Supporting Information

Predicting binary-interaction parameters of cubic equations of state for petroleum fluids containing pseudo-components

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Detailed results for the 174 pure compounds used in this study (accuracy of the developed GCM to estimate T_c, P_c and ω and accuracy of the reverse GCM to estimate the structure).

Table S1. Deviations on the estimation of T_c, P_c and ω by the developed GCM.

Compound	N			P_c		T_c		ω	
	N_{PAR}	N_{ARO}	N_{NAP}	AD* (kPa)	RD* (%)	AD (K)	RD (%)	AD	RD (%)
n-Octane	8	0	0	130.2	5.23	9.9	1.74	0.0709	17.75
n-Nonane	9	0	0	97.9	4.28	7.7	1.30	0.0725	16.35
n-Decane	10	0	0	79.4	3.76	5.7	0.93	0.0782	15.88
n-Undecane	11	0	0	68.3	3.50	4.3	0.67	0.0722	13.61
n-Dodecane	12	0	0	49.9	2.74	2.6	0.39	0.0736	12.78
n-Tridecane	13	0	0	60.3	3.59	0.5	0.07	0.0695	11.26
n-Tetradecane	14	0	0	56.4	3.59	0.9	0.12	0.0496	7.71
n-Pentadecane	15	0	0	45.8	3.10	0.6	0.08	0.0469	6.84
n-Hexadecane	16	0	0	36.6	2.61	1.0	0.13	0.0318	4.43
n-Heptadecane	17	0	0	17.0	1.27	2.4	0.33	0.0377	4.90
n-Octadecane	18	0	0	15.7	1.24	5.0	0.67	0.0328	4.04
n-Nonadecane	19	0	0	11.6	0.96	6.9	0.91	0.0270	3.16
n-Eicosane	20	0	0	3.8	0.33	9.1	1.19	0.0349	3.84
3-Ethylhexane	8	0	0	10.2	0.39	6.6	1.17	0.0341	9.41
2,2-Dimethylhexane	8	0	0	90.2	3.56	9.0	1.64	0.0092	2.71
2,3-Dimethylhexane	8	0	0	9.8	0.37	4.6	0.81	0.0186	5.34
2,4-Dimethylhexane	8	0	0	60.2	2.35	5.3	0.96	0.0150	4.35
2,5-Dimethylhexane	8	0	0	130.2	5.23	8.8	1.60	0.0289	8.09
3,3-Dimethylhexane	8	0	0	29.8	1.13	3.2	0.57	0.0084	2.63
3,4-Dimethylhexane	8	0	0	69.8	2.60	10.0	1.76	0.0095	2.80
2-Methyl-3-ethylpentane	8	0	0	79.8	2.96	8.2	1.44	0.0008	0.23
3-Methyl-3-ethylpentane	8	0	0	189.8	6.76	17.7	3.07	0.0236	7.74
2-Methylheptane	8	0	0	136.2	5.48	0.8	0.15	0.0486	12.88
3-Methylheptane	8	0	0	74.2	2.91	4.9	0.86	0.0432	11.62
4-Methylheptane	8	0	0	78.2	3.07	2.9	0.52	0.0419	11.31
2,2,3-Trimethylpentane	8	0	0	109.8	4.02	4.7	0.83	0.0316	10.63
2,2,4-Trimethylpentane	8	0	0	52.2	2.03	14.8	2.73	0.0265	8.75
2,3,3-Trimethylpentane	8	0	0	199.8	7.09	14.7	2.56	0.0384	13.21
2,3,4-Trimethylpentane	8	0	0	109.8	4.02	7.5	1.32	0.0125	3.96
2,2,3,3-Tetramethylbutane	8	0	0	249.8	8.71	9.2	1.62	0.0837	34.17
2,2,3,3-Tetramethylpentane	9	0	0	347.9	12.71	24.0	3.92	0.0910	32.50
2,2,3,4-Tetramethylpentane	9	0	0	175.6	6.85	5.3	0.89	0.0604	19.43
2,2,4,4-Tetramethylpentane	9	0	0	27.0	1.15	15.5	2.72	0.0550	17.42
2,3,3,4-Tetramethylpentane	9	0	0	328.1	12.08	20.8	3.43	0.0583	18.64
2,2-Dimethyl-3-ethylpentane	9	0	0	182.1	7.08	3.1	0.53	0.0357	10.64
2,4-Dimethyl-3-ethylpentane	9	0	0	142.1	5.61	4.1	0.70	0.0179	5.08
3-ethylheptane	9	0	0	2.1	0.09	3.1	0.53	0.0370	9.08
3,3-Diethylpentane	9	0	0	287.1	10.73	23.2	3.80	0.0329	9.72
2,2,4-Trimethylhexane	9	0	0	6.8	0.29	13.3	2.32	0.0210	5.99
2,2,5-Trimethylhexane	9	0	0	57.9	2.49	18.8	3.31	0.0113	3.14
2,3,3-Trimethylhexane	9	0	0	165.5	6.48	9.2	1.54	0.0410	12.41
2,4,4-Trimethylhexane	9	0	0	72.1	2.93	5.9	1.01	0.0188	5.32
3,3,4-Trimethylhexane	9	0	0	236.4	9.01	15.4	2.55	0.0460	14.14
2,3,5-Trimethylhexane	9	0	0	13.5	0.56	7.7	1.33	0.0070	1.91
2,2-Dimethylheptane	9	0	0	37.9	1.61	10.1	1.75	0.0190	4.87
2,6-Dimethylheptane	9	0	0	87.9	3.82	7.9	1.36	0.0218	5.55
2-Methyloctane	9	0	0	97.9	4.28	0.1	0.02	0.0502	11.92

