SUPPORTING INFORMATION

Fast Hydrolysis for Chemical Recycling of Polyethylene Terephthalate (PET)

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Table S1. Experimental reactor loadings.

T_{SP} (°C)	*Water loading (mL)	PET loading (g)
300	3.00	0.300
350	2.58	0.258
400	1.43	0.143
450	0.59	0.059
480	0.50	0.050
		0.063
500	0.46	0.046
		0.058
510	0.44	0.044
		0.055
		0.073
		0.110
		0.220
540	0.40	0.040
		0.050
550	0.39	0.039
		0.049
570	0.37	0.037

* water loading is such that reactor pressure would be 30 MPa at the set point temperature.

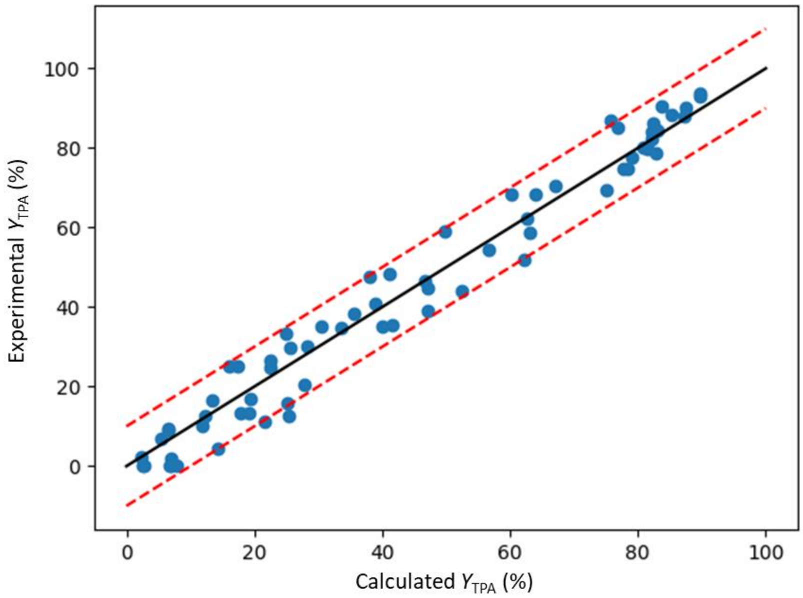

Figure S1. Comparison of experimental TPA yield with calculations made by Random Forest Regression, based on the dataset utilized for model training.

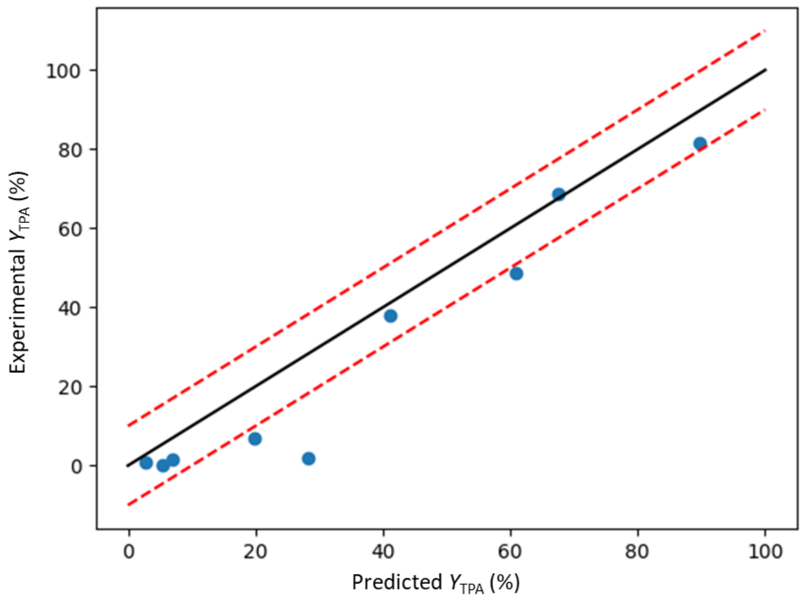

Figure S2. Comparison of experimental TPA yield with predictions made by Random Forest Regression, based on the dataset utilized for model predictions.

Table S2. Conditions and results for fast hydrolysis experiments. Uncertainties are measured standard deviations. T_{final} is the temperature calculated from equation 1 and N is the number of independent runs.

