Supporting Information

Thermodynamics fundamentals and energy efficiency for separation and high-valued utilization of light naphtha from Fischer-Tropsch synthesis

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Table S1. Specification of the vapor-liquid equilibrium experimental reagents

Chemical name	CAS No.	Source	Mass fraction purity
1-hexene	592-41-6	Macklin	>99%
n-hexane	110-54-3	Jiangtian Co., Ltd	>98%
2-hexene	592-43-8	TCI	>98%
2-methylpentane	107-83-5	Macklin	>99%
3-methylpentane	96-14-0	TCI	>99%
1-octene	111-66-0	Macklin	>98%
2-octene	111-67-1	TCI	>98%
3-methylheptane	589-81-1	TCI	>97%

Table S2. Experimental VLE data for 1-hexene (1) + 2-hexene (2) at 101.3kPa

					Wilson		NRTL		UNIQUAC	
T/K	x_1	y_1	γ_1	γ_2	ΔT	Δ y	ΔT	Δ y	ΔT	Δ y
333.17	0.9408	0.9452	1.0105	1.0362	0.25	-0.0016	0.00	-0.0014	0.24	-0.0016
333.28	0.8858	0.8878	1.0045	1.0958	0.23	0.0033	0.01	0.0049	0.23	0.0038
333.44	0.8223	0.8300	1.0065	1.0613	0.19	0.0006	0.01	0.0030	0.19	0.0018
333.62	0.7602	0.7758	1.0118	1.0310	0.14	-0.0045	0.00	-0.0017	0.14	-0.0023
333.80	0.6998	0.7133	1.0048	1.0469	0.10	0.0002	-0.01	0.0029	0.11	0.0033
333.94	0.6418	0.6613	1.0112	1.0318	0.10	-0.0034	0.02	-0.0010	0.11	0.0006
334.07	0.5995	0.6137	1.0005	1.0480	0.08	0.0034	0.01	0.0053	0.10	0.0079
334.27	0.5476	0.5655	1.0029	1.0366	0.03	0.0017	-0.02	0.0027	0.05	0.0067
334.43	0.5019	0.5204	1.0018	1.0338	0.01	0.0025	-0.03	0.0027	0.04	0.0078
334.58	0.4557	0.4776	1.0078	1.0254	0.01	0.0003	-0.02	-0.0005	0.04	0.0057
334.76	0.4034	0.4217	0.9995	1.0295	0.01	0.0049	-0.02	0.0029	0.04	0.0101
335.17	0.2976	0.3150	0.9991	1.0219	0.00	0.0061	-0.05	0.0018	0.03	0.0103
335.38	0.2451	0.2638	1.0092	1.0149	0.01	0.0038	-0.05	-0.0013	0.03	0.0072
335.60	0.1883	0.2061	1.0192	1.0106	0.05	0.0025	-0.04	-0.0030	0.06	0.0049
335.77	0.1479	0.1578	0.9882	1.0156	0.07	0.0078	-0.04	0.0026	0.08	0.0095
335.94	0.1066	0.1197	1.0345	1.0069	0.09	0.0013	-0.01	-0.0031	0.10	0.0022
336.12	0.0585	0.0667	1.0445	1.0070	0.16	0.0008	0.06	-0.0008	0.16	0.0011
336.24	0.0238	0.0281	1.0776	1.0075	0.21	-0.0003	0.18	-0.0001	0.21	-0.0002

*Standard uncertainties are u(T) = 0.01 K and u(x_1) = u(y_1) = 0.001.

Table S3. Experimental VLE data for 2-methlypentane (1) + 1-hexene (2) at 101.3kPa