3-Methyloctane	9	0	0	47.9	2.05	3.3	0.55	0.0414	10.04
4-Methyloctane	9	0	0	47.9	2.05	0.8	0.13	0.0420	10.17
2,2-Dimethyloctane	10	0	0	29.4	1.36	10.0	1.66	0.0146	3.40
2,3-Dimethyloctane	10	0	0	20.6	0.93	1.0	0.17	0.0186	4.29
2,4-Dimethyloctane	10	0	0	19.4	0.89	12.0	2.00	0.0203	4.68
2,5-Dimethyloctane	10	0	0	19.4	0.89	9.0	1.49	0.0262	5.94
2,6-Dimethyloctane	10	0	0	19.4	0.89	6.0	0.99	0.0244	5.57
2,7-Dimethyloctane	10	0	0	59.4	2.79	8.0	1.32	0.0278	6.29
3-Methylnonane	10	0	0	29.4	1.36	1.0	0.17	0.0508	10.92
2-Methylnonane	10	0	0	69.4	3.27	2.0	0.32	0.0582	12.32
4-Methylnonane	10	0	0	29.4	1.36	2.0	0.32	0.0509	10.95
5-Methylnonane	10	0	0	29.4	1.36	2.0	0.32	0.0420	9.21
2,2,3,3-Tetramethylhexane	10	0	0	323.5	12.87	11.1	1.78	0.0542	15.05
3,3,5-Trimethylheptane	10	0	0	130.9	5.64	2.4	0.39	0.0262	6.74
2,2,4,6,6-Pentamethylheptane	12	0	0	75.5	3.88	30.4	4.86	0.0728	16.92
1,2-Dimethylcyclopentane	2	0	5	127.5	3.70	2.3	0.40	0.0360	13.52
1,3-Dimethylcyclopentane	2	0	5	127.4	3.70	11.9	2.16	0.0440	16.05
1,1-Dimethylcyclopentane	2	0	5	127.4	3.70	15.9	2.91	0.0421	15.46
Ethylcyclopentane	2	0	5	80.4	2.37	6.6	1.16	0.0414	15.23
Methylcyclohexane	1	0	6	56.2	1.62	2.7	0.48	0.0158	6.73
1,2-Dimethylcyclopentane	2	0	5	127.5	3.70	9.7	1.76	0.0396	14.66
1,3-Dimethylcyclopentane	2	0	5	127.4	3.70	9.9	1.79	0.0397	14.71
1,1,2-Trimethylcyclopentane	3	0	5	36.7	1.25	11.0	1.89	0.0185	7.37
1,1,3-Trimethylcyclopentane	3	0	5	148.1	5.24	21.0	3.68	0.0585	27.73
1-methyl-2-ethylcyclopentane	3	0	5	36.7	1.25	5.6	0.95	0.0205	7.07
1,2-Dimethylcyclohexane	2	0	6	117.6	4.00	9.8	1.61	0.0256	11.00
1,3-Dimethylcyclohexane	2	0	6	117.6	4.00	5.2	0.88	0.0214	9.06
1,4-Dimethylcyclohexane	2	0	6	117.6	4.00	1.8	0.30	0.0269	11.62
1-Methyl-3-ethylcyclopentane	3	0	5	36.7	1.25	3.4	0.57	0.0115	4.09
1,2,4-Trimethylcyclopentane	3	0	5	87.3	3.02	10.4	1.79	0.0175	6.09
1,2,3-Trimethylcyclopentane	3	0	5	36.7	1.25	4.4	0.74	0.0375	12.21
1,1-Dimethylcyclohexane	2	0	6	117.6	4.00	5.2	0.88	0.0254	10.94
Ethylcyclohexane	2	0	6	16.0	0.53	12.8	2.10	0.0125	5.08
Isopropylcyclopentane	3	0	5	64.9	2.13	2.5	0.42	0.0335	11.05
1-methyl-1-ethylcyclopentane	3	0	5	44.9	1.49	8.5	1.46	0.0603	18.28
n-propylcyclopentane	3	0	5	44.9	1.49	5.5	0.92	0.0571	17.49
1-methyl-2-ethylcyclopentane	3	0	5	36.7	1.25	2.4	0.40	0.0025	0.94
1-methyl-3-ethylcyclopentane	3	0	5	77.2	2.66	3.4	0.57	0.0065	2.35
1,2-Dimethylcyclohexane	2	0	6	117.6	4.00	0.2	0.04	0.0202	8.47
1,3-Dimethylcyclohexane	2	0	6	117.6	4.00	1.6	0.27	0.0246	10.51
1,4-Dimethylcyclohexane	2	0	6	117.6	4.00	6.2	1.05	0.0210	8.85
1,2,3-Trimethylcyclopentane	3	0	5	148.1	5.24	18.4	3.21	0.0025	0.92
1,2,4-Trimethylcyclopentane	3	0	5	163.3	5.81	19.4	3.39	0.0255	10.45
n-Butylcyclopentane	4	0	5	31.6	1.16	5.8	0.93	0.0617	16.59
n-Propylcyclohexane	3	0	6	50.6	1.80	18.6	2.91	0.0388	14.93
n-Isopropylcyclohexane	3	0	6	93.6	3.29	6.5	1.03	0.0312	9.47
1,3,5-Trimethylcyclohexane	3	0	6	96.4	3.62	18.3	3.05	0.0347	10.42
n-Butylcyclohexane	4	0	6	66.3	2.58	24.5	3.68	0.0655	23.87
Isobutylcyclohexane	4	0	6	617.1	19.77	16.5	2.51	0.0208	6.53
Hexylcyclopentane	6	0	5	101.3	4.74	2.0	0.30	0.0812	17.05
Heptylcyclopentane	7	0	5	116.0	5.96	2.0	0.29	0.0765	14.85
Octylcyclopentane	8	0	5	113.9	6.35	0.5	0.07	0.0812	14.39
Nonylcyclopentane	9	0	5	121.4	7.35	0.3	0.04	0.0822	13.48
Decylcyclopentane	10	0	5	135.3	8.90	2.2	0.31	0.0808	12.36
Dodecylcyclopentane	12	0	5	162.3	12.52	3.9	0.51	0.0540	7.51
Tridecylcyclopentane	13	0	5	48.4	3.39	5.6	0.74	0.0437	5.78