T_{SP} (°C)	t (sec)	m_{PET}/m_w	T_{final} (°C)	log SI	Y_{TPA} (%)	Y_{US} (%)	$Y_{isophthalic\ acid}$ (%)	$Y_{phthalic\ acid}$ (%)	Y_{BHET} (%)	$Y_{Benzoic\ Acid}$ (%)	Ring Bal (%)	ξ (°C·min)	N
300	15	1/10	105	-1.7	0 ± 0	100 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	100 ± 0	inf	3
300	60		241	9.6	0 ± 0	98 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	95 ± 3	inf	3
300	85		272	11.8	0 ± 0	96 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	97 ± 3	inf	3
300	115		289	13.2	0 ± 0	97 ± 3	0 ± 0	0 ± 0	0 ± 0	0 ± 0	98 ± 3	inf	3
300	175		298	14.5	2 ± 1	79 ± 7	5 ± 0	0 ± 0	8 ± 0	0 ± 0	94 ± 9	$(6.8 \pm 6.0) \times 10^{6}$	4
350	55		270	10.9	0 ± 0	93 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	91 ± 2	Inf	4
350	60		281	11.5	0 ± 0	92 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	92 ± 0	Inf	4
350	65		290	12.1	0 ± 0	87 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	89 ± 5	Inf	4
350	75		306	13.1	0 ± 0	90 ± 3	1 ± 0	0 ± 0	1 ± 0	0 ± 0	*92 ± 2	$(1.2 \pm 1.4) \times 10^{9}$	3
350	115		337	15.2	11 ± 10	80 ± 12	3 ± 4	1 ± 0	4 ± 3	0 ± 0	99 ± 12	$(2.5 \pm 4.4) \times 10^{7}$	5
350	175		348	16.5	35 ± 13	61 ± 5	7 ± 4	0 ± 0	7 ± 4	1 ± 0	111 ± 15	$(9.7 \pm 4.8) \times 10^{3}$	6
400	45		277	10.9	1 ± 1	87 ± 9	4 ± 3	0 ± 0	5 ± 4	0 ± 0	96 ± 11	$(1.6 \pm 2.8) \times 10^{6}$	6
400	55		308	12.6	2 ± 1	88 ± 7	2 ± 0	0 ± 0	1 ± 0	0 ± 0	93 ± 7	$(7.8 \pm 5.0) \times 10^{5}$	3
400	60		320	13.2	1 ± 0	79 ± 3	5 ± 1	0 ± 0	4 ± 2	0 ± 0	89 ± 5	$(1.4 \pm 0.8) \times 10^{7}$	3
400	65		331	13.8	10 ± 1	74 ± 12	3 ± 3	0 ± 0	0 ± 1	0 ± 0	87 ± 13	$(2.4 \pm 0.4) \times 10^{6}$	5
400	75		349	14.8	13 ± 3	76 ± 14	18 ± 7	0 ± 0	1 ± 0	1 ± 1	110 ± 6	$(2.0 \pm 0.8) \times 10^{4}$	3
400	85		362	15.5	12 ± 2	70 ± 12	10 ± 6	0 ± 0	4 ± 2	2 ± 1	99 ± 9	$(2.0 \pm 0.1) \times 10^{4}$	3
400	95		372	16.1	35 ± 12	59 ± 7	14 ± 8	0 ± 0	1 ± 0	0 ± 0	109 ± 5	$(4.7 \pm 2.7) \times 10^{3}$	3
400	115		385	16.9	68 ± 5	28 ± 6	13 ± 7	0 ± 0	2 ± 1	0 ± 0	*112 ± 4	$(1.3 \pm 0.2) \times 10^{3}$	3
400	175		398	18.2	87 ± 9	2 ± 1	12 ± 8	1 ± 0	3 ± 2	2 ± 1	106 ± 5	$(1.4 \pm 0.3) \times 10^{3}$	6
450	45		311	12.4	7 ± 5	78 ± 8	3 ± 1	0 ± 0	6 ± 1	1 ± 1	95 ± 15	$(2.0 \pm 1.9) \times 10^{5}$	4
450	55		345	14.1	1 ± 0	73 ± 10	3 ± 1	0 ± 0	9 ± 4	10 ± 4	96 ± 1	$(2.3 \pm 0.3) \times 10^{6}$	4
450	60		359	14.7	30 ± 29	45 ± 33	10 ± 6	0 ± 0	6 ± 5	0 ± 0	90 ± 28	$(1.0 \pm 1.5) \times 10^{5}$	7
450	65		372	15.3	41 ± 9	48 ± 2	10 ± 1	0 ± 0	2 ± 2	1 ± 1	103 ± 9	$(1.9 \pm 0.9) \times 10^{3}$	3
450	75		392	16.3	49 ± 5	48 ± 1	12 ± 1	0 ± 0	4 ± 2	0 ± 0	113 ± 5	$(1.5 \pm 0.3) \times 10^{3}$	4
450	85		407	17.0	40 ± 17	18 ± 7	14 ± 4	1 ± 0	8 ± 3	2 ± 1	*83 ± 13	$(3.5 \pm 1.8) \times 10^{3}$	3
450	105		427	18.0	84 ± 8	6 ± 1	11 ± 2	0 ± 0	2 ± 2	0 ± 0	103 ± 5	$(8.3 \pm 1.3) \times 10^{2}$	5
450	135		441	19.0	77 ± 14	3 ± 2	13 ± 2	2 ± 1	1 ± 1	1 ± 0	97 ± 13	$(1.5 \pm 0.6) \times 10^{3}$	5