					Wilson		NRTL		UNIQUAC	
T/K	x_1	y_1	γ_1	γ_2	ΔT	Δ y	ΔT	Δ y	ΔT	Δ y
333.17	0.9408	0.9452	1.0105	1.0362	0.25	-0.0017	0.01	-0.0013	0.24	-0.0016
333.28	0.8858	0.8878	1.0045	1.0958	0.22	0.0032	0.01	0.0051	0.22	0.0037
333.44	0.8223	0.8300	1.0065	1.0613	0.18	0.0004	0.01	0.0033	0.18	0.0017
333.62	0.7602	0.7758	1.0118	1.0310	0.13	-0.0046	0.00	-0.0013	0.14	-0.0024
333.80	0.6998	0.7133	1.0048	1.0469	0.09	0.0001	-0.01	0.0033	0.10	0.0033
333.94	0.6418	0.6613	1.0112	1.0318	0.09	-0.0034	0.02	-0.0006	0.11	0.0006
334.07	0.5995	0.6137	1.0005	1.0480	0.07	0.0035	0.02	0.0057	0.09	0.0080
334.27	0.5476	0.5655	1.0029	1.0366	0.02	0.0018	-0.02	0.0032	0.05	0.0068
334.43	0.5019	0.5204	1.0018	1.0338	0.00	0.0027	-0.03	0.0032	0.03	0.0079
334.58	0.4557	0.4776	1.0078	1.0254	0.00	0.0006	-0.03	0.0000	0.03	0.0058
334.76	0.4034	0.4217	0.9995	1.0295	0.00	0.0052	-0.03	0.0034	0.03	0.0102
334.95	0.3498	0.3847	1.0453	0.9988	0.01	-0.0108	-0.02	-0.0138	0.04	-0.0061
335.17	0.2976	0.3150	0.9991	1.0219	0.00	0.0064	-0.05	0.0023	0.03	0.0104
335.38	0.2451	0.2638	1.0092	1.0149	0.02	0.0040	-0.05	-0.0008	0.03	0.0073
335.60	0.1883	0.2061	1.0192	1.0106	0.05	0.0026	-0.04	-0.0026	0.06	0.0049
335.77	0.1479	0.1578	0.9882	1.0156	0.08	0.0078	-0.04	0.0029	0.08	0.0095
335.94	0.1066	0.1197	1.0345	1.0069	0.10	0.0012	-0.01	-0.0027	0.10	0.0022
336.12	0.0585	0.0667	1.0445	1.0070	0.16	0.0007	0.06	-0.0006	0.16	0.0011
336.24	0.0238	0.0281	1.0776	1.0075	0.21	-0.0003	0.18	-0.0001	0.22	-0.0003

*Standard uncertainties are u(T) = 0.01 K and u(x_1) = u(y_1) = 0.001.

Table S4. Experimental VLE data for 3-methlypentane (1) + 1-hexene (2) at 101.3kPa

					Wilson		NRTL		UNIQUAC	
T/K	x_1	y_1	γ_1	γ_2	ΔT	Δ y	ΔT	Δ y	ΔT	Δ y
336.25	0.0205	0.0208	1.0200	1.0111	0.28	0.0012	0.27	0.0012	0.27	0.0012
336.22	0.0567	0.0635	1.1226	1.0054	0.24	-0.0029	0.23	-0.0029	0.23	-0.0029
336.19	0.0995	0.1029	1.0394	1.0096	0.18	0.0022	0.18	0.0022	0.18	0.0022
336.10	0.1891	0.2001	1.0659	1.0027	0.12	-0.0035	0.12	-0.0035	0.12	-0.0035
336.07	0.2398	0.2503	1.0529	1.0035	0.09	-0.0030	0.09	-0.0031	0.09	-0.0030
336.04	0.2919	0.3031	1.0478	1.0025	0.06	-0.0041	0.06	-0.0042	0.06	-0.0042
335.96	0.4105	0.4143	1.0214	1.0144	0.05	0.0003	0.05	0.0002	0.05	0.0003
335.89	0.7188	0.7147	1.0083	1.0385	0.07	0.0002	0.13	0.0001	0.13	0.0002
335.91	0.7765	0.7738	1.0099	1.0352	0.12	-0.0018	0.15	-0.0018	0.15	-0.0018
335.94	0.8379	0.8314	1.0048	1.0624	0.14	0.0020	0.17	0.0020	0.17	0.0020
335.97	0.9053	0.9049	1.0112	1.0253	0.16	-0.0029	0.22	-0.0029	0.21	-0.0029
335.99	0.9508	0.9507	1.0110	1.0211	0.21	-0.0020	0.25	-0.0020	0.25	-0.0020
336.02	1.0000	1.0000	1.0101		0.25	0.0000	0.29	0.0000	0.29	0.0000

*Standard uncertainties are u(T) = 0.01 K and u(x_1) = u(y_1) = 0.001.

