

Machine learning for revealing the relationship between process- structure-property of polypropylene in-reactor alloy

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Table S1 The process conditions of gas-phase copolymerization

Entry	C2 in	C3 in	H2 in	Initial P (MPa)	flowrate (kg/h)	time (min)
Run 1	0.403	0.597	0.000	0.84	1.86	75
Run 2	0.397	0.596	0.007	1.12	2.52	45
Run 3	0.393	0.593	0.015	1.12	2.79	75
Run 4	0.423	0.567	0.010	1.40	2.27	60
Run 5	0.377	0.613	0.010	1.40	2.29	30
Run 6	0.397	0.593	0.010	1.40	2.44	75
Run 7	0.397	0.593	0.010	1.40	2.18	45
Run 8	0.397	0.594	0.009	1.40	2.22	90
Run 9	0.393	0.598	0.009	1.40	2.15	45
Run 10	0.495	0.495	0.010	1.40	2.05	75
Run 11	0.502	0.498	0.000	0.93	2.16	75
Run 12	0.302	0.698	0.000	1.27	1.40	75
Run 13	0.371	0.623	0.006	0.93	1.84	75
Run 14	0.300	0.695	0.005	1.27	1.74	75
Run 15	0.393	0.602	0.005	1.12	1.59	75
Run 16	0.350	0.645	0.005	1.20	2.02	75
Run 17	0.399	0.598	0.002	1.12	2.24	75
Run 18	0.396	0.597	0.007	1.12	2.16	75
Run 19	0.384	0.611	0.005	1.12	2.57	75
Run 20	0.298	0.697	0.005	1.27	2.23	75
Run 21	0.496	0.499	0.005	0.93	3.81	75
Run 22	0.396	0.599	0.005	1.12	3.54	75
Run 23	0.388	0.602	0.010	1.12	2.99	75
Run 24	0.391	0.596	0.012	1.12	2.83	75
Run 25	0.397	0.595	0.007	1.12	3.15	30
Run 26	0.391	0.599	0.011	1.12	3.17	75
Run 27	0.445	0.550	0.005	1.03	2.35	75

Table S2 Structure and mechanical properties of polymer alloys

Entry	Rubber (wt%)	MI (wt%)	Ethylene (wt%)	F1 (wt%)	F2 (wt%)	F3 (wt%)	Xc (%)	FS (MPa)	IS (kJ/m2)
Run 1	16.23	11.97	29.87	12.07	4.16	83.77	43.97	22.40	10.81
Run 2	31.75	8.04	22.76	26.57	5.18	68.25	36.85	16.49	45.37
Run 3	43.98	25.92	28.75	34.93	9.05	56.02	29.84	11.61	36.83
Run 4	19.76	20.76	7.45	14.64	5.12	80.24	44.36	22.22	4.83
Run 5	17.12	19.96	8.32	13.19	3.94	82.88	48.33	24.53	5.89
Run 6	27.24	24.23	10.93	19.93	7.31	72.76	43.43	18.96	7.22
Run 7	14.94	20.66	7.37	9.54	5.41	85.06	50.86	28.72	4.38
Run 8	26.34	18.18	11.31	21.58	4.75	73.66	43.41	19.11	8.68
Run 9	16.55	19.86	3.96	11.59	4.96	83.45	44.62	25.21	7.26
Run 10	7.63	25.04	11.43	4.01	3.62	92.37	49.93	32.76	3.37
Run 11	15.96	13.65	29.81	11.29	4.67	84.04	43.95	22.62	7.56
Run 12	17.48	14.53	13.08	12.70	4.78	82.52	46.27	21.22	7.76
Run 13	20.02	9.48	25.93	12.34	7.68	79.98	42.57	21.56	10.64
Run 14	29.03	11.72	21.36	20.81	8.22	70.97	40.83	17.73	9.62
Run 15	17.60	16.27	10.71	8.83	8.77	82.40	48.15	27.01	6.76
Run 16	36.47	8.10	21.58	26.03	10.44	63.53	37.51	14.27	51.73
Run 17	35.41	6.99	27.09	24.75	10.66	64.59	35.23	14.53	52.80
Run 18	37.73	7.60	28.22	27.35	10.39	62.27	35.06	15.30	52.06
Run 19	36.90	6.62	24.63	25.02	11.88	63.10	35.71	15.97	52.31
Run 20	39.59	9.45	19.81	29.43	10.16	60.41	31.76	14.07	48.01
Run 21	28.98	3.74	37.73	17.90	11.09	71.02	31.33	15.32	50.75
Run 22	38.84	4.35	29.98	27.31	11.53	61.16	30.67	14.06	54.78
Run 23	38.49	7.85	12.91	29.01	9.48	61.51	32.54	14.66	47.98
Run 24	40.59	14.22	24.16	31.95	8.65	59.41	31.66	13.89	41.40
Run 25	26.60	9.78	23.06	20.69	5.92	73.40	41.50	20.04	11.15
Run 26	39.13	8.55	26.75	30.40	8.73	60.87	33.42	13.88	46.55
Run 27	34.50	6.20	23.09	22.23	12.27	65.50	36.08	14.92	55.87