Supporting Information

C₂/C₃ HYDROCARBON SEPARATION BY PRESSURE SWING ADSORPTION ON MIL-100(FE)

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<u>Tables</u>

Table S1. Main physical properties of MIL-100(Fe) sample in granule form.

Property	Granules
BET Surface area (m ² ·g ⁻¹)	1568
Micropore area $(m^2 \cdot g^{-1})$	1457
External Surface area $(m^2 \cdot g^{-1})$	110.9
Micropore volume (cm ³ ·g ⁻¹)	0.58

Table S2. Experimental conditions of breakthrough curves performed at 323 K and 150 kPa.

Run	Step	Feed composition	Q _{Feed} (SLPM)	Bed initial state
Single Co	mponent			
1	Adsorption	C ₂ H ₆	0.5	Filled with He
1	Desorption	Не	0.5	Filled with C ₂ H ₆
2	Adsorption	C ₂ H ₄	0.5	Filled with He
2	Desorption	Не	0.5	Filled with C ₂ H ₄
3	Adsorption	C ₃ H ₈	0.5	Filled with He
5	Desorption	Не	0.5	Filled with C ₃ H ₈
Binary				
	Adsorption	$0.30C_2H_6\!/0.70C_3H_8$	0.15/0.35	Filled with He
4	Desorption	Не	0.5	Filled with
			0.5	$0.30C_2H_6\!/0.70C_3H_8$
	Adsorption	$0.30C_2H_4\!/\!0.70C_3H_8$	0.15/0.35	Filled with He
5	December	Ца	0.5	Filled with
	Description	110	0.5	$0.30C_{2}H_{4}\!/0.70C_{3}H_{8}$
Pseudo-B	inary			
6	Adsorption	C ₂ H ₆	0.5	Filled with C ₃ H ₈
0	Desorption	C_3H_8	0.5	Filled with C ₂ H ₆
7	Adsorption	C ₂ H ₄	0.5	Filled with C ₃ H ₈
/	Desorption	C_3H_8	0.5	Filled with C ₂ H ₄

Step	Step Counter-current pressurization		Adsorption Rinse		Purge
		Cycle scheme 1			
Time, s	235	480	300	300	100
Pressure, kPa	150	150	150	10	10
Feed, SLPM	0.6 (C ₂ H ₆)	0.18/0.42 (C ₂ H ₆ / C ₃ H ₈)	0.6 (C ₃ H ₈)		0.15 (C ₂ H ₆)
Bed initial state		Filled with (C_2H_6 at 150) kPa	
		Cycle scheme 2	2		
Time, s	235	480	300	300	150
Pressure, kPa	150	150	150	10	10
Feed, SLPM	0.6 (C ₂ H ₄)	0.18/0.42 (C ₂ H ₄ / C ₃ H ₈)	0.6 (C ₃ H ₈)		0.15 (C ₂ H ₄)
Bed initial state	Filled with C ₂ H ₄ at 150 kPa				

Table S3. Experimental conditions for the VPSA cycles performed at 323 K.

Table S4. Henry's law constants for MIL-100(Fe) granules at three different temperatures.

Adsorbate	Henry cons	stants, K_H (mol kg	$-\Delta H_o$ (kJ mol ⁻¹)	<i>K_{Ho}</i> (mol kg ⁻¹ kPa ⁻¹)	
	323 K	373 K	423 K		
Ethane	9.87×10^{-3}	3.85×10^{-3}	2.03×10^{-3}	18.02	1.19×10^{-5}
Ethylene	9.40×10^{-3}	4.50×10^{-3}	2.24×10^{-3}	16.23	2.29×10^{-5}
Propane	3.50×10^{-2}	1.09×10^{-2}	4.19×10^{-3}	24.09	4.51×10^{-6}