Tetradecylcyclopentane	14	0	5	51.8	3.82	6.8	0.88	0.0312	3.95
Pentadecylcyclopentane	15	0	5	53.9	4.17	10.3	1.32	0.0285	3.42
Hexadecylcyclopentane	16	0	5	55.5	4.50	10.3	1.31	0.0098	1.14
Decylclohexane	10	0	6	73.6	4.46	7.8	1.03	0.0570	8.60
Pentylcyclohexane	5	0	6	47.4	2.03	11.4	1.70	0.0306	7.41
Hexylcyclohexane	6	0	6	29.1	1.36	10.7	1.55	0.0302	6.62
Heptylcyclohexane	7	0	6	11.7	0.60	10.3	1.46	0.0280	5.63
Octylcyclohexane	8	0	6	5.3	0.30	9.3	1.28	0.0233	4.32
nonylcyclohexane	9	0	6	21.6	1.30	8.4	1.14	0.0170	2.95
undecylcyclohexane	11	0	6	52.5	3.68	4.9	0.64	0.0057	0.88
dodecylcyclohexane	12	0	6	66.1	4.97	3.4	0.44	0.0229	3.40
tridecylcyclohexane	13	0	6	79.7	6.41	1.9	0.25	0.0444	6.34
tetradecylcyclohexane	14	0	6	92.0	7.92	0.1	0.01	0.0720	10.01
dicyclohexylmethane	1	0	12	169.8	7.18	29.5	3.94	0.0089	2.30
1,1-dicyclohexylethane	2	0	12	134.8	6.24	27.5	3.61	0.0085	1.98
2,2-dicyclohexylpropane	3	0	12	104.0	5.25	18.4	2.40	0.0108	2.30
1,1-dicyclohexylbutane	4	0	12	75.3	4.14	6.6	0.86	0.0147	2.88
1,1-dicyciohexylpentane	5	0	12	49.7	2.96	2.4	0.31	0.0211	3.83
1,1-dicyclohexylhexane	6	0	12	25.7	1.65	2.1	0.26	0.0289	4.91
1.1-dicyclohexylheplane	7	0	12	4.3	0.30	6.7	0.85	0.0410	6.58
1,1-dicyclohexyloctane	8	0	12	15.7	1.17	10.3	1.29	0.0573	8.77
Benzene	0	6	0	197.1	4.02	8.6	1.52	0.0122	5.83
Toluene	1	6	0	0.6	0.02	5.7	0.96	0.0009	0.35
Ethylbenzene	2	6	0	17.8	0.49	4.4	0.71	0.0010	0.33
m-Xylene	2	6	0	87.8	2.48	4.5	0.73	0.0242	7.44
o-Xylene	2	6	0	110.2	2.95	8.8	1.39	0.0088	2.85
p-Xylene	2	6	0	112.9	3.21	5.3	0.86	0.0199	6.18
o-ethyltoluene	3	6	0	189.2	6.22	7.7	1.19	0.0500	17.05
m-ethyltoluene	3	6	0	389.0	13.70	6.3	0.98	0.0207	6.41
p-ethyltoluene	3	6	0	4.0	0.12	3.2	0.50	0.0231	6.30
1,2,3-Trimethylbenzene	3	6	0	225.2	6.52	21.1	3.18	0.0232	6.33
1,2,4-Trimethylbenzene	3	6	0	3.0	0.09	5.7	0.88	0.0341	9.04
n-Propylbenzene	3	6	0	29.0	0.91	5.0	0.79	0.0015	0.43
n-Butylbenzene	4	6	0	14.2	0.49	2.9	0.44	0.0079	2.01
m-Diethylbenzene	4	6	0	21.2	0.74	0.4	0.06	0.0318	8.99
p-Diethylbenzene	4	6	0	98.2	3.50	5.5	0.83	0.0171	4.25
3-Ethyl-o-xylene	4	6	0	21.2	0.74	16.6	2.44	0.0238	6.56
2-Ethyl-m-xylene	4	6	0	118.8	3.93	7.6	1.13	0.0207	5.10
4-Ethyl-m-xylene	4	6	0	21.2	0.74	1.6	0.24	0.0281	6.79
5-Ethyl-m-xylene	4	6	0	151.2	5.50	8.4	1.29	0.0311	7.45
4-Ethyl-o-xylene	4	6	0	21.2	0.74	3.6	0.54	0.0255	6.20
2-Ethyl-p-xylene	4	6	0	21.2	0.74	0.4	0.06	0.0256	6.21
Isobutylbenzene	4	6	0	138.8	4.56	13.3	2.04	0.0062	1.63
1-Methyl-2-n-propylbenzene	4	6	0	38.8	1.32	1.4	0.22	0.0212	5.20
1-Methyl-3-n-propylbenzene	4	6	0	91.2	3.25	9.4	1.44	0.0269	6.52
1-Methyl-4-n-propylbenzene	4	6	0	91.2	3.25	7.4	1.13	0.0276	6.67
m-Cymene	4	6	0	28.8	0.98	6.4	0.98	0.0447	13.11
o-Cymene	4	6	0	28.8	0.98	1.4	0.22	0.0487	14.44
p-Cymene	4	6	0	101.2	3.62	10.3	1.57	0.0191	5.21
o-Diethylbenzene	4	6	0	21.2	0.74	4.6	0.68	0.0463	13.64
1,2,4,5-Tetramethylbenzene	4	6	0	38.8	1.32	11.7	1.74	0.0482	11.10
1,2,3,4-Tetramethylbenzene	4	6	0	208.8	6.71	29.6	4.27	0.0313	7.51
1,2,3,5-Tetramethylbenzene	4	6	0	68.8	2.32	15.6	2.29	0.0383	9.03
n-Pentylbenzene	5	6	0	22.2	0.85	2.0	0.29	0.0084	1.92
Indane	0	6	3	428.3	10.84	27.6	4.04	0.0021	0.69
Cumene	3	6	0	20.0	0.62	12.3	1.95	0.0174	5.35