Table S5. Experimental VLE data for 1-octene (1) + 2-octene (2) at 101.3kPa

					Wilson		NRTL		UNIQUAC	
T/K	x_1	y_1	γ_1	γ_2	ΔT	Δ y	ΔT	Δ y	ΔT	Δ y
398.53	0.0000	0.0000		1.0076	0.25	0.0000	0.25	0.0000	0.25	0.0000
398.23	0.0566	0.0652	1.0406	1.0067	0.19	0.0007	0.21	0.0004	0.18	0.0004
398.03	0.1039	0.1186	1.0367	1.0047	0.13	0.0009	0.15	0.0006	0.12	-0.0006
397.81	0.1604	0.1839	1.0476	0.9990	0.08	-0.0017	0.10	-0.0019	0.06	-0.0051
397.57	0.2127	0.2388	1.0326	1.0002	0.07	0.0003	0.08	0.0002	0.06	-0.0051
397.33	0.2594	0.2951	1.0532	0.9912	0.10	-0.0058	0.11	-0.0058	0.10	-0.0131
397.11	0.3175	0.3497	1.0258	0.9982	0.08	0.0010	0.08	0.0009	0.09	-0.0083
396.86	0.3652	0.4008	1.0291	0.9957	0.13	-0.0002	0.13	-0.0005	0.15	-0.0109
396.70	0.4145	0.4427	1.0058	1.0084	0.09	0.0088	0.09	0.0081	0.12	-0.0031
396.51	0.4657	0.5007	1.0179	0.9954	0.09	0.0031	0.09	0.0019	0.13	-0.0097
396.36	0.5032	0.5393	1.0186	0.9916	0.09	0.0024	0.09	0.0007	0.13	-0.0107
396.21	0.5603	0.5986	1.0197	0.9804	0.03	0.0000	0.03	-0.0024	0.08	-0.0132
395.97	0.6214	0.6623	1.0240	0.9642	0.03	-0.0039	0.04	-0.0070	0.10	-0.0165
395.81	0.6734	0.7019	1.0060	0.9912	0.00	0.0062	0.02	0.0027	0.07	-0.0054
395.58	0.7257	0.7590	1.0156	0.9601	0.02	-0.0018	0.05	-0.0053	0.09	-0.0118
395.40	0.7746	0.8064	1.0161	0.9434	0.01	-0.0042	0.05	-0.0075	0.08	-0.0124
395.24	0.8177	0.8432	1.0109	0.9489	0.00	-0.0023	0.04	-0.0049	0.07	-0.0086
395.03	0.8570	0.8788	1.0111	0.9405	0.04	-0.0032	0.09	-0.0049	0.11	-0.0075
394.83	0.9106	0.9242	1.0062	0.9460	0.02	-0.0020	0.07	-0.0025	0.08	-0.0038
394.70	0.9462	0.9528	1.0020	0.9825	0.02	0.0000	0.07	0.0003	0.06	-0.0003
394.55	1.0000	1.0000	0.9991		-0.03	0.0000	-0.03	0.0000	-0.03	0.0000

*Standard uncertainties are u(T) = 0.01 K and u(x_1) = u(y_1) = 0.001.

Table S6. Experimental VLE data for 3-methlyheptane (1) + 1-octene (2) at 101.3kPa

					Wilson		NRTL		UNIQUAC	
T/K	x_1	y_1	γ_1	γ_2	ΔT	Δ y	ΔT	Δ y	ΔT	Δ y
391.38	1.0000	1.0000	1.0214		0.67	0.0000	0.67	0.0000	0.67	0.0000
391.63	0.8832	0.8900	1.0221	1.0211	0.47	-0.0060	0.43	-0.0063	0.46	-0.0059
391.77	0.8167	0.821	1.0156	1.0546	0.36	-0.0026	0.33	-0.0022	0.36	-0.0019
391.9	0.7630	0.7661	1.0107	1.0620	0.27	-0.0003	0.24	0.0008	0.27	0.0009
392.05	0.6996	0.7093	1.0163	1.0369	0.19	-0.0052	0.16	-0.0033	0.19	-0.0033
392.23	0.6400	0.6482	1.0102	1.0418	0.08	-0.0019	0.07	0.0008	0.10	0.0006
392.37	0.5849	0.5956	1.0117	1.0345	0.02	-0.0025	0.02	0.0007	0.04	0.0005
392.51	0.5316	0.5431	1.0111	1.0318	-0.02	-0.0014	-0.02	0.0021	0.00	0.0020
392.66	0.4731	0.4852	1.0108	1.0291	-0.05	0.0002	-0.05	0.0035	-0.03	0.0038
392.83	0.4077	0.4170	1.0033	1.0318	-0.07	0.0052	-0.06	0.0081	-0.04	0.0089
392.98	0.3496	0.3670	1.0255	1.0159	-0.05	-0.0011	-0.06	0.0010	-0.03	0.0023
393.14	0.3016	0.3154	1.0170	1.0187	-0.06	0.0034	-0.07	0.0046	-0.04	0.0065
393.3	0.2393	0.2555	1.0338	1.0125	0.00	0.0014	-0.04	0.0014	0.02	0.0039
393.43	0.1963	0.2105	1.0345	1.0126	0.05	0.0028	-0.01	0.0021	0.05	0.0049
393.59	0.1447	0.1584	1.0514	1.0098	0.11	0.0015	0.02	0.0001	0.12	0.0029
393.8	0.0832	0.0944	1.0835	1.0078	0.20	-0.0003	0.06	-0.0020	0.20	0.0004
394.06	0.0000	0.0000		1.0129	0.41	0.0000	0.41	0.0000	0.41	0.0000

*Standard uncertainties are u(T) = 0.01 K and u(x_1) = u(y_1) = 0.001.

