Kinetic study of hydrogen production by the high temperature water gas shift reaction of reformate gas in conventional and membrane packed bed reactors over Ca-promoted CeO_2-ZrO_2 supported Ni-Cu catalyst

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Supporting Information

Table S1. Experimental kinetic data

Run	T	r_{CO}	TOF*	N_{CO} ($x10^{-5}$)	N_{H2O} ($x10^{-4}$)	N_{H2} ($x10^{-5}$)	N_{CO2} ($x10^{-5}$)	K_{eq}	1-β
	K	mol/ (g-cat*hr)	(1/s)	mol/s	mol/s	mol/s	mol/s		
			Packed Bed Tubular Reactor – Atmospheric Pressure						
1	673	0.619	0.001145	5.6	1.6	1.1	5.3	11.85	0.994
2	673	0.618	0.001144	6.9	1.9	1.4	6.4	11.85	0.994
3	673	0.618	0.001144	8.6	2.3	1.7	7.8	11.85	0.994
4	673	0.619	0.001145	12	3.2	2.2	11	11.85	0.995
5	673	0.619	0.001145	23	6.2	4.4	20	11.85	0.995
6	723	0.717	0.001327	5.0	1.5	1.9	6.1	7.40	0.979
7	723	1.52	0.002813	5.8	1.8	2.2	7.2	7.40	0.979
8	723	4.7	0.008697	7.2	2.2	2.8	8.9	7.40	0.980
9	723	14.8	0.027385	8.6	2.5	3.1	9.7	7.40	0.982
10	723	20.7	0.038302	12	3.3	3.1	12	7.40	0.988
11	773	6.28	0.01162	2.8	1.1	3.3	6.9	4.91	0.844
12	773	12.1	0.022389	3.6	1.5	3.9	8.6	4.91	0.873
13	773	24	0.044408	5.6	2.0	4.4	11	4.91	0.915
14	773	42.8	0.079194	7.8	2.6	4.4	12	4.91	0.947
15	773	51	0.094367	11	3.2	3.9	13	4.91	0.972

Packed Bed Tubular Reactor – High Pressure (200 psi)									
16	673	4.81	0.0089	4.7	1.4	0.56	5.0	11.85	0.991
17	673	4.8	0.008882	5.6	1.6	0.56	5.6	11.85	0.992
18	673	4.8	0.008882	6.9	1.9	0.28	6.7	11.85	0.993
19	673	4.81	0.0089	8.3	2.3	0.28	7.8	11.85	0.994
20	673	4.81	0.0089	12	3.3	0.28	11	11.85	0.995
21	723	0.916	0.001695	4.2	1.3	1.1	5.6	7.40	0.975
22	723	0.927	0.001715	4.7	1.5	1.1	6.1	7.40	0.975
23	723	0.913	0.001689	5.8	1.8	1.4	7.5	7.40	0.976
24	723	0.906	0.001676	7.2	2.2	1.7	8.9	7.40	0.976
25	723	0.92	0.001702	10	3.2	2.2	13	7.40	0.977
26	773	1.85	0.003423	3.3	1.4	2.8	8.1	4.91	0.872
27	773	3.42	0.006328	4.4	1.7	3.3	9.7	4.91	0.878
28	773	14.7	0.0272	5.0	2.0	3.6	11	4.91	0.884
29	773	39	0.072163	6.4	2.4	3.6	12	4.91	0.911
30	773	49.3	0.091221	9.7	3.1	2.8	14	4.91	0.956
Membrane Reactor (200 psi)									
31	673	1.61	0.002979	3.6	1.3	2.5	6.1	11.85	0.971
32	673	3.18	0.005884	4.4	1.6	3.1	7.8	11.85	0.972
33	673	9.45	0.017486	6.1	2.1	3.9	10	11.85	0.975