Mesitylene	3	6	0	102.0	3.26	6.0	0.95	0.0558	13.99
n-Hexylbenzene	6	6	0	13.1	0.55	1.0	0.15	0.0054	1.13
n-Hepthylbenzene	7	6	0	13.8	0.63	1.0	0.14	0.0088	1.67
1,2-Diphenylethane	2	12	0	17.8	0.67	17.4	2.22	0.0456	9.33
n-Octylbenzene	8	6	0	2.1	0.11	1.0	0.14	0.0034	0.59
n-Nonylbenzene	9	6	0	21.8	1.15	3.1	0.42	0.0237	3.74
n-Decylbenzene	10	6	0	26.8	1.52	4.4	0.58	0.0243	3.58
n-Undecylbenzene	11	6	0	43.1	2.58	6.0	0.79	0.0316	4.31
n-Dodecylbenzene	12	6	0	31.9	2.05	2.0	0.25	0.0149	2.03
n-Tetradecylbenzene	14	6	0	41.3	2.95	4.3	0.53	0.0286	3.51
n-Tridecylbenzene	13	6	0	41.5	2.80	3.4	0.43	0.0149	1.91
n-Pentadecylbenzene	15	6	0	42.7	3.21	5.6	0.70	0.0316	3.68
n-Hexadecylbenzene	16	6	0	46.9	3.69	6.6	0.81	0.0355	3.95
n-Heptadecylbenzene	17	6	0	44.9	3.71	8.2	0.99	0.0624	6.79
n-Octadecylbenzene	18	6	0	47.3	4.08	9.4	1.13	0.0781	8.22
average				**85.3**	**3.45**	**7.9**	**1.23**	**0.0332**	**8.33**

* AD = absolute deviation ; RD = relative deviation

Table S2. Accuracy of the reverse GCM to estimate the structure (N_{PAR}, N_{ARO} and N_{NAP}) of 174 pure components.