Table S2. Continued.

T_{SP} (°C)	t (sec)	m_{PET}/m_w	T_{final} (°C)	log*SI*	Y_{TPA} (%)	Y_{US} (%)	$Y_{isophthalic\ acid}$ (%)	$Y_{phthalic\ acid}$ (%)	Y_{BHET} (%)	$Y_{Benzoic\ Acid}$ (%)	Ring Bal (%)	ξ (°C·min)	N
450	175	1/10	447	19.7	85 ± 9	4 ± 3	12 ± 5	2 ± 1	2 ± 1	1 ± 0	106 ± 9	$(1.6 \pm 0.4) \times 10^3$	6
480	35		283	10.8	7 ± 3	80 ± 10	6 ± 3	6 ± 3	4 ± 1	1 ± 0	98 ± 3	$(3.9 \pm 2.4) \times 10^4$	3
480	45		331	13.2	17 ± 1	74 ± 4	8 ± 0	8 ± 0	7 ± 3	1 ± 0	109 ± 6	$(5.9 \pm 1.2) \times 10^3$	4
480	55		368	14.9	25 ± 2	68 ± 3	6 ± 0	6 ± 0	5 ± 1	3 ± 1	107 ± 5	$(3.7 \pm 1.0) \times 10^3$	4
480	65		396	16.1	47 ± 17	37 ± 12	3 ± 1	3 ± 1	3 ± 4	8 ± 3	100 ± 14	$(2.1 \pm 1.2) \times 10^3$	6
480	75		418	17.1	78 ± 2	16 ± 7	11 ± 5	0 ± 0	2 ± 2	0 ± 0	107 ± 6	$(5.4 \pm 0.2) \times 10^2$	3
480	95		446	18.4	88 ± 9	3 ± 3	9 ± 2	4 ± 1	1 ± 0	2 ± 1	108 ± 9	$(7.1 \pm 2.1) \times 10^2$	6
480	115		462	19.2	80 ± 11	5 ± 4	14 ± 10	2 ± 1	2 ± 1	1 ± 1	103 ± 13	$(1.1 \pm 0.4) \times 10^3$	8
480	175		477	20.5	58 ± 17	5 ± 3	11 ± 9	11 ± 9	8 ± 5	2 ± 2	*86 ± 11	$(4.6 \pm 2.5) \times 10^3$	9
500	30		266	9.8	1 ± 0	83 ± 10	0 ± 0	0 ± 0	0 ± 0	0 ± 0	*84 ± 10	$(1.1 \pm 0.8) \times 10^6$	3
500	45		344	13.7	33 ± 11	55 ± 12	8 ± 3	0 ± 0	1 ± 0	3 ± 4	100 ± 3	$(1.8 \pm 0.7) \times 10^3$	3
500	60		399	16.1	74 ± 10	9 ± 5	20 ± 6	0 ± 0	2 ± 0	8 ± 6	*115 ± 14	$(5.5 \pm 1.9) \times 10^2$	9
500	75		435	17.6	79 ± 9	4 ± 1	10 ± 4	0 ± 0	3 ± 1	0 ± 0	96 ± 6	$(6.7 \pm 1.4) \times 10^2$	3
500	100		470	19.1	56 ± 7	4 ± 2	12 ± 3	0 ± 0	2 ± 0	2 ± 2	*76 ± 11	$(2.0 \pm 0.6) \times 10^3$	3