	323 K (150 - 10 kPa)			373 K (373 K (150 - 10 kPa)			423 K (150 - 10 kPa)		
C_3/C_2 pair	$\Delta q_i / \Delta q_j$	$K_{\rm Hi}/K_{\rm Hj}$	$\mathbf{S}_{i/j}$	$\Delta q_i / \Delta q_j$	$K_{\rm Hi}/K_{\rm Hj}$	$S_{i\!/\!j}$	$\Delta q_i / \Delta q_j$	$K_{\rm Hi}/K_{\rm Hj}$	$S_{i\!/\!j}$	
Propane/Ethane (0.70/0.30)	6.6	3.5	23.3	7.7	2.8	21.6	7.2	2.1	14.9	
Propane/Ethylene (0.70/0.30)	7.5	3.7	28.0	8.8	2.4	21.3	8.2	1.9	15.3	
	323 K (150 - 50 kPa)			323 K (150 - 50 kPa) 373 K (150 - 50 kPa)			Pa)	423 K	(150 - 50 k	Pa)
Propane/Ethane (0.70/0.30)	4.0	3.5	14.2	5.2	2.8	14.7	5.1	2.1	10.4	
Propane/Ethylene (0.70/0.30)	4.6	3.7	17.1	6.0	2.4	14.5	5.7	1.9	10.7	

Table S5. Working capacities and selectivity parameters for MIL-100(Fe) granules at three different temperatures and different regeneration pressures.

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Parameter	Values
Overall heat transfer coefficient (U), $W \cdot m^{-2} \cdot K^{-1}$	20
Film (gas-wall) heat transfer coefficient (h_w), W·m ⁻² ·K ⁻¹	45
Film (gas-particle) heat transfer coefficient (h_f), W·m ⁻² ·K ⁻¹	40
Heat axial dispersion coefficient (λ), W·m ⁻¹ ·K ⁻¹	0.3
Film mass transfer coefficient (k_f), m·s-1	2 x 10 ⁻²
Axial dispersion coefficient (D_{ax}), m ² ·s ⁻¹	5 x 10 ⁻⁴
Wall specific heat at constant pressure (C_{pw}), J·kg ⁻¹ ·K ⁻¹	500
Particle specific heat at constant pressure (C_{ps}), J·kg ⁻¹ ·K ⁻¹	1456
	C ₂ H ₆ : 4.7 x 10 ⁻⁰⁹
Crystal diffusivity on site A (D_{cA}), m ² ·s ⁻¹	C ₂ H ₄ : 1.1 x 10 ⁻⁰⁸
	C ₃ H ₈ : 1.6 x 10 ⁻⁰⁹
	C ₂ H ₆ : 1.8 x 10 ⁻⁰⁹
Crystal diffusivity on site B (D_{cB}), m ² ·s ⁻¹	C ₂ H ₄ : 2.7 x 10 ⁻⁰⁹
	C ₃ H ₈ : 7.7 x 10 ⁻⁰⁹

Cycle	$Pu_R, \%$	$Rec_R, \%$	Prod _R , *	$Pu_X,\%$	$Rec_X, \%$	Prod _x , *
Scheme		C ₂ H ₆ or C	C_2H_4		C ₃ H ₈	
1	99.5	86.7	1.7	97.0	99.4	4.5
1: q _{sat} - 5%	97.6	86.6	1.7	97.9	96.8	4.3
1: q _{sat} + 5%	99.9	79.7	1.5	95.5	99.9	4.5
1: b∞ - 5%	98.8	85.8	1.7	97.6	98.4	4.4
1: $b_{\infty} + 5\%$	99.8	83.4	1.6	96.3	99.8	4.5
2	100.0	75.8	1.4	94.7	100.0	4.3
2: q _{sat} - 5%	99.3	78.7	1.5	95.9	99.1	4.3
2: q _{sat} + 5%	100.0	68.9	1.3	93.3	100.0	4.3
2: b _∞ - 5%	99.8	76.9	1.4	95.4	99.7	4.3
2: $b_{\infty} + 5\%$	100.0	72.2	1.3	93.9	100.0	4.3

Table S7. VPSA performance parameters comparison between the results obtained for the cycles designed with those obtained for the same cycles, but considering (b_{∞} a q_{sat}) by ±5%.

Porosimetry by Hg intrusion



Figure S1. Inter-crystalline macropore size distribution by mercury intrusion of MIL-100(Fe) granules.

Isotherm Equilibrium Data



Figure S2. Adsorption isotherms measured on MIL-100(Fe) granules. Closed and open symbols represent adsorption and desorption branches, respectively and the lines correspond to the fitted DSL model.



Figure S3. Adsorption isotherms comparison at 323 K, on different materials for: (a) ethane, and (b) ethylene [1-4].