Compound	Calculated structure			AD*		
	N_{PAR}	N_{ARO}	N_{NAP}	N_{PAR}	N_{ARO}	N_{NAP}
n-Octane	6.98	1.52	0.00	1.02	1.52	0.00
n-Nonane	7.80	1.65	0.00	1.20	1.65	0.00
n-Decane	8.60	1.82	0.00	1.40	1.82	0.00
n-Undecane	9.68	1.71	0.00	1.32	1.71	0.00
n-Dodecane	10.47	1.85	0.00	1.53	1.85	0.00
n-Tridecane	11.79	1.53	0.00	1.21	1.53	0.00
n-Tetradecane	13.43	0.88	0.00	0.57	0.88	0.00
n-Pentadecane	14.39	0.86	0.00	0.61	0.86	0.00
n-Hexadecane	15.80	0.39	0.00	0.20	0.39	0.00
n-Heptadecane	16.04	1.01	0.00	0.96	1.01	0.00
n-Octadecane	17.16	0.78	0.00	0.84	0.78	0.00
n-Nonadecane	18.21	0.62	0.00	0.79	0.62	0.00
n-Eicosane	18.58	1.09	0.00	1.42	1.09	0.00
3-Ethylhexane	6.92	1.26	0.00	1.08	1.26	0.00
2,2-Dimethylhexane	8.01	0.00	0.00	0.01	0.00	0.00
2,3-Dimethylhexane	7.20	0.89	0.00	0.80	0.89	0.00
2,4-Dimethylhexane	7.88	0.15	0.00	0.12	0.15	0.00
2,5-Dimethylhexane	7.96	0.14	0.00	0.04	0.14	0.00
3,3-Dimethylhexane	7.27	0.00	0.73	0.73	0.00	0.73
3,4-Dimethylhexane	7.03	1.05	0.00	0.97	1.05	0.00
2-Methyl-3-ethylpentane	7.25	0.78	0.00	0.75	0.78	0.00
3-Methyl-3-ethylpentane	5.70	0.52	1.78	2.30	0.52	1.78
2-Methylheptane	7.48	0.83	0.00	0.52	0.83	0.00
3-Methylheptane	7.17	1.11	0.00	0.83	1.11	0.00
4-Methylheptane	7.21	1.03	0.00	0.79	1.03	0.00
2,2,3-Trimethylpentane	5.63	0.00	2.24	2.37	0.00	2.24
2,2,4-Trimethylpentane	6.01	0.00	1.78	1.99	0.00	1.78
2,3,3-Trimethylpentane	5.00	0.00	2.91	3.00	0.00	2.91
2,3,4-Trimethylpentane	6.86	0.37	0.71	1.14	0.37	0.71
2,2,3,3-Tetramethylbutane	2.38	0.00	5.29	5.62	0.00	5.29
2,2,3,3-Tetramethylpentane	2.40	0.00	6.39	6.60	0.00	6.39
2,2,3,4-Tetramethylpentane	4.84	0.00	3.86	4.16	0.00	3.86
2,2,4,4-Tetramethylpentane	5.32	0.00	3.36	3.68	0.00	3.36
2,3,3,4-Tetramethylpentane	4.52	0.32	3.95	4.48	0.32	3.95
2,2-Dimethyl-3-ethylpentane	6.83	0.05	1.81	2.17	0.05	1.81
2,4-Dimethyl-3-ethylpentane	7.67	0.58	0.55	1.33	0.58	0.55
3-ethylheptane	7.72	1.39	0.00	1.28	1.39	0.00
3,3-Diethylpentane	5.65	1.29	2.00	3.35	1.29	2.00
2,2,4-Trimethylhexane	7.66	0.00	1.06	1.34	0.00	1.06
2,2,5-Trimethylhexane	8.30	0.00	0.43	0.70	0.00	0.43
2,3,3-Trimethylhexane	6.04	0.00	2.79	2.96	0.00	2.79
2,4,4-Trimethylhexane	8.09	0.00	0.64	0.91	0.00	0.64
3,3,4-Trimethylhexane	5.57	0.11	3.16	3.43	0.11	3.16
2,3,5-Trimethylhexane	8.80	0.00	0.01	0.20	0.00	0.01
2,2-Dimethylheptane	8.51	0.39	0.00	0.49	0.39	0.00
2,6-Dimethylheptane	9.00	0.05	0.00	0.00	0.05	0.00
2-Methyloctane	8.25	1.01	0.00	0.75	1.01	0.00
3-Methyloctane	8.05	1.16	0.00	0.95	1.16	0.00
4-Methyloctane	8.02	1.15	0.00	0.98	1.15	0.00
2,2-Dimethyloctane	9.63	0.24	0.00	0.37	0.24	0.00

