Supporting Information

Application of a biodegradable poly(butylene adipate-co-terephthalate) membrane for phenol pervaporation recovery

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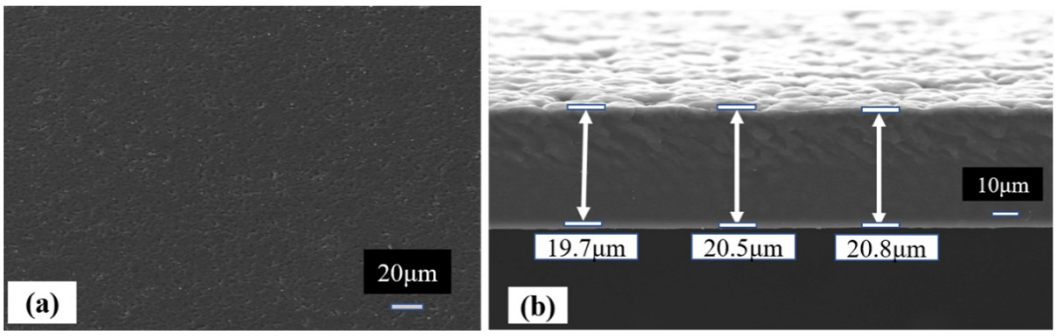

Fig. S1 SEM images of the surface (a) and the cross-section (b) of pure PBAT membrane.

Table S1 Number of phenol and water molecules and PBAT chains in each cell

Models	Total sorption uptake (g/g membrane)	Phenol content (wt%)	Cell component		
			PBAT	Phenol	Water
PBAT-0.000	-	-	2	-	-
PBAT-0.002	0.0481	66	2	16	42
PBAT-0.004	0.0632	76	2	24	39
PBAT-0.006	0.0869	79	2	34	47
PBAT-0.008	0.1074	83	2	44	47
PBAT-0.010	0.1308	85	2	57	50

PBAT-n represents the model at different feed concentrations.

Table S2 PBAT-phenol and PBAT-water model components.

Module	Cell component		
	PBAT	Phenol	Water
PBAT-phenol	2	40	-
PBAT-water	2	-	40

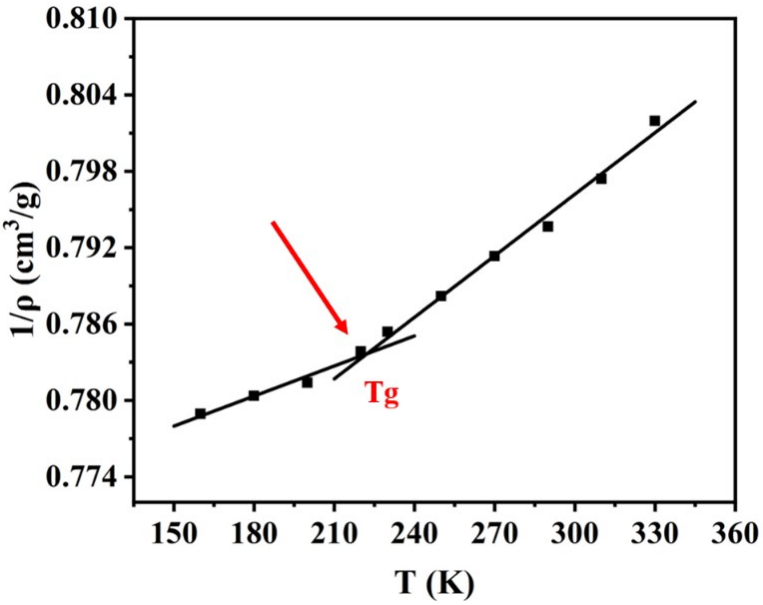

Fig. S2 Specific volume of PBAT membrane as a function of temperature.

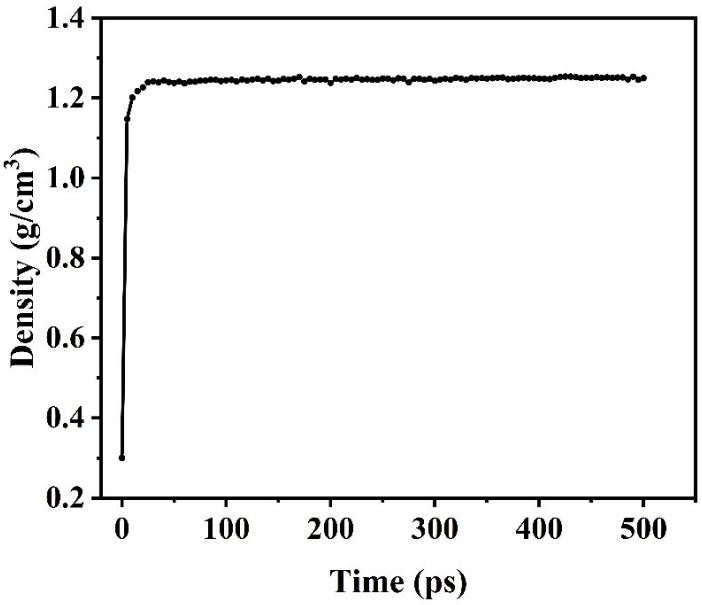

Fig. S3 Density of pure PBAT membrane model at 298 K.

