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Supporting Information

Towards a Better Understanding of Delamination of Multilayer Flexible Packaging Films by Carboxylic Acids

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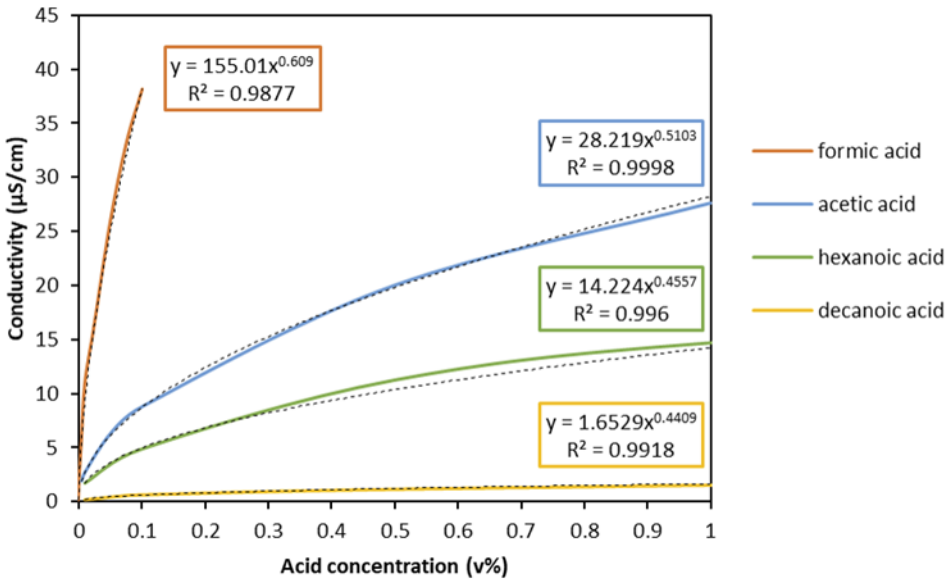

Figure S1. Calibration curves of formic acid, acetic acid, hexanoic acid and decanoic acid used for conversions of conductivity values to acid concentration.

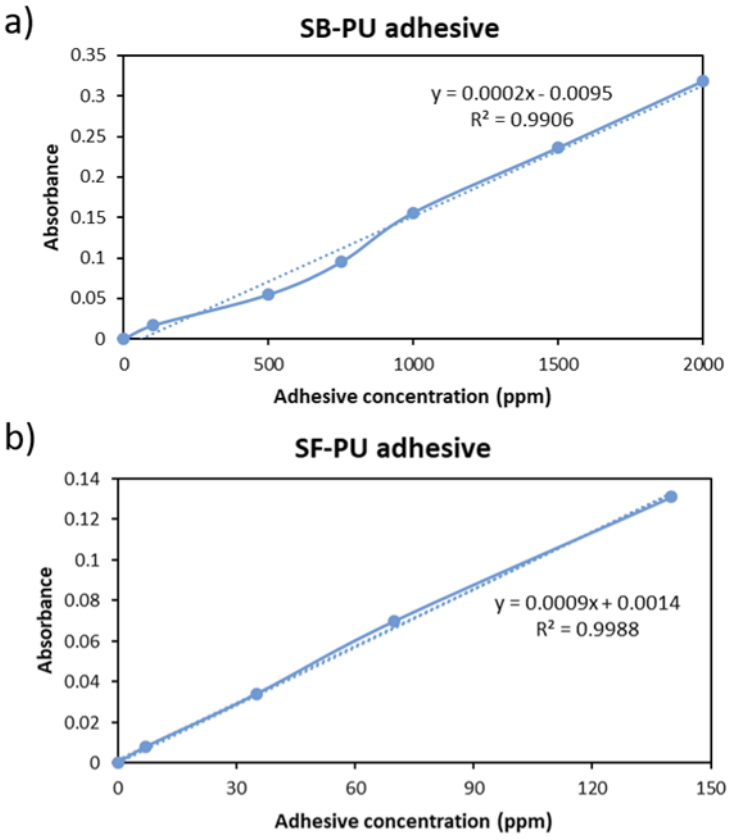

Figure S2. Calibration curves of a)SB-PU adhesive; b) SF-PU adhesive used to follow dissolution kinetics of adhesives in formic acid medium.