500	175		497	21.0	57 ± 13	3 ± 3	15 ± 2	0 ± 0	8 ± 6	0 ± 0	*79 ± 3	$(4.2 \pm 1.5) \times 10^3$	3
510	35		300	11.6	10 ± 3	82 ± 11	7 ± 5	0 ± 0	4 ± 2	0 ± 0	103 ± 6	$(1.7 \pm 1.0) \times 10^4$	3
510	45		351	14.0	35 ± 1	50 ± 11	17 ± 7	0 ± 0	4 ± 5	0 ± 0	107 ± 4	$(1.4 \pm 0.1) \times 10^3$	3
510	55		390	15.7	36 ± 2	43 ± 5	21 ± 3	1 ± 1	0 ± 0	1 ± 1	103 ± 1	$(1.9 \pm 0.2) \times 10^3$	3
510	75		443	17.8	94 ± 3	1 ± 1	11 ± 0	0 ± 0	2 ± 1	0 ± 0	107 ± 4	$(4.6 \pm 0.3) \times 10^2$	3
510	95		473	19.1	80 ± 6	1 ± 1	11 ± 4	1 ± 1	5 ± 3	0 ± 0	99 ± 3	$(9.0 \pm 1.2) \times 10^2$	3
510	115		491	19.9	76 ± 4	1 ± 0	11 ± 0	0 ± 0	3 ± 0	0 ± 0	*90 ± 4	$(1.3 \pm 0.1) \times 10^3$	3
510	175		507	21.2	30 ± 5	1 ± 1	12 ± 2	0 ± 0	0 ± 0	44 ± 6	*86 ± 2	$(1.6 \pm 0.5) \times 10^4$	3
540	35		317	12.3	25 ± 3	53 ± 2	13 ± 0	1 ± 0	1 ± 0	1 ± 0	94 ± 6	$(1.9 \pm 0.5) \times 10^3$	4
540	45		371	14.7	30 ± 6	55 ± 5	12 ± 6	0 ± 0	2 ± 1	0 ± 0	100 ± 9	$(2.1 \pm 0.7) \times 10^3$	3
540	55		413	16.4	68 ± 4	20 ± 8	18 ± 1	1 ± 0	1 ± 1	1 ± 1	108 ± 4	$(5.4 \pm 0.5) \times 10^2$	3
540	65		445	17.6	81 ± 3	2 ± 1	27 ± 0	4 ± 1	3 ± 0	0 ± 0	*116 ± 4	$(5.1 \pm 0.3) \times 10^2$	4
540	75		470	18.5	93 ± 4	0 ± 0	10 ± 2	3 ± 0	2 ± 0	0 ± 0	109 ± 7	$(4.8 \pm 0.4) \times 10^2$	4
540	85		488	19.2	88 ± 10	0 ± 0	10 ± 2	0 ± 0	1 ± 0	0 ± 0	100 ± 8	$(6.9 \pm 1.7) \times 10^2$	4
540	105		512	20.2	62 ± 8	2 ± 1	18 ± 2	1 ± 0	2 ± 0	3 ± 0	89 ± 10	$(1.8 \pm 0.4) \times 10^3$	3
540	135		529	21.2	42 ± 4	3 ± 2	10 ± 1	1 ± 0	6 ± 0	3 ± 0	*66 ± 6	$(5.2 \pm 0.8) \times 10^3$	3

Table S2. Continued.