2,3-Dimethyloctane	9.01	0.99	0.00	0.99	0.99	0.00
2,4-Dimethyloctane	9.27	0.54	0.00	0.73	0.54	0.00
2,5-Dimethyloctane	9.12	0.76	0.00	0.88	0.76	0.00
2,6-Dimethyloctane	9.21	0.73	0.00	0.79	0.73	0.00
2,7-Dimethyloctane	9.56	0.44	0.00	0.44	0.44	0.00
3-Methylnonane	8.66	1.50	0.00	1.34	1.50	0.00
2-Methylnonane	8.86	1.33	0.00	1.14	1.33	0.00
4-Methylnonane	8.63	1.46	0.00	1.37	1.46	0.00
5-Methylnonane	8.85	1.23	0.00	1.15	1.23	0.00
2,2,3,3-Tetramethylhexane	6.17	0.98	2.39	3.83	0.98	2.39
3,3,5-Trimethylheptane	8.66	0.25	0.73	1.34	0.25	0.73
2,2,4,6,6-Pentamethylheptane	8.57	0.00	2.36	3.43	0.00	2.36
1,2-Dimethylcyclopentane	3.55	2.76	0.64	1.55	2.76	4.36
1,3-Dimethylcyclopentane	4.01	2.71	0.00	2.01	2.71	5.00
1,1-Dimethylcyclopentane	4.06	2.59	0.00	2.06	2.59	5.00
Ethylcyclopentane	3.66	2.80	0.64	1.66	2.80	4.36
Methylcyclohexane	1.61	1.23	4.17	0.61	1.23	1.83
1,2-Dimethylcyclopentane	4.04	2.71	0.00	2.04	2.71	5.00
1,3-Dimethylcyclopentane	4.04	2.71	0.00	2.04	2.71	5.00
1,1,2-Trimethylcyclopentane	2.31	0.00	5.49	0.69	0.00	0.49
1,1,3-Trimethylcyclopentane	0.84	0.00	6.86	2.16	0.00	1.86
1-methyl-2-ethylcyclopentane	3.74	0.86	3.59	0.74	0.86	1.41
1,2-Dimethylcyclohexane	0.26	0.00	8.07	1.74	0.00	2.07
1,3-Dimethylcyclohexane	1.09	0.00	6.92	0.91	0.00	0.92
1,4-Dimethylcyclohexane	0.55	0.00	7.60	1.45	0.00	1.60
1-Methyl-3-ethylcyclopentane	3.79	0.32	3.88	0.79	0.32	1.12
1,2,4-Trimethylcyclopentane	4.53	0.21	3.20	1.53	0.21	1.80
1,2,3-Trimethylcyclopentane	5.10	1.69	1.22	2.10	1.69	3.78
1,1-Dimethylcyclohexane	0.91	0.00	7.10	1.09	0.00	1.10
Ethylcyclohexane	0.62	0.00	7.66	1.38	0.00	1.66
Isopropylcyclopentane	4.40	2.27	1.34	1.40	2.27	3.66
1-methyl-1-ethylcyclopentane	5.07	2.79	0.00	2.07	2.79	5.00
n-propylcyclopentane	5.00	3.14	0.00	2.00	3.14	5.00
1-methyl-2-ethylcyclopentane	2.90	0.00	5.10	0.10	0.00	0.10
1-methyl-3-ethylcyclopentane	3.50	0.00	4.55	0.50	0.00	0.45
1,2-Dimethylcyclohexane	0.94	0.00	7.18	1.06	0.00	1.18
1,3-Dimethylcyclohexane	0.66	0.00	7.49	1.34	0.00	1.49
1,4-Dimethylcyclohexane	1.15	0.00	6.84	0.85	0.00	0.84
1,2,3-Trimethylcyclopentane	3.75	0.00	4.09	0.75	0.00	0.91
1,2,4-Trimethylcyclopentane	2.19	0.00	5.62	0.81	0.00	0.62
n-Butylcyclopentane	5.96	3.20	0.00	1.96	3.20	5.00
n-Propylcyclohexane	0.00	0.00	9.32	3.00	0.00	3.32
n-Isopropylcyclohexane	3.94	2.45	2.67	0.94	2.45	3.33
1,3,5-Trimethylcyclohexane	5.89	0.85	2.06	2.89	0.85	3.94
n-Butylcyclohexane	0.00	0.00	10.45	4.00	0.00	4.45
Isobutylcyclohexane	0.91	4.15	4.44	3.09	4.15	1.56
Hexylcyclopentane	8.90	2.49	0.00	2.90	2.49	5.00
Heptylcyclopentane	10.47	1.99	0.00	3.47	1.99	5.00
Octylcyclopentane	11.56	1.87	0.00	3.56	1.87	5.00
Nonylcyclopentane	13.02	1.50	0.00	4.02	1.50	5.00
Decylcyclopentane	14.26	0.70	0.61	4.26	0.70	4.39
Dodecylcyclopentane	13.76	0.00	4.02	1.76	0.00	0.98
Tridecylcyclopentane	14.39	3.18	0.00	1.39	3.18	5.00
Tetradecylcyclopentane	15.49	2.96	0.00	1.49	2.96	5.00
Pentadecylcyclopentane	16.28	2.94	0.00	1.28	2.94	5.00
Hexadecylcyclopentane	17.32	2.48	0.33	1.32	2.48	4.67