3.3 Physical property analysis

3.3.1 Non-bond interaction energy

The non-bond interaction energy consists of three components, which are van der Waals force interaction energy, polar interaction energy and hydrogen bond energy. This paper focused on the non-bond interaction energy of PBAT membrane with phenol

and water, respectively. It could be calculated from Eq. 1

$$E_{i-j} = E_{total} - E_i - E_j \quad (1)$$

where E_{i-j} (KJ/mol) is the non-interaction energy between components i and j, E_{total} (KJ/mol) is the total energy of the model, and E_i and E_j (KJ/mol) are the energy of component i and j, respectively.

3.3.2 Fractional accessible volume (FAV) and fractional cavity volume (FCV)

The formula for calculating the FAV value of the PBAT membrane in the pure membrane model and the swollen model is as shown in Eq. 2.

$$FAV(r) = \frac{V - V_c}{V} \times 100\% \quad (2)$$

where V is the volume of the cell and V_c is the occupied volume which circled by the Connally surface. And FAV is FFV when the probe radius is zero. The Connally surface was obtained by a hard spherical particle which has specific radius.[36,37] This process was carried out in Materials Studio.

The cavity size distribution inside the membrane can be further obtained by the Connolly surface. The specific formula for the FCV(r) with radius in the range of r-r+Δr is as Eq. 3.

$$FCV(r) = \frac{AccV(r) - AccV(r + \Delta r)}{V} \quad (3)$$

where AccV(r) is the accessible volume when the probe radius is r, AccV(r+Δr) is the accessible volume when the probe radius is r+Δr. And V is the cell volume. Δr was taken as 0.1 Å and r was set from 0 to 3.0 Å.

3.3.3 Mean-squared displacement (MSD)

The MSD of phenol and water molecules are analyzed using the Einstein relationship:

$$MSD = \frac{1}{N}\sum_{i=1}^{N} < [r_i(t_0 + t) - r_i(t_0)]^2 > \quad (4)$$

where N is the total number of atoms, $r_i(t_0 + t)$ and $r_i(t_0)$ are the positions at time $t_0 + t$ and time t_0, respectively.

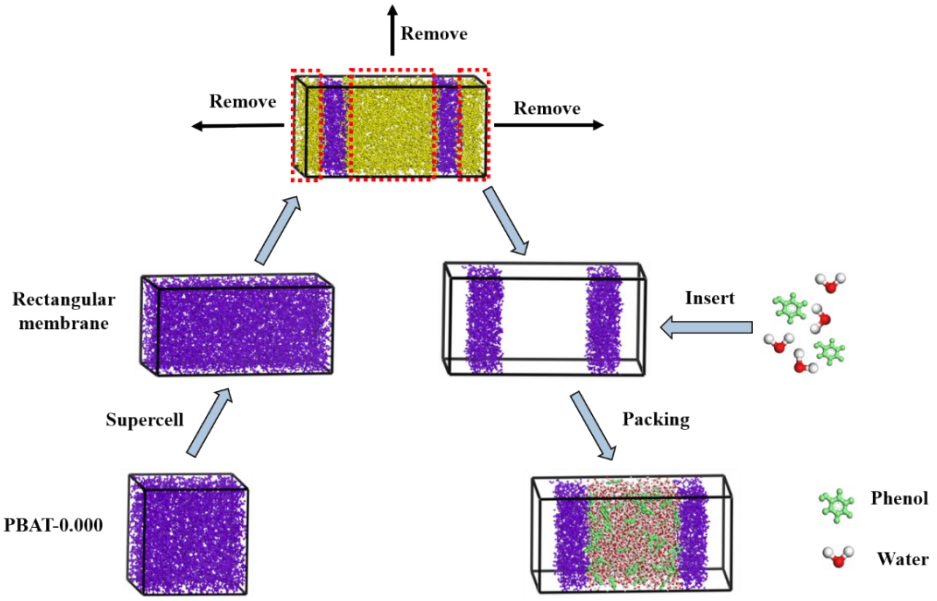

Fig. S4 The schematic diagram of the detailed simulation process for adsorption, diffusion and permeation analysis.

