

Supplementary Materials

Fischer–Tropsch Synthesis: Computational Sensitivity Modeling for Series of Cobalt Catalysts

Harrison Williams ¹, Muthu K. Gnanamani ², Gary Jacobs ³, Wilson D. Shafer ¹ and David Coulliette ^{1,*}

¹. Asbury University, One Macklem Drive, Wilmore, KY, 40390, USA

². Center for Applied Energy Research, University of Kentucky, 2540 Research Park Dr., Lexington, KY, 40511, USA

³. University of Texas at San Antonio, Dept. of Biomedical Engineering and Chemical Engineering / Dept. of Mechanical Engineering, 1 UTSA Circle, San Antonio, TX, 78249, USA

* Correspondence: david.coulliette@asbury.edu; Tel.: 859-858-3511

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Category 1 Data:

Data Set 1A:

Figure S1A: Conversion % vs. TOS

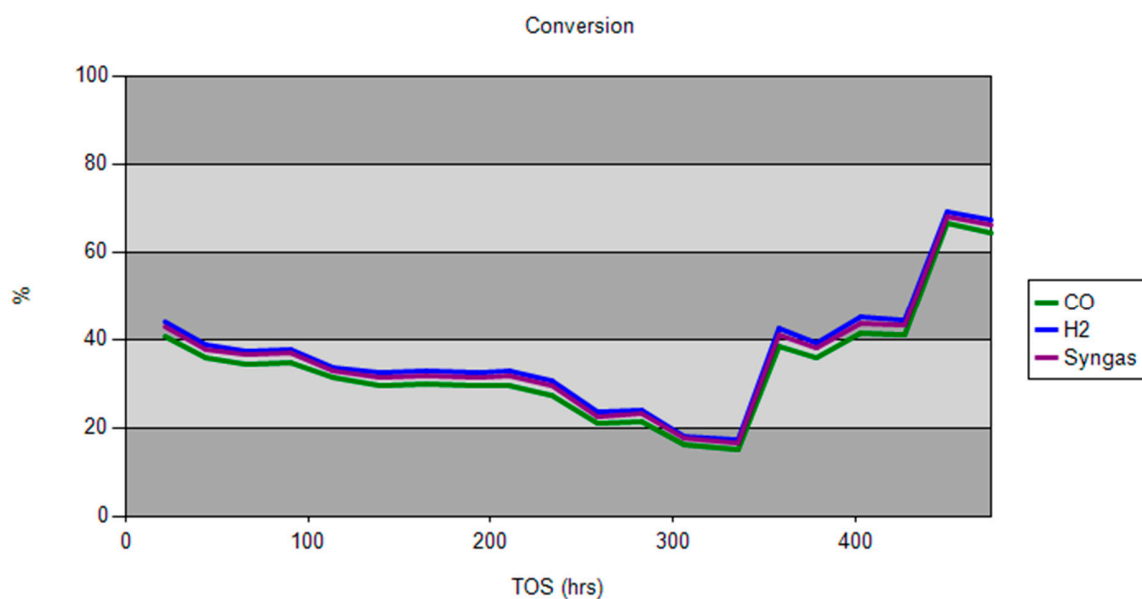


Table S1A: Experimental Data

TOS (hrs)	H ₂ :CO Ratio	Temperature (K)	Pressure (psig)	Gasfeed Flowrate (slph)	Tailgas Flowrate (slph)	Oil (g)	Wax (g)	Water (g)
21.50	2.0000	493	275	40.80	25.86	14.00	4.05	101.80
43.75	2.0000	493	275	40.80	27.81	12.40	7.20	81.50
66.25	2.0000	493	275	40.80	28.36	13.00	7.40	76.30

