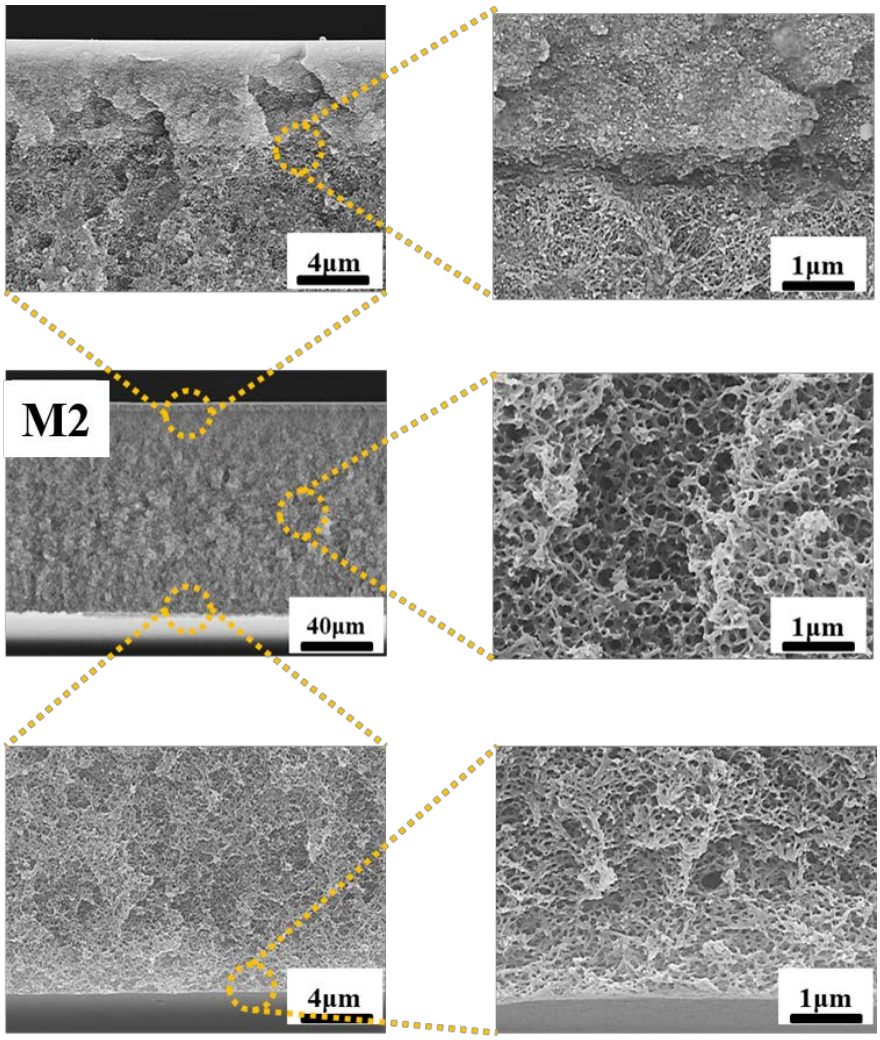

Fig. S2. SEM images of the cross-section of M2 at high magnification.