Figure S4. C_2/C_3 mixtures selectivity on MIL-100(Fe) granules as a function of the total pressure at 323, 373, and 423 K predicted by the ExDSL model: (a) 0.30/0.70 ethane/propane mixture, and (b) 0.30/0.70 ethylene/propane mixture.

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Multicomponent adsorption equilibrium models



Figure S5. Binary ethane/propane adsorption equilibrium estimated by the ExDSL model and by the IAS theory as a function of the gas phase ethane molar fraction at 150 kPa, and at (a) 323, (b) 373, and (c) 423 K.



Figure S6. Binary ethylene/propane adsorption equilibrium estimated by the ExDSL model and by the IAS theory as a function of the gas phase ethylene molar fraction at 150 kPa, and at (a) 323, (b) 373, and (c) 423 K.

Transport Parameters:

To obtain the transport parameters included in the model it was necessary to estimate general properties of the gases and gas mixtures, like density, viscosity, molar specific heat and thermal conductivity. Viscosity of the pure components was obtained by the method of Chung et al. and the viscosity of the gas mixtures was calculated from the method of Wilke [5]. The thermal conductivities of the pure gases and gas mixtures were determined by the use of Eucken and Wassiljewa equations, respectively [5,6]. The transport parameters such molecular diffusivity and macropore diffusivity were estimated by the Chapman-Enskog and Bosanquet equations, respectively [6]. The values calculated for the micropore diffusivity according to the previously mentioned correlations are summarized in Table S4. The Wakao and Funazkri correlation was used to obtain the axial mass and heat dispersion coefficients [6]. The film heat transfer coefficient between the gas and the column wall was calculated with the Wasch and Froment correlation [6]. The only parameters that were adjusted to the experimental results were U and h_w, adjusted by the breakthrough experiments and then used in the simulations of the PSA cycles. The transport parameters obtained are summarized in Table S4.

Breakthrough curves



Figure S7. Molar flow rates (a) adsorption of ethane over a bed initially full of helium at 323 K and 150 kPa; (b) desorption of previously adsorbed ethane in flowing helium at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.



Figure S8. Molar flow rates (a) adsorption of ethylene over a bed initially full of helium at 323 K and 150 kPa; (b) desorption of previously adsorbed ethylene in flowing helium at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.



Figure S9. Molar flow rates (a) adsorption of propane over a bed initially full of helium at 323 K and 150 kPa; (b) desorption of previously adsorbed propane in flowing helium at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.



Figure S10. Molar flow rates (a) adsorption of a mixture 0.30/0.70 ethane/propane over a bed initially full of helium at 323 K and 150 kPa; (b) desorption of previously adsorbed mixture in flowing helium at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.



Figure S11. Molar flow rates (a) adsorption of a mixture 0.30/0.70 ethylene/propane over a bed initially full of helium at 323 K and 150 kPa; (b) desorption of previously adsorbed mixture in flowing helium at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.



Figure S12. Molar flow rates (a) adsorption of ethane over a bed initially full of propane at 323 K and 150 kPa; (b) desorption of previously adsorbed ethane in flowing propane at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.



Figure S13. Molar flow rates (a) adsorption of ethylene over a bed initially full of propane at 323 K and 150 kPa; (b) desorption of previously adsorbed ethylene in flowing propane at 323 K and 150 kPa; gas temperature history along the (c) adsorption and (d) desorption at 0.17 m, 0.42 m and 0.67 m from the bottom end of the column. Symbols represent experimental results and solid lines simulation results.