Decylclohexane	11.32	4.39	0.38	1.32	4.39	5.62
Pentylcyclohexane	5.43	2.17	3.66	0.43	2.17	2.34
Hexylcyclohexane	6.41	1.97	3.92	0.41	1.97	2.08
Heptylcyclohexane	7.31	1.64	4.40	0.31	1.64	1.60
Octylcyclohexane	8.17	1.12	5.08	0.17	1.12	0.92
nonylcyclohexane	8.99	0.46	5.97	0.01	0.46	0.03
undecylcyclohexane	9.60	0.00	7.85	1.40	0.00	1.85
dodecylcyclohexane	9.46	0.00	9.02	2.54	0.00	3.02
tridecylcyclohexane	9.16	0.00	10.36	3.84	0.00	4.36
tetradecylcyclohexane	8.70	0.00	11.84	5.30	0.00	5.84
dicyclohexylmethane	0.00	1.58	12.16	1.00	1.58	0.16
1,1-dicyclohexylethane	0.00	1.59	13.16	2.00	1.59	1.16
2,2-dicyclohexylpropane	0.21	1.36	13.89	2.79	1.36	1.89
1,1-dicyclohexylbutane	2.35	0.76	12.90	1.65	0.76	0.90
1,1-dicyciohexylpentane	3.61	0.07	13.21	1.39	0.07	1.21
1,1-dicyclohexylhexane	4.69	0.00	13.07	1.31	0.00	1.07
1.1-dicyclohexylheplane	5.52	0.00	13.09	1.48	0.00	1.09
1,1-dicyclohexyloctane	5.99	0.00	13.51	2.01	0.00	1.51
Benzene	0.00	5.58	0.12	0.00	0.42	0.12
Toluene	1.27	5.62	0.00	0.27	0.38	0.00
Ethylbenzene	2.24	5.68	0.00	0.24	0.32	0.00
m-Xylene	2.74	5.27	0.00	0.74	0.73	0.00
o-Xylene	1.62	6.50	0.00	0.38	0.50	0.00
p-Xylene	2.78	5.24	0.00	0.78	0.76	0.00
o-ethyltoluene	0.34	2.17	6.85	2.66	3.83	6.85
m-ethyltoluene	2.97	2.08	4.26	0.03	3.92	4.26
p-ethyltoluene	3.34	5.60	0.00	0.34	0.40	0.00
1,2,3-Trimethylbenzene	1.97	7.38	0.00	1.03	1.38	0.00
1,2,4-Trimethylbenzene	3.21	5.98	0.00	0.21	0.02	0.00
n-Propylbenzene	3.30	5.61	0.00	0.30	0.39	0.00
n-Butylbenzene	4.21	5.74	0.00	0.21	0.26	0.00
m-Diethylbenzene	2.60	4.22	3.16	1.40	1.78	3.16
p-Diethylbenzene	4.70	5.32	0.00	0.70	0.68	0.00
3-Ethyl-o-xylene	1.68	4.78	4.01	2.32	1.22	4.01
2-Ethyl-m-xylene	3.48	6.60	0.00	0.52	0.60	0.00
4-Ethyl-m-xylene	4.22	5.89	0.00	0.22	0.11	0.00
5-Ethyl-m-xylene	5.01	5.02	0.00	1.01	0.98	0.00
4-Ethyl-o-xylene	4.15	6.01	0.00	0.15	0.01	0.00
2-Ethyl-p-xylene	4.26	5.79	0.00	0.26	0.21	0.00
Isobutylbenzene	3.81	5.64	0.00	0.19	0.36	0.00
1-Methyl-2-n-propylbenzene	4.03	5.91	0.00	0.03	0.09	0.00
1-Methyl-3-n-propylbenzene	4.76	5.15	0.00	0.76	0.85	0.00
1-Methyl-4-n-propylbenzene	4.72	5.24	0.00	0.72	0.76	0.00
m-Cymene	2.36	3.90	3.47	1.64	2.10	3.47
o-Cymene	1.81	3.74	4.31	2.19	2.26	4.31
p-Cymene	4.01	4.14	1.68	0.01	1.86	1.68
o-Diethylbenzene	1.55	3.52	5.02	2.45	2.48	5.02
1,2,4,5-Tetramethylbenzene	3.87	6.48	0.00	0.13	0.48	0.00
1,2,3,4-Tetramethylbenzene	2.47	8.17	0.00	1.53	2.17	0.00
1,2,3,5-Tetramethylbenzene	3.56	6.84	0.00	0.44	0.84	0.00
n-Pentylbenzene	5.21	5.78	0.00	0.21	0.22	0.00
Indane	0.00	6.80	2.61	0.00	0.80	0.39
Cumene	3.02	4.88	0.80	0.02	1.12	0.80
Mesitylene	3.89	5.16	0.00	0.89	0.84	0.00
n-Hexylbenzene	6.12	5.88	0.00	0.12	0.12	0.00
n-Hepthylbenzene	7.11	5.90	0.00	0.11	0.10	0.00