Table S7. Extend Antoine equation parameters of involved component

reagent	1-hexene	2-hexene	2-mehylpentane	3-mehylpentane	1-octene	2-octene	3-mehylheptane
T unit	K	K	K	K	K	K	K
P unit	kPa	kPa	kPa	kPa	kPa	kPa	kPa
C_{1i}	45.0692	47.7642	46.6712	50.1822	68.0282	120.4922	89.1622
C_{2i}	-5104.7	-5250.2	-5041.2	-5239.7	-7155.9	-8285.1	-7700.9
C_{3i}	0	0	0	0	0	0	0
C_{4i}	0	0	0	0	0	0	0
C_{5i}	-4.3484	-4.7627	-4.6404	-5.1592	-7.5843	-17.078	-11.067
C_{6i}	1.17E-17	1.63E-17	1.94E-17	2.17E-17	1.71E-17	1.80E-02	7.69E-06
C_{7i}	6	6	6	6	6	1	2
C_{8i}	133.39	140.17	119.55	110.25	171.45	172.95	152.6
C_{9i}	504.00	509.80	497.70	504.60	566.90	572.00	563.60

*Obtained from the Aspen property database

Table S8. Van Ness test results of the binary systems

system	Wilson		NRTL		UNIQUAC	
	Δp	Δy	Δp	Δy	Δp	Δy
1-hexene(1) + 2-hexene(2)	0.0412	0.2034	0.0663	0.2944	0.0453	0.4586
2-methlypentane (1) + 1-hexene (2)	0.0307	0.2711	0.0157	0.2311	0.0333	0.4825
3-methlypentane (1) + 1-hexene (2)	0.0529	0.2011	0.0530	0.2003	0.0529	0.2011
1-octene (1) + 2-octene (2)	0.0262	0.2314	0.0324	0.2789	0.0371	0.6983
3-methlyheptane (1) + 1-octene (2)	0.0684	0.2105	0.0577	0.2289	0.0638	0.2872

Table S9. The Wilson interaction parameters of some other components involved in this paper

Component i	1-pentene	n-pentane	n-pentane	1-hexene	1-hexene
Component j	n-pentane	2-methly-1-butene	n-hexane	n-hexane	n-octane
Temperature units	C	C	C	C	C
AIJ	0	0	0	-0.8895	0
AJI	0	0	0	-1.3753	0
BIJ	91.6395	-35.0643	157.0057	341.2918	138.2886
BJI	-174.2314	-8.3298	-177.5244	388.2634	-138.0379
TLOWER	0	5	25	55	55
TUPPER	25	25	68.2	67.9	55
Component i	n-hexane	n-hexane	n-hexane	n-hexane	
Component j	2-methylpentane	3-methylpentane	n-heptane	n-octane	
Temperature units	C	C	C	C	
AIJ	0	0	0	1.0178	
AJI	0	0	0	0.3288	
BIJ	-215.3085	-157.9951	54.7213	-165.5737	
BJI	150.9864	123.9267	-48.226	-255.819	
TLOWER	10	10	14	14	
TUPPER	40	40	98.6	124.3	
Component i	n-hexane	2-methylpentane	3-methylpentane	1-heptene	
Component j	n-decane	n-octane	n-octane	n-heptane	
Temperature units	C	C	C	C	
AIJ	0	0	0	0.3476	
AJI	0	0	0	0.1661	
BIJ	151.193	-37.6949	20.6325	-88.495	
BJI	-177.5945	3.667	-44.6721	-107.0888	
TLOWER	35	10	10	55	
TUPPER	144.8	40	40	98.44	
Component i	1-heptene	n-heptane	1-octene	n-octane	
Component j	n-octane	n-octane	n-octane	2-octene	
Temperature units	C	C	C	C	
AIJ	0	0.5957	0	0	
AJI	0	0.2943	0	0	
BIJ	177.0212	-62.0158	-33.0609	113.717	
BJI	-357.996	-308.2502	37.1995	-122.8106	
TLOWER	55	39.5	100.2	116.88	
TUPPER	55	124.3	125.28	125.49	