90.25	2.0000	493	275	40.80	28.12	12.80	7.30	83.00
114.00	2.0000	493	275	40.80	29.52	12.10	5.60	79.10
140.00	2.0000	493	275	40.80	29.99	11.85	4.65	77.60
165.00	2.0000	493	275	40.80	29.93	11.35	5.30	75.30
193.00	2.0000	493	275	40.80	29.94	12.56	5.76	78.58
210.75	2.0000	493	275	40.80	29.93	6.50	6.00	52.10
234.00	2.0000	493	275	40.80	30.83	10.00	5.70	68.00
258.25	2.0000	493	275	51.00	41.48	11.70	6.40	66.70
282.50	2.0000	493	275	51.00	41.17	11.15	6.55	66.35
306.50	2.0000	493	275	61.20	52.48	11.30	6.80	61.40
335.25	2.0000	493	275	61.20	52.93	12.80	6.90	71.15

Experimental Data for Data Set 1A. Includes the reaction conditions at each sample. While the experiment lasted for over 400 hours (Figure 1A), the data was truncated to avoid dramatic flowrate changes that caused significant error with the model.

Data Set 1B:

Figure S1B: Conversion % vs. TOS

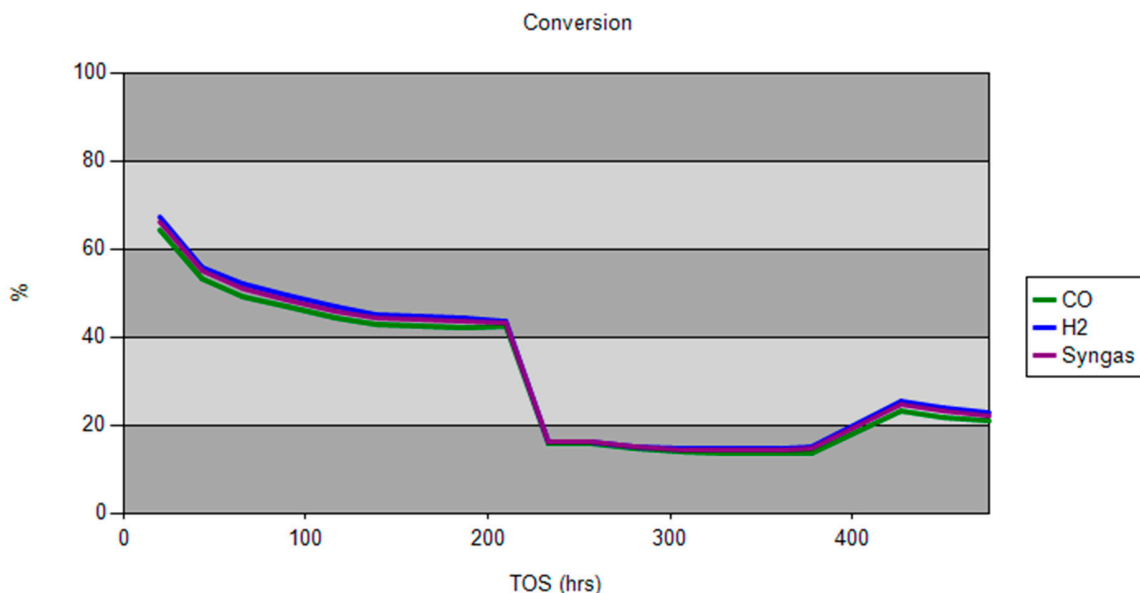


Table S1B: Experimental Data

TOS (hrs)	H ₂ :CO Ratio	Temperature (K)	Pressure (psig)	Gasfeed Flowrate (slph)	Tailgas Flowrate (slph)	Oil (g)	Wax (g)	Water (g)
19.50	2.0000	493	275	43.20	18.15	14.40	8.88	137.11
43.25	2.0000	493	275	43.20	22.59	14.85	12.00	138.70
65.75	2.0000	493	275	43.20	24.04	13.05	11.30	114.50
90.00	2.0000	493	275	43.20	24.95	13.00	11.50	108.60
116.75	2.0000	493	275	43.20	25.92	13.55	12.40	117.40
139.00	2.0000	493	275	43.20	26.61	10.85	10.90	95.50
164.00	2.0000	493	275	43.20	26.65	11.15	12.70	104.80
187.75	2.0000	493	275	43.20	26.87	10.92	10.37	98.04
209.50	2.0000	493	275	43.20	26.93	9.55	9.60	90.50

Experimental Data for Data Set 1B. Includes the reaction conditions and some products at each sample. While the experiment lasted for over 400 hours (Figure 1B), the data was truncated to avoid error caused by intentional ammonia poisoning of the catalyst.