1,2-Diphenylethane	0.00	8.96	5.70	2.00	3.04	5.70
n-Octylbenzene	8.02	5.95	0.00	0.02	0.05	0.00
n-Nonylbenzene	8.61	6.24	0.00	0.39	0.24	0.00
n-Decylbenzene	9.47	6.29	0.00	0.53	0.29	0.00
n-Undecylbenzene	10.10	6.53	0.00	0.90	0.53	0.00
n-Dodecylbenzene	11.46	6.05	0.24	0.54	0.05	0.24
n-Tetradecylbenzene	13.12	5.85	0.57	0.88	0.15	0.57
n-Tridecylbenzene	12.37	6.26	0.00	0.63	0.26	0.00
n-Pentadecylbenzene	14.18	5.87	0.37	0.82	0.13	0.37
n-Hexadecylbenzene	15.12	5.97	0.20	0.88	0.03	0.20
n-Heptadecylbenzene	15.24	4.80	2.11	1.76	1.20	2.11
n-Octadecylbenzene	15.75	4.33	2.91	2.25	1.67	2.91
average				**1.37**	**0.93**	**1.54**

* AD = absolute deviation

Components used to model the distillation cuts

Table S3. Components used to model the distillation cuts.

Cut	Component	*NBP* (K)	*MW*	*SG*
C_7	2,4-Dimethylpentane	353.64	100.20	0.67638
	Cyclohexane	353.87	84.16	0.78229
	Benzene	353.24	78.11	0.88319
C_8	2,2,3-Trimethylpentane	382.99	114.23	0.72005
	1-trans-2-cis-3-Trimethylcyclopentane	383.55	112.22	0.75750
	Toluene	383.78	92.14	0.87407
C_9	2,2,3,3-Tetramethylpentane	413.44	128.26	0.76069
	1-trans-3,5-Trimethylcyclohexane	413.70	126.24	0.77564
	m-Xylene	412.27	106.17	0.86909
C_{10}	n-Decane	447.30	142.28	0.73424
	Isobutylcyclohexane	444.50	140.27	0.79810
	Isobutylbenzene	445.94	134.22	0.85773
C_{11}	n-Undecane	469.08	156.31	0.74391
	cis-Decahydronaphthalene	468.96	138.25	0.90182
	3-Ethyl-o-xylene	467.11	134.22	0.89657
C_{12}	n-Dodecane	489.47	170.34	0.75241
	1-methyl-2-pentylcyclohexane	490.65	168.32	0.81873
	p-tert-Butylethylbenzene	485.25	162.27	0.86827
C_{13}	n-Tridecane	508.62	184.37	0.76109
	2-Butyl-1,1,3-trimethylcyclohexane	510.52	182.35	0.83227
	1,2,3-Trimethylindene	509.00	158.24	1.02040
C_{14}	n-Tetradecane	526.73	198.39	0.76649
	Dicyclohexylmethane	525.95	180.33	0.87965
	1,2,3,4-Tetraethylbenzene	524.16	190.32	0.89078
C_{15}	n-Pentadecane	543.84	212.42	0.77175
	1,1-Dicyclohexylethane	544.32	194.36	0.89648
	1,1-Diphenylethane	545.78	182.27	1.00410
C_{16}	n-Hexadecane	560.01	226.45	0.77663
	2,2-Dicyclohexylpropane	559.15	208.38	0.90571
	2-Butylnaphthalene	561.15	184.28	0.96472
C_{17}	n-Heptadecane	575.3	240.47	0.78019
	Decylcyclohexane	570.75	224.43	0.82228
	n-Decylbenzene	571.04	218.38	0.85898
C_{18}	n-Octadecane	589.86	254.50	0.78414
	Dodecylcyclopentane	584.10	238.46	0.85420
	n-Undecylbenzene	586.40	232.41	0.85870
C_{19}	n-Nonadecane	603.05	268.53	0.78804
	Tetradecylcyclopentane	599.00	266.51	0.87017
	n-Dodecylbenzene	600.76	246.44	0.85954
C_{20}+	n-Pentatetracontane	827.15	633.21	0.82972
	n-Pentatriacontane	763.15	492.95	0.81651
	Naphthalene	491.14	128.17	1.02880