T_{SP} (°C)	t (sec)	m_{PET}/m_w	T_{final} (°C)	log*SI*	Y_{TPA} (%)	Y_{US} (%)	$Y_{isophthalic\ acid}$ (%)	$Y_{phthalic\ acid}$ (%)	Y_{BHET} (%)	$Y_{Benzoic\ Acid}$ (%)	Ring Bal (%)	ξ (°C·min)	N
540	175	1/10	537	21.9	30 ± 1	1 ± 0	15 ± 0	1 ± 0	8 ± 1	11 ± 2	*65 ± 2	(1.5 ± 0.1) x 10^4	2
550	15		178	4.1	0 ± 0	81 ± 1	1 ± 0	0 ± 0	1 ± 0	0 ± 0	*83 ± 1	(2.3 ± 0.5) x 10^5	3
550	30		291	11.0	9 ± 2	81 ± 9	5 ± 5	0 ± 0	4 ± 3	2 ± 1	102 ± 2	(1.9 ± 1.8) x 10^4	3
550	35		323	12.5	13 ± 9	66 ± 3	11 ± 5	0 ± 0	2 ± 1	3 ± 1	96 ± 6	(2.7 ± 2.9) x 10^4	4
550	45		378	14.9	17 ± 10	50 ± 12	15 ± 6	0 ± 0	1 ± 0	2 ± 1	85 ± 14	(1.5 ± 1.5) x 10^4	4
550	55		421	16.6	41 ± 8	25 ± 1	26 ± 9	0 ± 0	3 ± 1	25 ± 6	*121 ± 8	(1.8 ± 0.8) x 10^3	4
550	60		438	17.3	41 ± 15	1 ± 0	36 ± 2	0 ± 0	0 ± 3	0 ± 0	*77 ± 5	(2.2 ± 0.6) x 10^3	3
550	65		453	17.8	23 ± 3	1 ± 1	33 ± 3	0 ± 0	5 ± 0	0 ± 1	*62 ± 13	(2.4 ± 2.2) x 10^4	2
570	15		184	4.5	11 ± 0	100 ± 1	1 ± 0	0 ± 0	2 ± 0	0 ± 0	114 ± 15	(1.0 ± 0.7) x 10^6	3
570	30		301	11.4	2 ± 1	86 ± 12	2 ± 1	0 ± 0	3 ± 0	1 ± 0	94 ± 12	(2.3 ± 0.9) x 10^5	3
570	35		334	13.0	15 ± 13	19 ± 14	13 ± 11	0 ± 0	1 ± 1	23 ± 15	*71 ± 26	(4.9 ± 9.5) x 10^6	5
570	45		391	15.4	48 ± 7	31 ± 11	13 ± 11	0 ± 0	6 ± 3	1 ± 1	98 ± 16	(9.5 ± 3.5) x 10^2	5
570	55		436	17.0	47 ± 16	1 ± 2	23 ± 17	0 ± 0	5 ± 2	4 ± 2	*79 ± 10	(1.9 ± 1.4) x 10^3	6
570	60		454	17.7	24 ± 0	7 ± 2	23 ± 2	0 ± 0	0 ± 0	6 ± 0	*60 ± 5	(5.4 ± 0.1) x 10^3	3
570	65		470	18.3	20 ± 1	3 ± 2	1 ± 2	0 ± 0	0 ± 0	47 ± 17	*72 ± 19	(8.6 ± 0.7) x 10^3	3
570	175		567	22.5	13 ± 1	0 ± 0	16 ± 1	6 ± 0	4 ± 0	32 ± 1	87 ± 13	(6.9 ± 1.4) x 10^4	3
510	45	1/8	351	14.0	48 ± 7	37 ± 0	15 ± 2	0 ± 0	12 ± 1	1 ± 0	113 ± 10	(6.5 ± 0.2) x 10^2	3
510	55		390	15.7	35 ± 5	25 ± 11	40 ± 3	0 ± 0	10 ± 2	0 ± 0	109 ± 11	(1.7 ± 0.5) x 10^3	3
510	65		421	16.9	69 ± 13	1 ± 0	32 ± 13	0 ± 0	4 ± 2	0 ± 0	106 ± 4	(5.9 ± 1.9) x 10^2	3
510	75		443	17.8	86 ± 7	1 ± 0	3 ± 1	0 ± 0	5 ± 0	3 ± 0	99 ± 8	(4.4 ± 0.7) x 10^2	4
510	85		461	18.5	75 ± 9	1 ± 0	18 ± 2	0 ± 0	5 ± 2	0 ± 0	99 ± 8	(7.2 ± 1.6) x 10^2	3
510	45	1/6	351	14.0	38 ± 6	37 ± 6	7 ± 2	0 ± 0	9 ± 2	1 ± 0	93 ± 4	(7.9 ± 2.3) x 10^2	3
510	55		390	15.7	36 ± 13	28 ± 0	42 ± 13	0 ± 0	14 ± 4	0 ± 0	*120 ± 5	(1.7 ± 1.1) x 10^3	2
510	65		421	16.9	55 ± 2	4 ± 4	43 ± 4	0 ± 0	6 ± 4	0 ± 0	108 ± 5	(6.4 ± 0.5) x 10^2	3
510	75		443	17.8	71 ± 6	4 ± 3	14 ± 14	0 ± 0	6 ± 2	5 ± 2	99 ± 8	(4.9 ± 0.8) x 10^2	4
510	85		461	18.5	59 ± 7	1 ± 0	32 ± 8	0 ± 0	7 ± 3	0 ± 0	98 ± 4	(8.7 ± 2.1) x 10^2	3
510	45	1/4	351	14.0	33 ± 8	24 ± 24	12 ± 4	0 ± 0	10 ± 11	4 ± 3	*82 ± 19	(7.4 ± 2.8) x 10^2	3
510	55		390	15.7	24 ± 27	9 ± 0	33 ± 2	0 ± 0	9 ± 2	0 ± 0	*76 ± 30	(2.5 ± 1.9) x 10^4	3
510	65		421	16.9	45 ± 6	0 ± 0	39 ± 7	0 ± 0	10 ± 5	0 ± 0	94 ± 14	(6.7 ± 1.7) x 10^2	3
510	75		443	17.8	44 ± 5	1 ± 0	37 ± 6	0 ± 0	6 ± 1	0 ± 0	89 ± 2	(8.5 ± 2.0) x 10^2	3