VPSA Cycles



Figure S14. Last (8th) cycle performed for the VPSA scheme 1 on MIL-100(Fe) granules: pressure history; molar flow rates of ethane and propane at the column exit considering a q_{sat} of 95% (left) and a q_{sat} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S15. Last (8th) cycle performed for the VPSA scheme 1 on MIL-100(Fe) granules: gas temperature history at 0.17 m (bottom), 0.42 m (middle) from the bottom end of the column; and column wall temperature at 0.67 m (top) from the bottom end of the column considering a q_{sat} of 95% (left) and a q_{sat} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S16. Last (8th) cycle performed for the VPSA scheme 1 on MIL-100(Fe) granules: pressure history; molar flow rates of ethane and propane at the column exit considering a b_{∞} of 95% (left) and a b_{∞} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S17. Last (8th) cycle performed for the VPSA scheme 1 on MIL-100(Fe) granules: gas temperature history at 0.17 m (bottom), 0.42 m (middle) from the bottom end of the column; and column wall temperature at 0.67 m (top) from the bottom end of the column considering a b_{∞} of 95% (left) and a b_{∞} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S18. Last (8th) cycle performed for the VPSA scheme 2 on MIL-100(Fe) granules: pressure history; molar flow rates of ethylene and propane at the column exit considering a q_{sat} of 95% (left) and a q_{sat} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S19. Last (8th) cycle performed for the VPSA scheme 2 on MIL-100(Fe) granules: gas temperature history at 0.17 m (bottom), 0.42 m (middle) from the bottom end of the column; and column wall temperature at 0.67 m (top) from the bottom end of the column considering a q_{sat} of 95% (left) and a q_{sat} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S20. Last (8th) cycle performed for the VPSA scheme 2 on MIL-100(Fe) granules: pressure history; molar flow rates of ethylene and propane at the column exit considering a b_{∞} of 95% (left) and a b_{∞} of 105% (right). Symbols represent the experimental results and lines the simulation results.



Figure S21. Last (8th) cycle performed for the VPSA scheme 2 on MIL-100(Fe) granules: gas temperature history at 0.17 m (bottom), 0.42 m (middle) from the bottom end of the column; and column wall temperature at 0.67 m (top) from the bottom end of the column considering a b_{∞} of 95% (left) and a b_{∞} of 105% (right). Symbols represent the experimental results and lines the simulation results.

RAW DATA

Equilibrium isotherms data:

P (kPa)	q (mol/kg)
24.490	0.206
61.340	0.519
204.210	1.523
403.550	2.609
816.600	4.100
597.790	3.403
95.980	0.825



P (kPa)	q (mol/kg)
18.820	0.084
49.580	0.208
195.800	0.660
402.460	1.228
790.700	2.267
590.510	1.705
95.600	0.433





P (kPa)	q (mol/kg)
13.070	0.022
52.330	0.097
198.820	0.355
399.200	0.674
790.570	1.448
598.260	0.976
98.150	0.220

P (kPa)	q (mol/kg)
13.066	0.126
52.850	0.540
192.660	1.750
394.920	3.075
780.600	4.659
568.980	3.956
106.900	1.051



q (mol/kg)
0.056
0.180
0.673
1.302
2.257
1.815
0.380





P (kPa)	q (mol/kg)
12.990	0.043
48.113	0.104
197.018	0.344
399.126	0.654
797.123	1.175
593.570	0.929
98.336	0.207

P (kPa)	q (mol/kg)
9.952	0.427
93.673	3.198
193.772	4.437
393.512	5.550
784.991	6.226
594.553	6.030
67.482	2.621



q (mol/kg)
0.269
0.539
1.939
3.351
4.856
4.216
1.204





P (kPa)	q (mol/kg)
12.979	0.076
55.228	0.240
204.500	0.812
401.787	1.695
799.000	3.229
598.944	2.528
105.847	0.452

Breakthrough experiments data:

Single ethane:

Time, s	yethane	Time, s	yethane
214	0.003099134	5	0.916484988
297	0.000737907	13	1.039142268
303	0.004874727	21	1.023301724
310	0.086964795		
322	0.729318067	28	0.918192418
329	0.91081837	37	0.865185472
334	0.948244745	48	0.807590974
344	0.955749918	78	0.670590722
379	0.969921986	125	0.594946233
399	0.987930406	170	0 4 6 2 7 2 7 4 0 2
429	0.975798294	1/8	0.463/3/102
461	0.971325268	278	0.286146882
579	0.990250693	451	0.075227019
759	0.983873482	698	0.032148152
960	0.992426226	000	0 010520701
3429	1	999	0.010339791
3608	1	1398	0.005685132
3759	1	2001	0.003388899

