Supplementary Information for

Molecular Dynamic Simulations of Pressure-Driven Water Transport through Polyamide Nanofiltration Membranes at Different Membrane Densities

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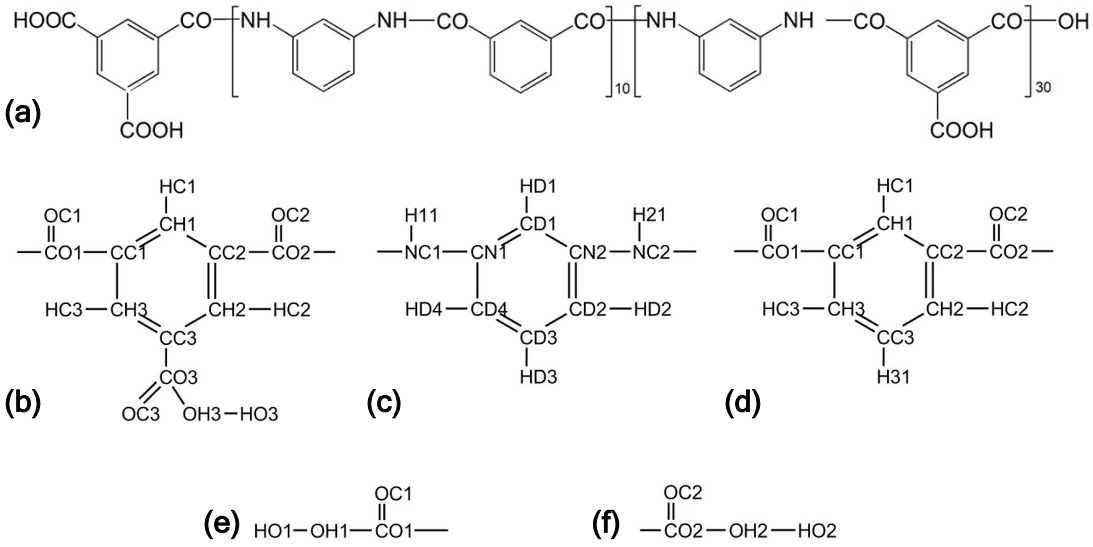

Fig. S1. The linear PA model (a) and the CHARMM models of the PA units: unit-1 (b), unit-2 (c), unit-3 (d), left terminal residue (e), and right terminal residues (f).

Table S1. The topology file of PA units for CHARMM with all patches

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* unit models of a single PA chain
* Charmm General Force Field v. 2b4 for below parameters

MASS     1    HGP1     1.00800    H ! O–H N–H
MASS     2    HGR61    1.00800    H ! aromatic H
MASS     3    CG2R61   12.01100    C ! 6-mem aromatic C
MASS     4    CG2O1    12.01100    C ! carbonyl C: amides
MASS     5    CG2O2    12.01100    C ! carbonyl C: carboxylic acids
MASS     6    NG2S1    14.00700    N ! CO–NH
MASS     7    OG311    15.99940    O ! hydroxyl oxygen
MASS     8    OG2D1    15.99940    O ! carbonyl O: amides carboxylic acids
MASS     9    OG2D2    15.99940    O ! carbonyl O: carboxylates, carbonate

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RESI unit1              0.00 ! unit-1
GROUP                        ! aromatic
ATOM CH1   CG2R61    -0.115   !
ATOM CH2   CG2R61    -0.115   !
ATOM CH3   CG2R61    -0.115   !
ATOM HC1   HGR61      0.115   !
ATOM HC2   HGR61      0.115   !
ATOM HC3   HGR61      0.115   !

GROUP                        !
ATOM CC1   CG2R61    0.0     !
ATOM CO1   CG2O1      0.52   !
ATOM OC1   OG2D1    -0.52    !
ATOM CC2   CG2R61    0.0     !
ATOM CO2   CG2O1      0.52   !
ATOM OC2   OG2D1    -0.52    !

GROUP                        !
ATOM CC3   CG2R61    -0.03   !
ATOM CO3   CG2O2      0.75   !
ATOM OC3   OG2D1    -0.55    !
ATOM OH3   OG311    -0.61    !
ATOM HO3   HGP1       0.44   !

BOND CC1 CH3 CC1 CO1
BOND CH1 CC2 CH2 CC3
BOND CH1 HC1 CH2 HC2
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BOND CH3 HC3
BOND CC2 CO2    CC3 CO3
BOND CO3 OH3 OH3 HO3
DOUBLE CC2 CH2 CC3 CH3
DOUBLE CC1 CH1 CO3 OC3
DOUBLE CO1 OC1 CO2 OC2


RESI unit2              0.00 ! unit-2
GROUP                        !
ATOM CD1    CG2R61     -0.115 !
ATOM CD2    CG2R61     -0.115 !
ATOM CD3    CG2R61     -0.115 !
ATOM CD4    CG2R61     -0.115 !
ATOM HD1    HGR61       0.115 !
ATOM HD2    HGR61       0.115 !
ATOM HD3    HGR61       0.115 !
ATOM HD4    HGR61       0.115  !