Table S2. Continued.

T_{SP} (˚C)	t (sec)	m_{PET}/m_w	T_{final} (˚C)	log*SI*	Y_{TPA} (%)	Y_{US} (%)	$Y_{isophthalic\ acid}$ (%)	$Y_{phthalic\ acid}$ (%)	Y_{BHET} (%)	$Y_{Benzoic\ Acid}$ (%)	Ring Bal (%)	*ξ* (˚C·min)	N
510	85	1/4	461	18.5	33 ± 3	0 ± 0	36 ± 16	0 ± 0	5 ± 1	0 ± 0	*74 ± 15	(1.8 ± 0.3) x 10^3	3
500	60	1/3	399	16.1	51 ± 17	18 ± 19	30 ± 28	0 ± 0	4 ± 4	0 ± 0	103 ± 28	(6.3 ± 4.2) x 10^2	9
510	45	1/2	351	14.0	20 ± 5	20 ± 15	27 ± 9	0 ± 0	24 ± 13	0 ± 0	91 ± 4	(1.1 ± 0.6) x 10^2	3
510	55		390	15.7	1 ± 1	1 ± 1	33 ± 11	0 ± 0	9 ± 4	0 ± 0	*43 ± 14	(3.0 ± 3.4) x 10^6	3
510	65		421	16.9	17 ± 6	5 ± 5	20 ± 15	0 ± 0	3 ± 3	0 ± 0	*45 ± 19	(3.2 ± 2.0) x 10^3	2
510	75		443	17.8	4 ± 0	0 ± 0	2 ± 0	0 ± 0	3 ± 0	1 ± 0	*14 ± 1	(4.0 ± 0.3) x 10^4	2
510	85		461	18.5	14 ± 8	0 ± 0	49 ± 5	0 ± 0	6 ± 1	0 ± 0	*69 ± 13	(4.2 ± 0.6) x 10^4	3
480	75	1/8	418	17.1	69 ± 6	0 ± 0	18 ± 2	0 ± 0	6 ± 2	0 ± 0	94 ± 4	(6.2 ± 1.2) x 10^2	3
500	60		399	16.1	66 ± 13	1 ± 0	27 ± 8	0 ± 0	0 ± 0	10 ± 1	104 ± 20	(5.7 ± 2.7) x 10^2	3
540	55		413	16.4	68 ± 6	8 ± 10	8 ± 6	0 ± 0	0 ± 0	13 ± 6	97 ± 20	(4.5 ± 0.1) x 10^2	3
550	35		323	12.5	27 ± 10	55 ± 9	16 ± 7	0 ± 0	1 ± 1	14 ± 6	112 ± 15	(1.9 ± 0.9) x 10^3	3

* ring balance differs by more than ± 15% from 100% or ring balance had a mean value that differed from 100% with statistical significance ($p < 0.05$).