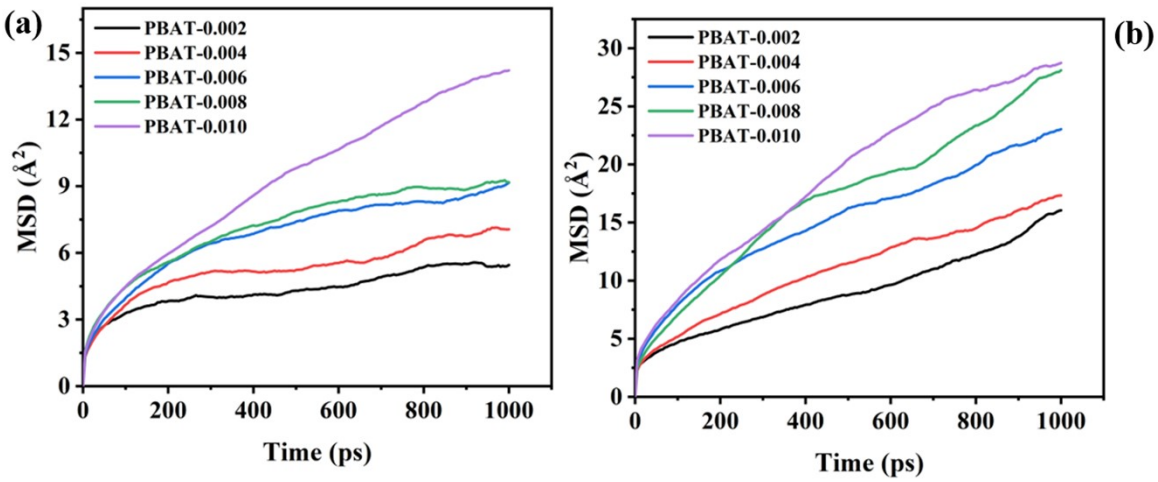

Fig. S5 Mean-squared displacement (MSD) diagrams of the (a) phenol and (b) water molecules in the five models swelled in 0.2 wt%, 0.4 wt%, 0.6 wt%, 0.8 wt% and 1.0 wt% phenol solutions during the 1000-ps molecular dynamics (MD) simulation at 343 K.

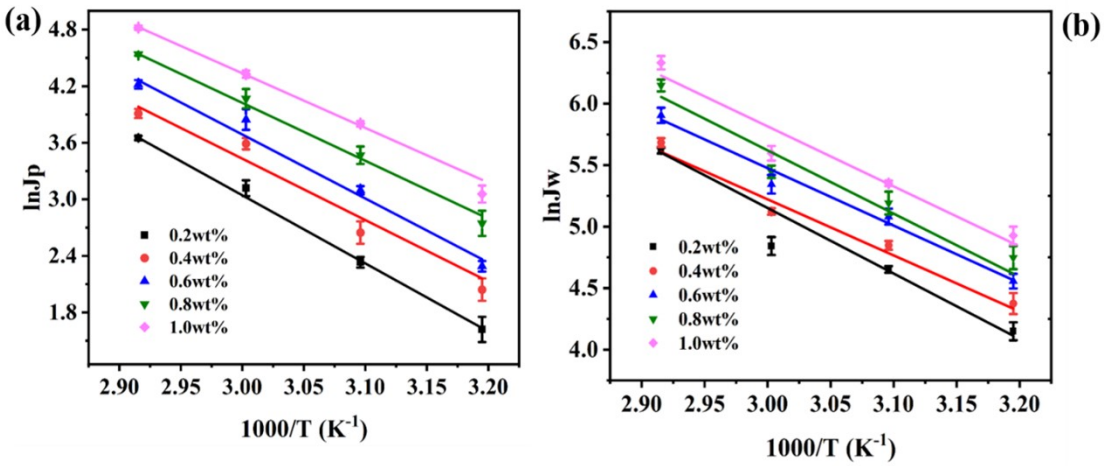

Fig. S6 Arrhenius curves of the (a) phenol flux and (b) water flux at various feed concentrations.

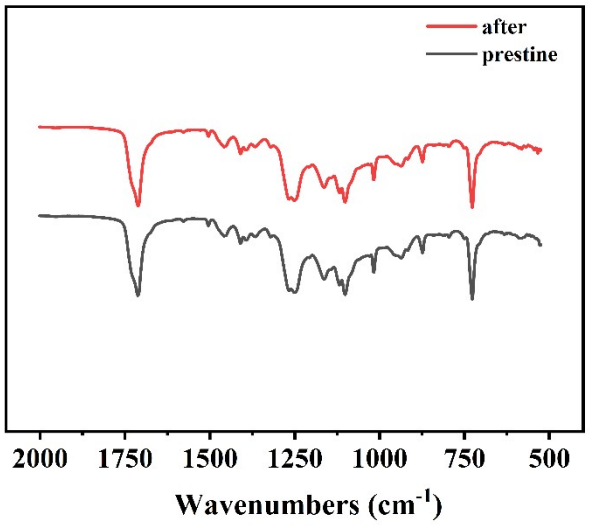

Fig. S7 FT-IR of PBAT membrane before and after reaction.