GROUP                        !
ATOM CN1    CG2R61      0.14    !
ATOM NC1    NG2S1      -0.47    !
ATOM H11    HGP1        0.33    !
ATOM CN2    CG2R61      0.14    !
ATOM NC2    NG2S1      -0.47    !
ATOM H21    HGP1        0.33    !

BOND CD1 CN2 CD2 CD3
BOND CD4 CN1
BOND CD1 HD1 CD2 HD2
BOND CD3 HD3 CD4 HD4
BOND CN1 NC1 NC1 H11
BOND CN2 NC2 NC2 H21
DOUBLE CN1 CD1 CN2 CD2 CD3 CD4


RESI unit3              0.00 ! unit-3
GROUP                        !
ATOM CH1    CG2R61     -0.115 !
ATOM CH2    CG2R61     -0.115 !
ATOM CH3    CG2R61     -0.115 !
ATOM HC1    HGR61       0.115 !
ATOM HC2    HGR61       0.115 !
ATOM HC3    HGR61       0.115 !
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ATOM CC3    CG2R61      -0.115
ATOM H31    HGR61        0.115

GROUP                           !
ATOM CC1    CG2R61       0.0     !
ATOM CO1    CG2O1        0.52    !
ATOM OC1    OG2D1       -0.52    !
ATOM CC2    CG2R61       0.0     !
ATOM CO2    CG2O1        0.52    !
ATOM OC2    OG2D1       -0.52    !

BOND CC1 CH3
BOND CH1 CC2 CH2 CC3
BOND CH1 HC1 CH2 HC2
BOND CH3 HC3 CC3 H31
BOND CC2 CO2 CC1 CO1
DOUBLE CC2 CH2 CC3 CH3
DOUBLE CC1 CH1
DOUBLE CO1 OC1 CO2 OC2
ANGLE CH2 CC3 H31    CH3 CC3 H31
DIHE HC2 CH2 CC3 H31    HC3 CH3 CC3 H31
DIHE CC2 CH2 CC3 H31    CC1 CH3 CC3 H31
IC CH2    CH3    *CC3    H31       0.0000    0.0000 180.0000    0.0000    0.0000


PRES COOH1                0.00    ! left terminal residue
ATOM CC1    CG2R61      -0.03
ATOM CO1    CG2O2        0.75    !
ATOM OC1    OG2D1       -0.55    !
ATOM OH1    OG311       -0.61    !
ATOM HO1    HGP1         0.44    !

BOND CO1 OH1    OH1 HO1
ANGLE OC1 CO1 OH1 CO1 OH1 HO1
ANGLE CC1 CO1 OH1
DIHE OC1 CO1 OH1 HO1    CC1 CO1 OH1 HO1
DIHE CH1 CC1 CO1 OH1    CH3 CC1 CO1 OH1
IMPR CO1 CC1 OH1 OC1


PRES COOH2                0.00    ! right terminal residue
ATOM CC2    CG2R61     -0.03
ATOM CO2    CG2O2        0.75    !
ATOM OC2    OG2D1       -0.55    !
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ATOM OH2    OG311      -0.61    !
ATOM HO2    HGP1        0.44    !

BOND CO2 OH2 OH2 HO2
ANGLE OC2 CO2 OH2 CO2 OH2 HO2
ANGLE CC2 CO2 OH2
DIHE OC2 CO2 OH2 HO2    CC2 CO2 OH2 HO2
DIHE CH1 CC2 CO2 OH2    CH2 CC2 CO2 OH2
IMPR CO2 CC2 OH2 OC2

PRES amide1                         ! linking CO2-NC1
BOND 1CO2 2NC1
ANGLE 1OC2 1CO2 2NC1    1CC2 1CO2 2NC1
ANGLE 1CO2 2NC1 2CN1    1CO2 2NC1 2H11
DIHE 1OC2 1CO2 2NC1 2H11    1OC2 1CO2 2NC1 2CN1
DIHE 1CC2 1CO2 2NC1 2H11    1CC2 1CO2 2NC1 2CN1
DIHE 1CH1 1CC2 1CO2 2NC1    1CH2 1CC2 1CO2 2NC1
DIHE 1CO2 2NC1 2CN1 2CD1    1CO2 2NC1 2CN1 2CD4
IMPR 1CO2 1CC2 2NC1 1OC2    2NC1 1CO2 2CN1 2H11


PRES amide2                         ! linking NC2-CO1
BOND 1NC2 2CO1
ANGLE 1NC2 2CO1 2OC1    1NC2 2CO1 2CC1
ANGLE 1CN2 1NC2 2CO1    1H21 1NC2 2CO1
DIHE 1H21 1NC2 2CO1 2OC1    1H21 1NC2 2CO1 2CC1
DIHE 1CN2 1NC2 2CO1 2OC1    1CN2 1NC2 2CO1 2CC1
DIHE 1NC2 2CO1 2CC1 2CH1    1NC2 2CO1 2CC1 2CH3
DIHE 1CD1 1CN2 1NC2 2CO1    1CD2 1CN2 1NC2 2CO1
IMPR 2CO1 2CC1 1NC2 2OC1    1NC2 2CO1 1CN2 1H21


PATCHING FIRS NONE LAST NONE

END
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