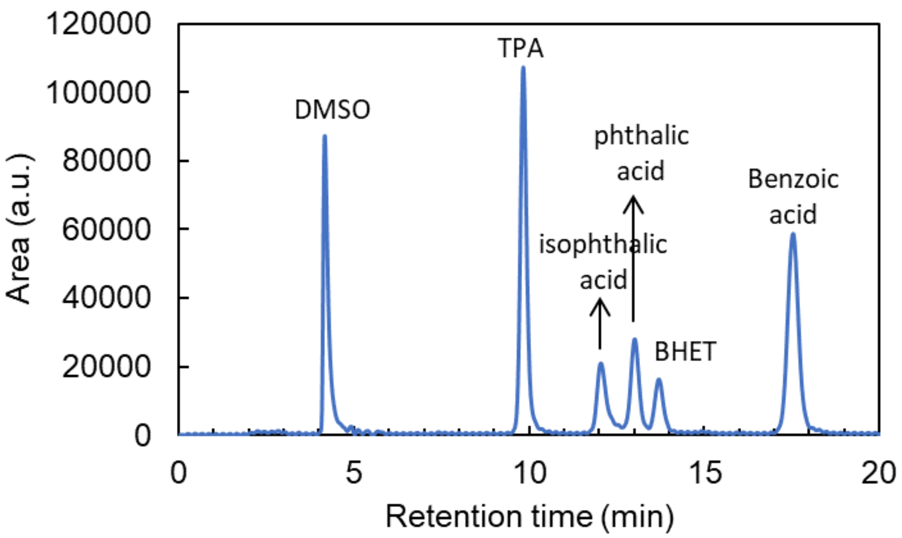

Figure S3. HPLC chromatogram of dissolved solids in aqueous filtrate from a representative PET hydrolysis experiment at set point temperature of 450 ˚C for 135 seconds, with 1/10 PET/water mass ratio.

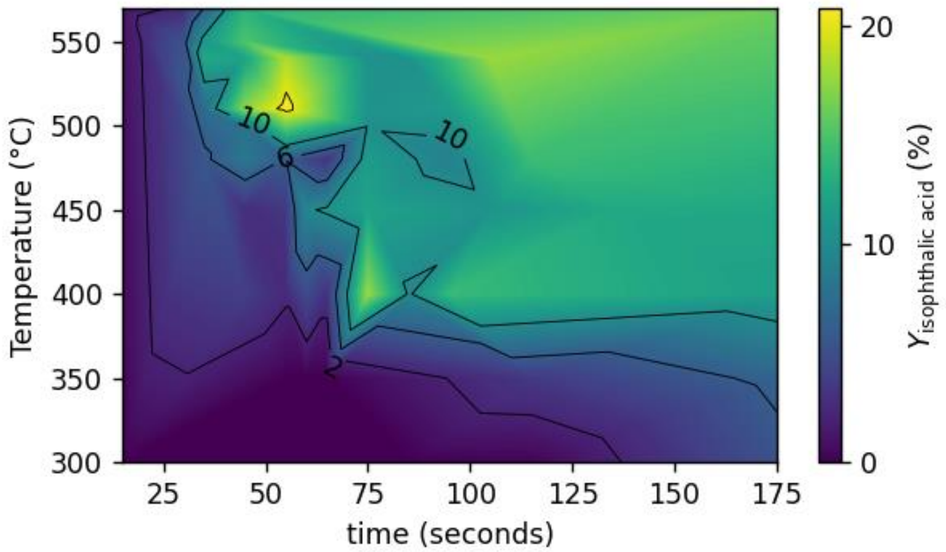

Figure S4. Contour plot illustrating effects of set point temperature and batch holding time on isophthalic acid yield from fast hydrolysis of PET (m_{PET}/m_W = 1/10).