34	673	20.4	0.037747	8.3	2.6	4.2	12	11.85	0.981
35	673	25	0.046258	10	3.2	4.4	13	11.85	0.985
36	723	5.09	0.009418	3.1	1.2	3.1	6.7	7.40	0.921
37	723	5.08	0.0094	3.6	1.4	3.6	7.8	7.40	0.927
38	723	5.09	0.009418	4.4	1.7	3.9	8.9	7.40	0.933
39	723	5.1	0.009437	5.6	2.0	4.7	11	7.40	0.938
40	723	5.09	0.009418	8.3	3.0	6.7	15	7.40	0.946
41	773	34.1	0.063096	6.4	3.1	10	20	4.91	0.779
42	773	41.7	0.077159	8.3	3.6	11	22	4.91	0.838
43	773	48.3	0.089371	13	4.9	12	26	4.91	0.897
44	773	52.6	0.097328	23	7.8	15	37	4.91	0.937
45	773	54.7	0.101213	53	16	25	70	4.91	0.959

*TOF = turnover frequency; $\mathbf{r_{CO}}$ = rate of CO conversion measured at reactor exit.

Table S2: Actual Reformate Gas Flow Rate and Mass Balance

Packed Bed Reactor (Atmospheric pressure)

CO (IN-OUT) mol/s	H_2O (IN-OUT) mol/s	CO_2 (IN-OUT) mol/s	**CO,0 (mol/s)**	**Reformate (mol/s)**	**Reformate (mL/min)**
3.24	6.10	-3.95	6.50	14.13	190.03
3.89	7.97	-4.76	7.56	16.44	221.09
4.70	10.26	-5.78	9.00	19.57	263.11
6.65	14.64	-8.16	12.50	27.17	365.43
11.88	25.20	-14.69	24.38	52.99	712.60
4.00	7.51	-4.73	6.25	13.59	182.72
4.74	8.36	-5.60	7.63	16.58	222.91
5.86	10.65	-6.91	9.25	20.11	270.42
6.24	12.11	-7.44	10.25	22.28	299.66
7.47	15.67	-9.04	13.13	28.53	383.71
5.00	8.50	-5.71	5.13	11.14	149.83
6.30	9.74	-7.09	7.13	15.49	208.30
7.85	13.63	-8.95	9.00	19.57	263.11
8.26	14.15	-9.56	11.38	24.73	332.55
8.47	16.67	-10.04	13.13	28.53	383.71

Packed Bed Reactor (200 psi)

3.17	5.67	-3.80	5.81	12.64	169.93
3.48	6.71	-4.22	6.50	14.13	190.03
4.13	8.58	-5.02	7.56	16.44	221.09
4.76	9.65	-5.81	9.19	19.97	268.59
6.66	13.64	-8.16	13.13	28.53	383.71
3.75	6.87	-4.39	5.50	11.96	160.79
4.06	6.90	-4.77	6.44	13.99	188.20
4.99	8.97	-5.86	7.63	16.58	222.91
5.86	10.65	-6.91	9.25	20.11	270.42
8.66	14.64	-10.16	13.75	29.89	401.98
5.95	9.12	-6.69	6.69	14.54	195.51
7.04	11.59	-7.96	7.88	17.12	230.22
7.98	12.45	-9.03	9.38	20.38	274.08
8.53	13.31	-9.73	11.00	23.91	321.58
9.52	17.06	-11.07	13.31	28.94	389.19

Membrane Reactor (200 psi)

4.27	6.67	-4.90	5.88	12.77	171.75
5.50	8.74	-6.29	7.25	15.76	211.95
6.96	11.65	-8.01	9.31	20.24	272.25
8.17	15.17	-9.49	11.06	24.05	323.41
8.65	14.63	-10.16	13.75	29.89	401.98
4.85	7.87	-5.49	5.56	12.09	162.62
5.65	9.12	-6.39	6.50	14.13	190.03
6.39	9.97	-7.26	7.88	17.12	230.22

7.85	13.63	-8.95
10.60	17.25	-12.12
15.01	22.54	-16.74
16.28	25.44	-18.26
18.63	30.09	-21.19
25.67	43.67	-29.59
46.77	89.43	-54.82

9.00	19.57	263.11
13.56	29.48	396.50
15.38	33.42	449.48
17.31	37.64	506.13
22.50	48.91	657.78
34.38	74.73	1004.94
66.88	145.38	1955.07