Data Set 1C:

Figure S1C: Conversion % vs. TOS

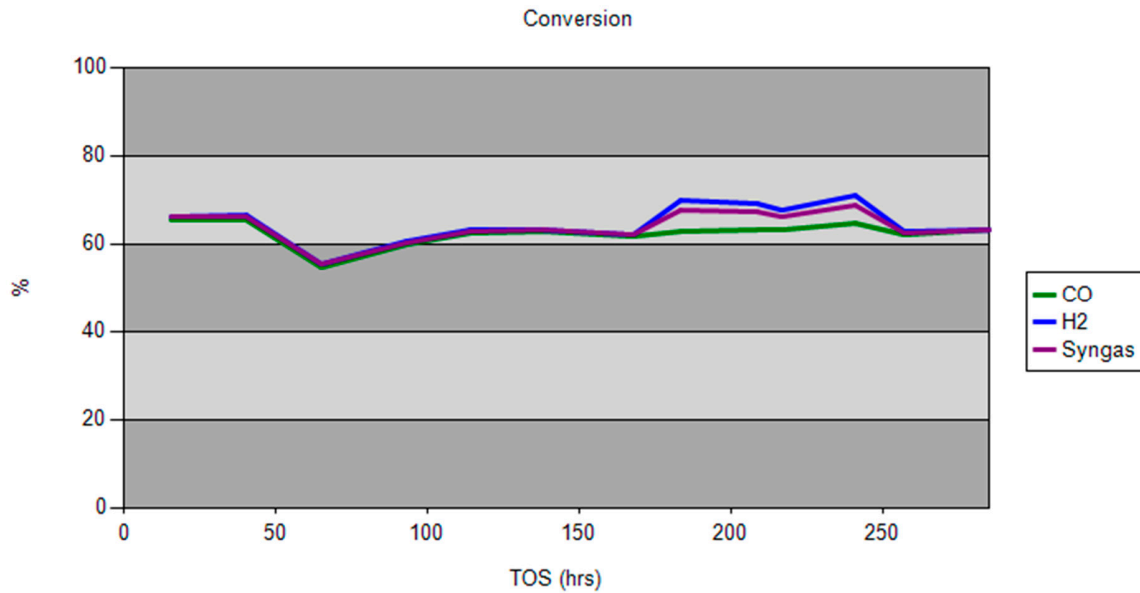


Table S1C: Experimental Data

TOS (hrs)	H2:CO Ratio	Temperature (K)	Pressure (psig)	Gasfeed Flowrate (slph)	Tailgas Flowrate (slph)	Oil (g)	Wax (g)	Water (g)
15.67	2.0000	493	275	33.30	12.11	6.25	4.30	85.99
40.67	2.0000	493	275	33.30	11.95	12.49	11.95	128.46
65.00	2.0000	493	275	33.30	15.61	10.87	13.11	126.97
93.00	2.0000	493	275	33.30	13.89	10.91	14.53	133.08
114.33	2.0000	493	275	33.30	13.08	8.59	11.67	111.63
138.17	2.0000	493	275	33.30	13.03	9.73	13.12	125.40
168.00	2.0000	493	275	33.30	13.41	11.58	15.99	153.82
183.50	1.8986	493	275	31.41	10.50	4.44	7.26	93.83
208.75	1.8986	493	275	31.41	10.49	10.56	13.59	155.12
216.92	1.8986	493	275	31.41	10.74	3.04	4.67	45.29
240.75	1.8986	493	275	31.41	10.03	8.18	14.61	140.55

Experimental Data for Data Set 1C. Includes the reaction conditions at each sample. While the experiment lasted for over 250 hours (Figure 1C), the data was truncated to avoid error caused by changing H2 to D2.