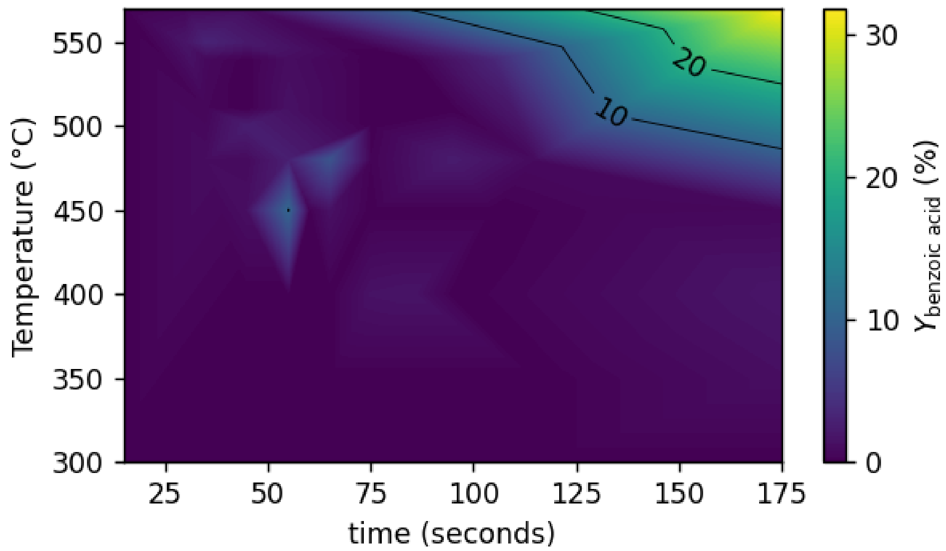

Figure S5. Contour plot illustrating effects of set point temperature and batch holding time on benzoic acid yield from fast hydrolysis of PET (m_{PET}/m_W = 1/10).

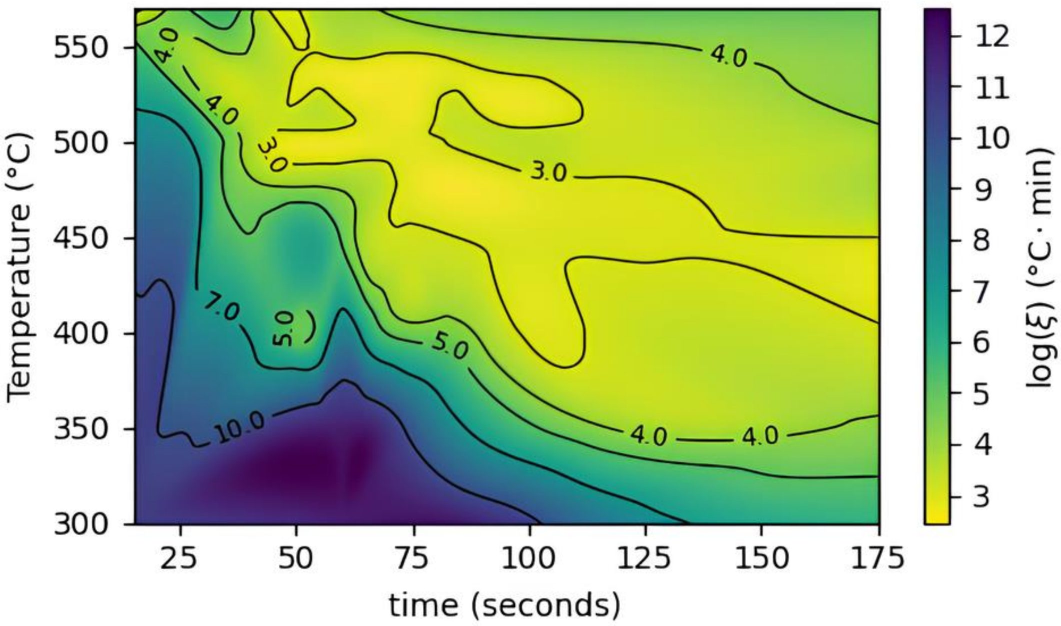

Figure S6. Contour plot illustrating effects of set point temperature and batch holding time on the logarithm of the environmental energy impact from fast hydrolysis of PET (m_{PET}/m_W = 1/10).