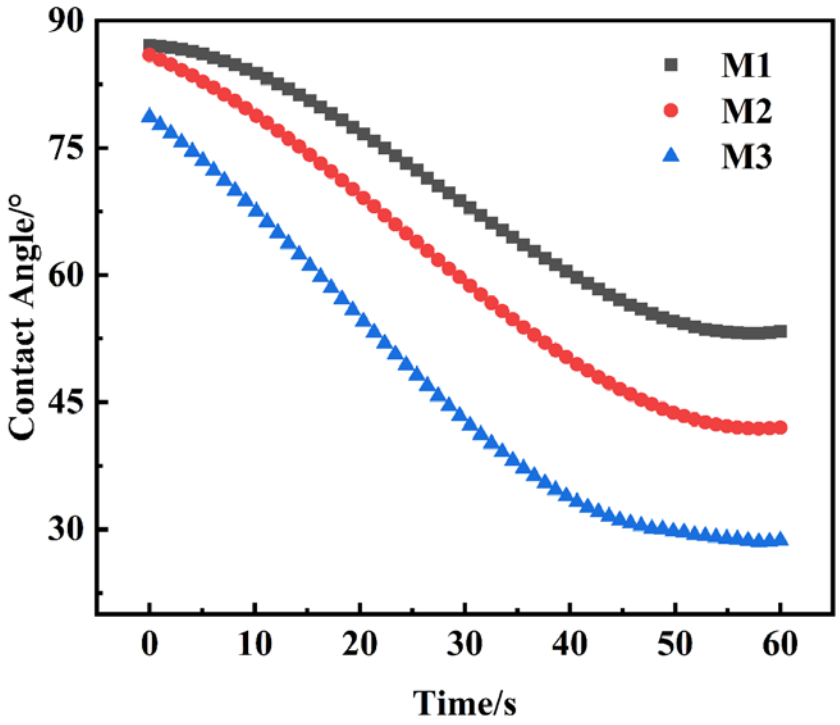

Fig. S3. Surface dynamic contact angle of the PES/SPSf/SPES blend membranes.

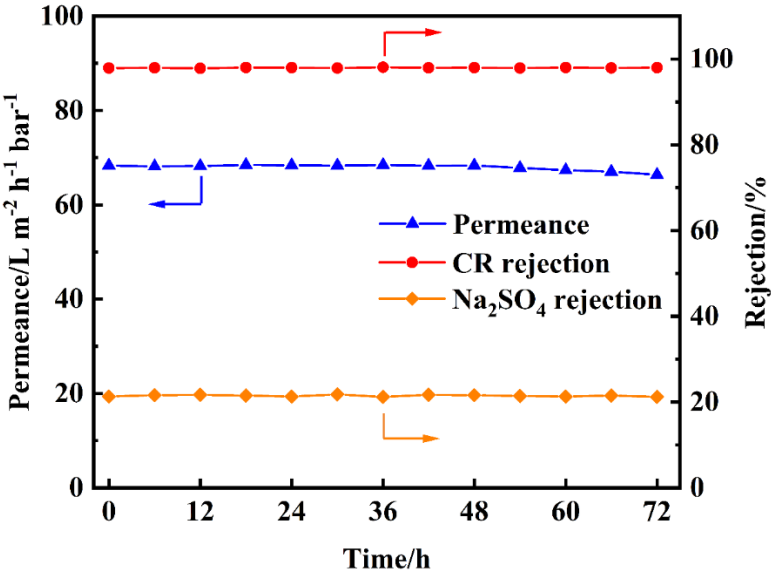

Fig. S4. Stability of M2 operation for CR/Na_2SO_4 mixed solution treatment

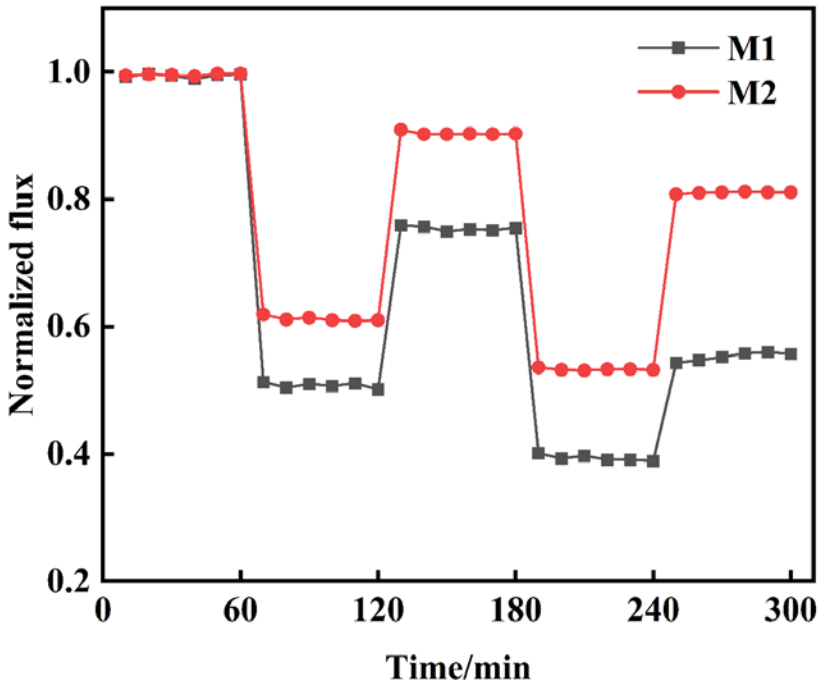

Fig. S5. Anti-fouling performance of PES/SPSf/SPES LNF membranes with a CR solution.