Easily Recoverable and Reusable p-toluenesulfonic Acid for Faster Hydrolysis of Waste Polyethylene Terephthalate

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Characterizing the intrinsic viscosity of recycled PET powders

The intrinsic viscosity (IV) (dL g^{-1}) of recycled PET powders was measured via Ubbelohde viscometer at 25 °C. First, 0.005 g/mL PET solution was obtained by dissolve certain amount of recycled PET in phenol/tetrachloroethane (w/w, 3/2). Then, the obtained PET solution was added into Ubbelohde viscometer to test its outflow time (t). Using the same method to determine the outflow time (t_0) of the phenol/tetrachloroethane (w/w, 3/2) solvent. The intrinsic viscosity (IV) (dL g^{-1}) was calculated from following equation:

$$Intrinsic\ viscosity = \frac{0.25(\frac{t}{t_0} - 1 + 3\ln\frac{t}{t_0})}{c} \quad (1)$$

where, c is the PET solution concentration (0.005 g/mL).

Characterizing the crystallinity of recycled PET powders

The crystallinity of recycled PET powders was calculated through Differential Scanning Calorimetry (DSC) measurements by using a NETZSCH DSC 200F3 under N_2 atmosphere. The sample was heated starting from 30 °C till 300 °C then cooled to 50 °C and again heated to 300 °C at a heating/cooling rate of 10 °C min^{-1}. The crystallinity of PET samples was calculated via following equation:

$$X_c = [(\Delta H_m - \Delta H_{cc})/ \Delta H°_m] \text{ x } 100 \quad (2)$$

where, X_c is the crystallinity (%), ΔH_m (J g^{-1}) and ΔH_{cc} (J g^{-1}) are the measured melt and cold crystallization enthalpy of waste PET, respectively, and $\Delta H°_m$ = 140.1 J g^{-1} is the melting enthalpy of 100% crystalline PET.

Characterizing the purity of generated TPA and recovered PTSA

Firstly, 0.1 g of TPA purchased from Aladin was weighed and dissolved in 6 mL of a 1 mol/L sodium hydroxide solution. The sodium terephthalate (NaTPA) solution was then diluted to a

series of certain concentrations to produce standard solutions of TPA. The standard curve was drawn by recording the absorbance of the standard solutions at 240 nm (Figure S1a). To detect the purity of the produced TPA, a solution of NaTPA was prepared by the same procedure as the standard solutions.

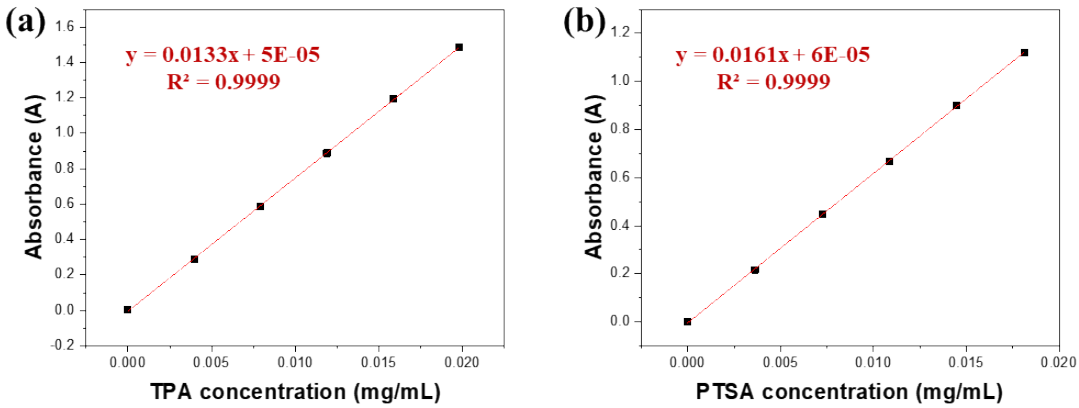

Figure S1. (a) The standard curve drawn based on the UV absorption values of vary concentrations of TPA at 240 nm wavelength. (b) The standard curve drawn based on the UV absorption values of vary concentrations of PTSA at 222 nm wavelength.