Category 2 Data:

Data Set 2A:

Figure S2A: Conversion % vs. TOS

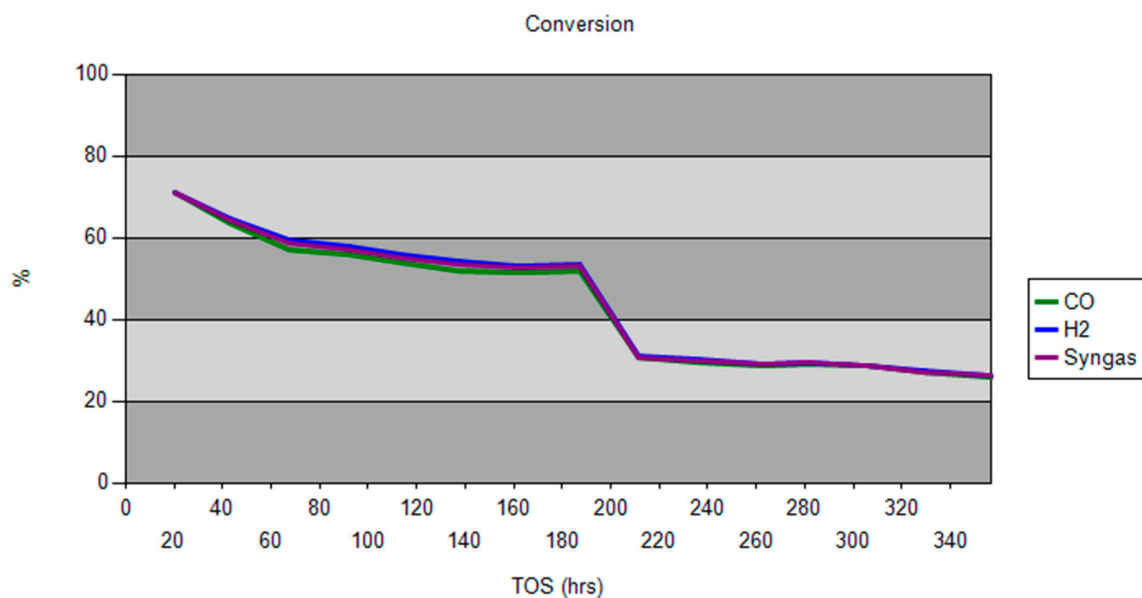


Table S2A: Experimental Data

TOS (hrs)	H ₂ :CO Ratio	Temperature (K)	Pressure (psig)	Gasfeed Flowrate (slph)	Tailgas Flowrate (slph)	Oil (g)	Wax (g)	Water (g)
20.50	2.0000	493	275	41.60	15.60	21.70	14.30	139.80
43.25	2.0000	493	275	41.60	18.09	20.80	21.50	144.00
67.50	2.0000	493	275	41.60	19.78	20.65	20.95	140.30
92.00	2.0000	493	275	41.60	20.58	19.40	21.73	131.95
113.75	2.0000	493	275	41.60	21.26	17.10	19.00	112.40
137.50	2.0000	493	275	41.60	22.32	17.80	19.75	120.50
162.50	2.0000	493	275	41.60	22.38	18.85	21.30	125.05
187.00	2.0000	493	275	41.60	22.39	18.00	20.10	117.10

Experimental Data for Data Set 2A. Includes the reaction conditions and some products at each sample. While the experiment lasted for over 340 hours (Figure 2A), the data was truncated to avoid error caused by intentional ammonia poisoning of the catalyst.