Time, s	yethane	Time, s	yethane
243	0.005545429	3	0.836500203
299	0.001690645	14	1.068182168
304	0.002547403	23	1.004894699
310	0.022717073		
315	0.280654939	59	0.812816382
320	0.665559466	89	0.662516439
325	0.84751748	151	0.521673783
330	0.93655201	242	0.357099207
335	0.942607941	349	0.193522273
340	0.961267834	E 0.0	0.052007050
373	1.006102016	598	0.053887656
448	0.981459297	899	0.0143904
597	0.942211118	1149	0.007234672
763	1.00967682	1699	0.003821829
1057	1.006703142	2100	0.002475210
4258	1.001467285	2190	0.002475515
4402	1.005309436	2498	0.001955562
4547	1.015607402	2811	0.001715846

Single ethylene:

Time, s	yethylene	Time, s	yethylene
18	0.0055		
48	0.000764305	15	0.772312473
64	0.000798207	25	1 014832575
83	0.003551028	25	1.014032373
113	0.001417989	39	0.88890327
143	0.000932155	60	0.760137853
173	0.001041249	86	0.648285636
223	0.003077968	120	0.537624527
273	0.044847055	180	0 424031755
323	0.785142352	100	0.424031733
423	0.972115303	280	0.274526284
483	0.978341605	359	0.156081023
583	0.985401354	450	0.109222695
704	0.962832397	700	0.040153869
883	0.982176367	000	0.015701595
3575	1	222	0.013101302
3838	1	1400	0.008257856
4126	1	1949	0.004001621

Time, s	yethylene
259	0.0041
274	0.001313977
284	0.003808557
294	0.04132217
304	0.727330923
314	0.926290886
324	0.980663546
333	0.982532299
344	0.9843169
359	0.989639006
370	1.019642706
390	1.001709975
404	1.011375525
420	0.993230742
819	1.012190682

Single propane:

Time, s	ypropane	Time, s	ypropane
198	0.001501592	5	0.91632793
723	0.000434279	19	1.031187564
733	0.001428521	39	0.878585879
743	0.020727742		0.07000075
754	0.477235065	61	0.772836817
764	0.820293404	78	0.717801303
778	0.925909947	110	0.660887234
794	0.91489762	129	0.62282029
808	0.944014396	179	0.580698181
838	0.948333362	275	0.544704626
868	1.005069592	275	0.511784626
918	0.951247203	359	0.465191568
1019	0.991180821	481	0.406555485
1218	0.97834973	769	0.348759068
1521	0.996419077	1000	0.261156551
4078	1	1000	0.201120221
4269	1	1399	0.187438824
4893	1	2105	0.042194214

Time, s	ypropane	Time, s	ypropane
704	0.003139417	2	0.856254861
		8	1.051903405
742	0.000998471	28	0.931681556
747	0.002171943		
752	0.001731095	87	0.726430347
757	0.009236173	221	0.568211439
762	0.145603057	318	0.485257673
767	0.56611247	447	0.428889766
772	0.833365652	597	0 384720637
777	0.899871326	557	0.504720057
797	0.953323985	748	0.346461501
829	0.953653826	870	0.301349857
889	0.956571383	1200	0.234004658
991	0.980843174	1610	0.14191155
1213	0.9911798	1000	0.070050474
4390	1.008107685	1800	0.078058474
4588	0.983815726	2402	0.01880579
4818	1.008076589	2901	0.004796531

Time, s	yethane	ypropane	Time, s	yethane	ypropane
456	0.002675114	0.001793	4	0 255670483	0.659663
510	0.000405386	0.000205	0	0.2021070105	0.770442
514	0.000524228	0.000231	9	0.30318/393	0.770442
520	0.001949643	0.000807	19	0.298687087	0.747127
525	0.00147662	0.000234	34	0.237054535	0.664256
530	0.00289334	0.000185	50	0.200195451	0.616201
535	0.03258732	0.000148	89	0.150927064	0.551575
544	0.624096313	0.00022	124	0 108727158	0 509972
559	0.905925871	0.000505		0.100727130	0.303372
589	0.981281654	0.000656			
639	1.006834224	0.003112	322	0.015842429	0.451128
749	0.9563	0.0437	449	0.004966499	0.400926
889	0.4863	0.5137	699	0.002617031	0.328803
1024	0.3619	0.6381	999	0.001859835	0 274825
1248	0.3207	0.6793	1200	0.001444011	0.201602
4888	0.2776	0.7224	1299	0.001444011	0.201603
5088	0.2810	0.7190	1599	0.001337138	0.119811
5289	0.2797	0.7203	2535	0.000772001	0.022222