Table S1. The diffusion coefficient constant, D_0 and the activation energy of the diffusivity, E_d of each constituent polymer layer and the boundary layer, calculated via pseudorandom-search algorithm.

	corona PET (Type A)	corona PET (Type B)	chemPET	PE trans.	PE white	PP	Boundary layer
D_0 [cm²/s]	4.40E-02	4.70E+08	2.90E-06	1.58E+03	5.41E+25	3.93E+24	4.36E-11
E_d [J/mol]	-6.11E+04	-1.24E+05	-3.43E+04	-8.99E+04	-2.40E+05	-2.31E+05	-1.12E+05

Table S2. The density and acid concentration of formic acid (mg/cm³) at different temperature and volumes.

	at 25 °C		at 50 °C		at 65 °C		at 75 °C	
V% acid	density of mixture [mg/cm³]	C_{acid} [mg/cm³]	density of mixture [mg/cm³]	C_{acid} [mg/cm³]	density of mixture [mg/cm³]	C_{acid} [mg/cm³]	density of mixture [mg/cm³]	C_{acid} [mg/cm³]
0	1027.45	0	1004.29	0	990.04	0	980.38	0
10	1046.11	121.40	1022.06	118.20	1007.23	116.20	997.24	114.90
20	1064.76	242.80	1039.83	236.40	1024.43	232.40	1014.10	229.80
30	1083.42	364.20	1057.60	354.60	1041.62	348.60	1030.96	344.70
40	1102.07	485.60	1075.37	472.80	1058.82	464.80	1047.82	459.60
50	1120.73	607.00	1093.14	591.00	1076.02	581.00	1064.69	574.50
60	1139.38	728.40	1110.92	709.20	1093.21	697.20	1081.55	689.40
70	1158.04	849.80	1128.69	827.40	1110.41	813.40	1098.41	804.30
75	1167.36	910.50	1137.57	886.50	1119.01	871.50	1106.84	861.75
80	1176.69	971.20	1146.46	945.60	1127.61	929.60	1115.28	919.20
85	1186.02	1031.90	1155.34	1004.70	1136.20	987.70	1123.71	976.65
90	1195.34	1092.60	1164.23	1063.80	1144.80	1045.80	1132.14	1034.10
100	1214.00	1214.00	1182.00	1182.00	1162.00	1162.00	1149.00	1149.00

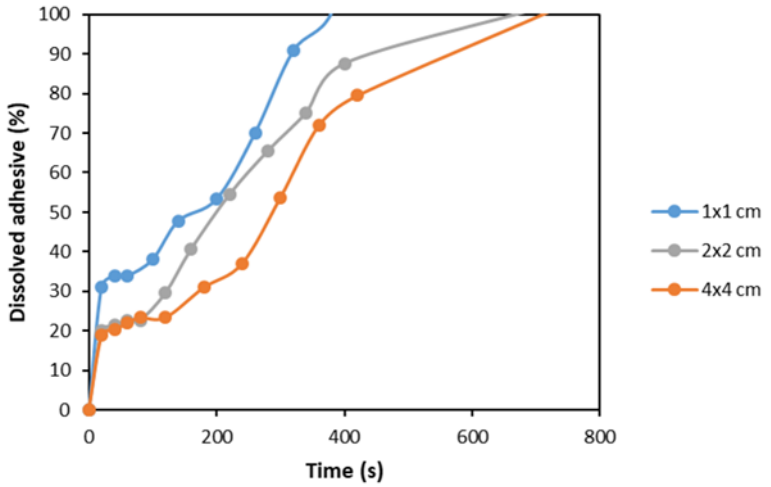

Figure S3. Delamination rate of sample B at different particle sizes under the same experimental conditions (at 100 °C, 100 v% formic acid, at 0.005 g/mL S/L ratio, stirring with a rotor at 400 rpm).

Table S3. SSE and TIC values of each case study.

sample	experimental conditions	SSE	TIC
A	at 75 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.025904067	0.173062
B	at 75 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.039762245	0.279267
C	at 75 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.002199464	0.154795
D	at 75 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.007381892	0.192268
E	at 75 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.001049302	0.126724
D	at 50 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.001744452	0.085850
D	at 65 °C, 100 v% formic acid, 0.005 g/mL of S/L	0.004474732	0.114847
B	at 75 °C, 85 v% formic acid, 0.005 g/mL of S/L	0.004011534	0.066406
B	at 75 °C, 75 v% formic acid, 0.005 g/mL of S/L	0.004723954	0.148119
B	at 75 °C, 50 v% formic acid, 0.005 g/mL of S/L	0.001650758	0.187504
B	at 75 °C, 100 v% formic acid, 0.12 g/mL of S/L	2.758340187	0.101994
D	at 75 °C, 100 v% formic acid, 0.025 g/mL of S/L	0.151356729	0.249143