Data Set 2B:

Figure S2B: Conversion % vs. TOS

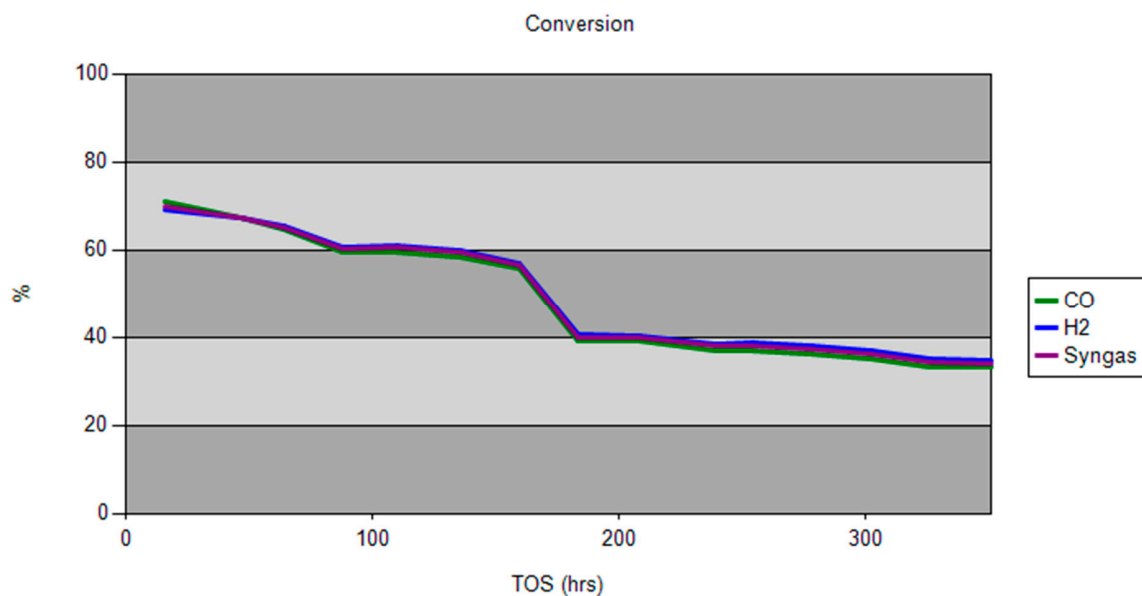


Table S2B: Experimental Data

TOS (hrs)	H2:CO Ratio	Temperature (K)	Pressure (psig)	Gasfeed Flowrate (slph)	Tailgas Flowrate (slph)	Oil (g)	Wax (g)	Water (g)
15.75	2.0000	493	275	32.80	12.81	13.40	7.10	85.80
47.25	2.0000	493	275	32.80	13.38	21.65	21.96	160.48
64.00	2.0000	493	275	32.80	14.08	11.70	10.60	82.00
88.25	2.0000	493	275	32.80	15.37	16.05	16.10	113.30
110.00	2.0000	493	275	32.80	15.26	14.40	15.05	99.30
135.50	2.0000	493	275	32.80	15.55	15.80	18.05	113.30
159.25	2.0000	493	275	32.80	16.37	14.40	16.60	105.00
183.50	2.0000	493	275	49.20	31.45	17.50	22.05	112.90
208.25	2.0000	493	275	49.20	31.68	17.50	21.15	111.60
239.50	2.0000	493	275	49.20	32.37	21.68	23.77	138.08
254.25	2.0000	493	275	49.20	32.41	10.30	10.10	65.20

Experimental Data for Data Set 2B. Includes the reaction conditions and some products at each sample. While the experiment lasted for over 300 hours (Figure 2B), the data was truncated to avoid error caused by intentional addition of 1-decene into the CSTR.