Firstly, 0.1 g of PTSA purchased from Aladin was dissolved in 6 mL water. Then, the PTSA aqueous solution was diluted to a series of concentrations to produce standard solutions of PTSA. The standard curve was drawn by recording the absorbance of the standard solutions at 222 nm (Figure S1b). To detect the purity of recovered PTSA (R-PTSA), a certain concentration (0.008-0.016 mg/mL) of R-PTSA aqueous solution was configured and detect its absorbance at 222 nm.

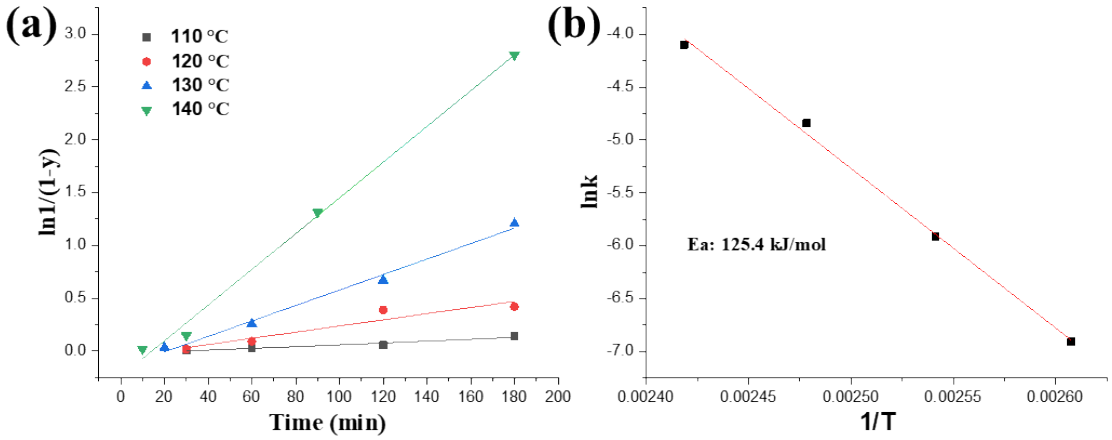

Figure S2. Hydrolysis kinetics of waste polyethylene terephthalate (PET) flakes with size of 1 cm x 1 cm in 80% *p*-toluenesulfonic acid (PTSA) aqueous solution. (a) Rate of waste PET hydrolysis at 110°C, 120°C, 130°C, and 140°C, respectively. (b) Arrhenius plot of the rate constant of waste PET hydrolysis. Reaction conditions: waste PET, 2.5 g; PTSA concentration, 80%; mass ratio of PTSA aqueous solution to waste PET, 20:1.

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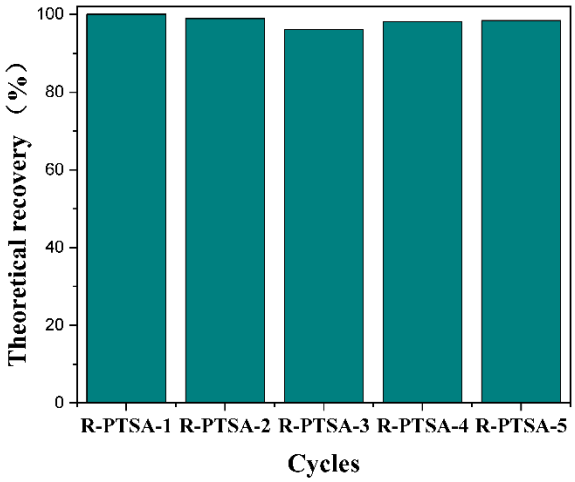

Figure S3. The theoretical recovery of R-PTSA at different cycles.

Table S1. Values used in Aspen Plus simulations of PET aicd-catalyzed hydrolysis.

Import			Output		
PET (kg/hr)	PTSA (kg/hr)	Water (kg/hr)	TPA (kg/hr)	EG (kg/hr)	Recycled PTSA (kg/hr)
125	2000	500	104.4	38.20	1828

Table S2. Energy recoveries and consumptions in Aspen Plus simulation.

	E0101	E0102	R0101	F0202	E0201	T0201-REB	T0201-COND
Heat duty (kW/hr))	446.13	8.12	-386.15	520.39	-41.62	90.50	-78.94