Binary 30ethane/70propane vs Helium:

Time, s	yethane	ypropane	Time, s	ethane	propane
446	0.002444882	0.001497	14	0.240495189	0.643614
512	0.000906352	0.000991	25	0.282284572	0 75 28/1
531	0.001482447	0.000807	25	0.202204572	0.752041
537	0.007349995	0.001688	39	0.237196079	0.679883
541	0.080793865	0.00103	69	0.171486248	0.596342
548	0.67606277	0.00102	99	0.129233137	0.541948
701	0.9992	0.0008	209	0.058625886	0.477794
767	0.9991	0.0009	249	0.029328803	0.453171
793	0.9977	0.0023	200	0.007077420	0.422265
838	0.9657	0.0343	500	0.007877429	0.452205
868	0.5456	0.4544	599	0.003317798	0.376809
961	0.3897	0.6103	870	0.001435653	0.300041
1148	0.3319	0.6681	1174	0.001560969	0.224297
1148	0.3021	0.6979	1399	0.001101347	0.171698
1755	0.2940	0.7060	1700	0.00110212	0.074490
5018	0.2778	0.7222	1799	0.00110213	0.074489
5246	0.2779	0.7221	2464	0.000869129	0.01641
5446	0.2684	0.7316	2950	0.000703188	0.003763

Time, s	yethane	ypropane
544	0.010847929	0.001403
556	0.723226581	0.000588
650	0.9995	0.0005
670	0.9990	0.0010
690	0.9994	0.0006
710	0.9995	0.0005
730	0.9995	0.0005
750	0.9994	0.0006
770	0.9992	0.0008
790	0.9991	0.0009
810	0.9980	0.0020
830	0.9965	0.0035
850	0.9697	0.0303
870	0.5989	0.4011
1080	0.3554	0.6446

Binary 30ethylene/70propane vs Helium:

Time, s	yethylene	ypropane	Time, s	yethane	ypropane
448	0.002578408	0.000465	8	0.247699519	0.635676
517	0.000448131	0.000281	10	0.200262405	0.707044
537	0.029462687	0.000401	18	0.309262105	0.787844
548	0.730824985	0.001768	28	0.26304086	0.709722
558	0.907301052	0.001398	48	0.205147275	0.633137
578	0.958437856	0.001426	73	0.162001191	0.582974
647	0.984870889	0.002637	98	0.126978935	0.542086
747	1.003020792	0.001512	148	0.087876098	0.499983
828	0.9981	0.0019	240	0.04720225	0.400000
848	0.9996	0.0004	249	0.04729325	0.462265
857	0.9971	0.0029	448	0.018086965	0.410915
867	0.9544	0.0456	698	0.006365823	0.341727
888	0.5575	0.4425	1111	0.002838056	0.244313
948	0.4171	0.5829	1508	0.001944434	0.153249
1047	0.3711	0.6289	2000	0.001544000	0.100210
4348	0.2976	0.7024	2008	0.001544909	0.037835
4357	0.2995	0.7005	2508	0.001231796	0.008342
4367	0.2990	0.7010	3008	0.000955565	0.002878

Time, s	yethylene	ypropane	Time, s	yethylene	ypropane
499	0.019577722	0.001645	4	0.24829889	0.646963
543	0.733386557	0.001448	9	0.298254651	0.782026
559	0.897359377	0.001983	24	0.275276455	0.727839
619	0.958154744	0.003588	35	0.232287396	0.666019
699	0.997374761	0.002625	54	0.19027833	0.615423
789	0.989231413	0.010769	79	0.148584083	0.565928
868	0.689888929	0.310111	124	0.104506957	0.516565
874	0.526894655	0.473105	199	0.062962379	0.47977
884	0.4521	0.5479	389	0.027686068	0.432088
998	0.3804	0.6196	550	0.010383511	0.375467
1099	0.3536	0.6464	899	0.003936398	0.290991
1198	0.3385	0.6615	1299	0.002237401	0.204792
1299	0.3280	0.6720	1749	0.001580929	0.088809
1398	0.3212	0.6788	2249	0.001392683	0.019855
1499	0.3161	0.6839	2800	0.001055269	0.004485

Pseudo-binary ethane vs propane:

Time, s	yethane	ypropane	Time, s	yethane	ypropane
4	0.005372423	0.994628	649	0.997801505	0.002198
9	0.001204587	0.998795	699	0.998948659	0.001051
29	0.00153667	0.998463	718	0.998614108	0.001386
69	0.007150661	0.992849	738	0.99755522	0.002445
119	0.015172255	0.984828	748	0.998503697	0.001496
199	0.142616342	0.857384	761	0.998220247	0.00178
299	0.322432749	0.677567	778	0.987812994	0.012187
449	0.490504057	0.509496	798	0.653612846	0.346387
598	0.602476375	0.397524	819	0.115704746	0.884295
799	0.701106081	0.298894	838	0.028001954	0.971998
1099	0.798841623	0.201158	858	0.016039747	0.98396
1498	0.9021	0.0979	949	0.009027367	0.990973
1998	0.9811	0.0189	1099	0.005367171	0.994633
2498	0.9954	0.0046	1298	0.003304445	0.996696
2998	0.9979	0.0021	1498	0.002557872	0.997442

Time, s	yethane	ypropane	Time, s	yethane	ypropane
7	0.005307903	0.994692	668	0.997503534	0.002496
19	0.001210822	0.998789	728	0.9989364	0.001064
49	0.002213584	0.997786	748	0.998491786	0.001508
89	0.014349946	0.98565	768	0.996866744	0.003133
169	0.075956539	0.924043	778	0.997499924	0.0025
249	0.242433432	0.757567	788	0.987201645	0.012798
369	0.410371508	0.589628	798	0.671011803	0.328988
499	0.537023986	0.462976	808	0.190768937	0.809231
700	0.650227609	0.349772	848	0.040673338	0.959327
898	0.741264783	0.258735	899	0.013382558	0.986617
1299	0.850576922	0.149423	1013	0.007398826	0.992601
1700	0.9442	0.0558	1198	0.004510324	0.99549
2249	0.9896	0.0104	1399	0.002878715	0.997121
2749	0.9966	0.0034	1604	0.002232301	0.997768
3249	0.9982	0.0018	1722	0.002028135	0.997972

Pseudo-binary ethylene vs propane:

Time, s	yethylene	ypropane	Time, s	yethylene	ypropane
4	0.006781829	0.993218	648	0.9983	0.0017
9	0.001174143	0.998826	698	0.9989	0.0011
28	0.001486582	0.998513	718	0.9991	0.0009
68	0.007623393	0.992377	738	0.9981	0.0019
118	0.018576719	0.981423	748	0.9986	0.0014
198	0.170522319	0.829478	758	0.9984	0.0016
298	0.365679432	0.634321	778	0.9869	0.0131
448	0.522613644	0.477386	799	0.4367	0.5633
598	0.6220819	0.377918	818	0.0954	0.9046
798	0.710929237	0.289071	838	0.0293	0.9707
1098	0.79782639	0.202174	870	0.0159	0.9841
1498	0.8970	0.1030	949	0.0096	0.9904
1998	0.9802	0.0198	1099	0.0065	0.9935
2498	0.9959	0.0041	1298	0.0041	0.9959
2998	0.9982	0.0018	1498	0.0032	0.9968

Time, s	yethylene	ypropane	Time, s	yethylene	ypropane
14	0.006937406	0.993063	668	0.997578577	0.002421
19	0.001309536	0.99869	729	0.999016476	0.000984
48	0.00191243	0.998088	769	0.998437194	0.001563
88	0.01056759	0.989432	789	0.983543971	0.016456
168	0.032375539	0.967624	799	0.499433028	0.500567
248	0.271218872	0.728781	809	0.132040859	0.867959
368	0.449714564	0.550285	819	0.051647661	0.948352
499	0.565354188	0.434646	829	0.03016535	0.969835
699	0.664719779	0.33528	839	0.0219205	0.978079
899	0.746433717	0.253566	849	0.017998479	0.982002
1299	0.846369407	0.153631	899	0.012812271	0.987188
1698	0.9397	0.0603	999	0.007952156	0.992048
2249	0.9893	0.0107	1198	0.005121752	0.994878
2749	0.9973	0.0027	1399	0.003230761	0.996769
3422	0.9985	0.0015	1610	0.002593632	0.997406

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