Data Set 2C:

Figure S2C: Conversion % vs. TOS

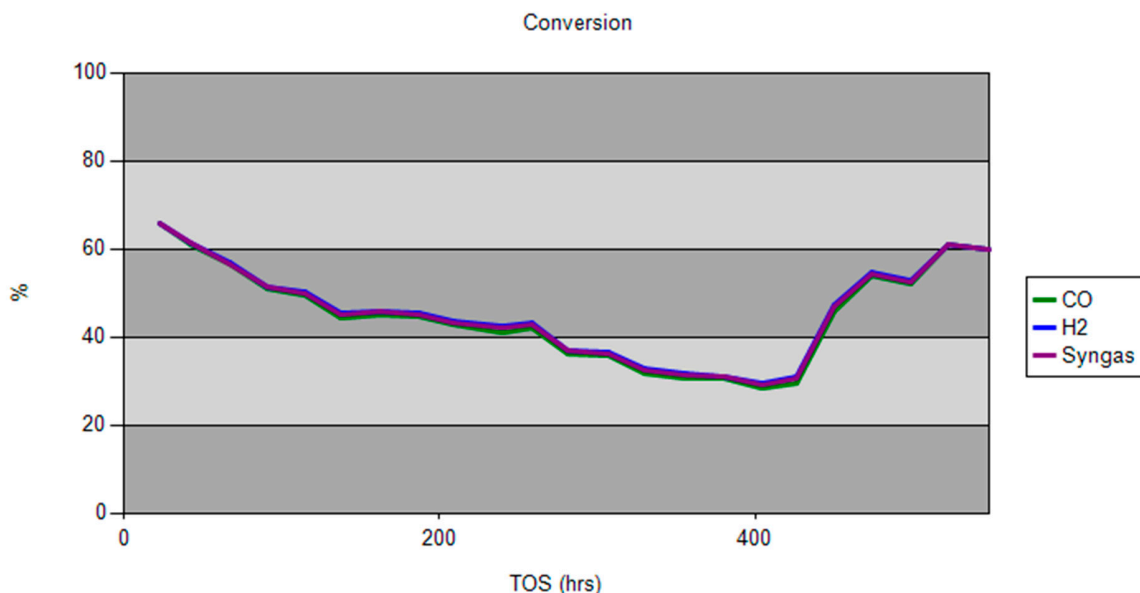


Table S2C: Experimental Data

TOS (hrs)	H2:CO Ratio	Temperature (K)	Pressure (psig)	Gasfeed Flowrate (slph)	Tailgas Flowrate (slph)	Oil (g)	Wax (g)	Water (g)
22.50	2.0000	493	275	38.40	15.84	16.10	17.00	139.40
43.00	2.0000	493	275	38.40	17.75	15.45	15.90	111.00
67.50	2.0000	493	275	38.40	19.59	17.28	17.58	125.09
90.75	2.0000	493	275	38.40	20.97	16.00	16.10	106.70
115.00	2.0000	493	275	38.40	21.80	16.80	17.40	108.15
137.50	2.0000	493	275	38.40	23.13	15.10	15.05	94.45
162.00	2.0000	493	275	38.40	22.87	15.80	16.30	101.00
187.50	2.0000	493	275	38.40	22.94	16.35	16.95	102.80
209.00	2.0000	493	275	38.40	24.21	13.40	13.25	80.45
239.75	2.0000	493	275	38.40	23.99	18.21	19.32	114.82
258.75	2.0000	493	275	38.40	24.04	11.70	11.70	70.45
281.50	2.0000	493	275	43.20	28.93	14.50	15.60	85.70
307.00	2.0000	493	275	43.20	29.16	15.60	16.60	94.00
330.00	2.0000	493	275	48.00	34.36	14.30	15.00	80.90
355.50	2.0000	493	275	48.00	34.41	15.25	16.20	90.40
380.00	2.0000	493	275	49.35	36.60	14.40	14.15	82.20
404.00	2.0000	493	275	49.35	36.39	13.82	13.60	78.37
425.75	2.0000	493	275	49.35	35.82	13.20	12.50	75.70

Experimental Data for Data Set 2C. Includes the reaction conditions at each sample. While the experiment lasted for over 450 hours (Figure 2C), the data was truncated to avoid dramatic flowrate changes that caused significant error with the model.