Table S10. The composition of the F-T oil feedstock

substance	mass content %	substance	mass content %	substance	mass content %
1-pentene	5.61	2-methylpentane	0.05	t-2-octane	0.17
n-pentane	2.53	3-methylpentane	0.06	2-methylheptane	0.07
c-2-pentene	0.13	1-heptene	15.79	3-methylheptane	0.10
t-2-pentene	0.12	n-heptane	5.69	1-nonene	15.03
2-methyl-1-butene	0.06	c-2-heptene	0.21	n-nonene	5.33
3-methyl-1-butene	0.06	t-2-heptene	0.20	c-2-nonene	0.16
1-hexene	9.64	2-methyl-1-hexene	0.08	c-2-nonene	0.15
n-hexane	4.48	2-methylhexane	0.07	1-decene	7.61
c-2-hexene	0.17	3-methylhexane	0.12	n-decane	2.02
t-2-hexene	0.17	1-octene	18.15	2-methylnonane	0.03
3-methyl-1-pentene	0.06	n-octane	5.86	3-methylnonane	0.05

Table S11. Summary of the two F-T synthesis oil separation processes

column	NS	Q_R/ Gcal • h^{-1}	Q_C/ Gcal·h^{-1}	product	purity wt. %	yield wt. %
			TDS process			
Col-11	33	3.6868	-1.8916	C6	91.60	94.48
Col-12	26	0.7513	-0.6645	C7	97.60	98.27
Col-13	39	2.6440	-2.4943	C8	94.40	96.45
Col-14	39	2.4207	-2.4122	C9	90.10	91.42
Col-15	40	1.4711	-1.5008	——	——	——
total	177	10.9739	-8.9633	——	——	——
			DWC process			
Col-21	53	5.6629	-3.8141	C6	91.50	94.48
Col-22	26	0.7513	-0.6645	C7	97.50	98.25
Col-23	53	3.2718	-3.1081	C8	94.40	96.41
total	132	9.6860	-7.5866	C9	90.30	91.57

Table S12. The composition of the C6 fraction feedstock

substance	mass content%	substance	mass content%
1-pentene	0.1	3-methyl-1-pentene	0.3
n-pentane	0.9	2-methylpentane	0.3
c-2-pentene	497 PPM	3-methylpentane	0.4
t-2-pentene	396 PPM	1-heptene	596 PPM
2-methyl-1-butene	18 PPM	n-heptane	9 PPM
3-methyl-1-butene	1PPB	c-2-heptene	460 PPB
1-hexene	65.3	t-2-heptene	460 PPB
n-hexane	30.3	2-methyl-1-hexene	8 PPM
c-2-hexene	1.2	2-methylhexane	21 PPM
t-2-hexene	1.1	3-methylhexane	13 PPM

Table S13. The composition of the C8 fraction feedstock

substance	mass content%	substance	mass content%
1-heptene	0.2	t-2-octane	0.7
n-heptane	0.9	2-methylheptane	0.3
c-2-heptene	289 PPM	3-methylheptane	0.3
t-2-heptene	199 PPM	1-nonene	3.8
2-methyl-1-hexene	4 PPM	n-nonene	0.3
2-methylhexane	1 PPM	c-2-nonene	94 PPM
3-methylhexane	5 PPM	c-2-nonene	114 PPM
1-octene	71.2	1-decene	175 PPB
n-octane	22.3	——	——

Table S14. Summary of narrow fraction separation processes

column	NS	Q_R/ Gcal·h^{-1}	Q_C/ Gcal·h^{-1}	purity wt. %	yield wt. %
		C6 fraction TC process			
Col-31	200	4.3090	-4.2875	95.0	96.67
		C6 fraction DPTC process			
Col-32	150	0	-4.0235	95.0	96.71
Col-33	50	3.5142	0	——	——
		C8 fraction TC process			
Col-41	200	5.7104	-5.7409	95.0	96.32
		C8 fraction DPTC process			
Col-42	110	0	-5.0755	95.0	96.35
Col-43	90	5.0184	0	——	——

Table S15. Details of columns and heat exchangers price in each process

columns	column price / 10^3 \$	condenser price / 10^3 \$	reboiler price / 10^3 \$
Col-11	492.63	31.42	31.47
Col-12	150.63	25.20	16.10
Col-13	456.22	28.14	27.97
Col-14	430.67	30.51	25.54
Col-15	318.29	21.72	31.75
Col-21	906.28	74.91	132.10
Col-22	150.63	25.20	16.10
Col-23	642.44	43.04	44.85
Col-31	2102.68	56.58	45.05
Col-32	1673.86	20.80	0
Col-33	739.63	0	82.74
Col-41	2572.67	78.33	56.18
Col-42	1603.12	32.40	0
Col-43	1419.53	0	162.78