Supporting information

Synergistic effect of Fe-Co bimetallic catalyst on FTS and WGS activity in the Fischer Tropsch process: A kinetic study

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Table S1: Detail FTS reaction model

`FT1RDS-4	$r_{FT} = \frac{kK_1K_2K_7K_6K_3^{3/2}P_{CO}P_{H_2}^{3/2}}{P_{H_2O}(1+K_1P_{CO}+\sqrt{K_3P_{H_2}})^3}$	FT3 RDS-10	$r_{FT} = \frac{kK_1K_3^{1/2}P_{CO}P_{H_2}^{1/2}}{(1+K_1P_{CO}+\sqrt{K_3P_{H_2}})^2}$
FT1RDS-5	$r_{FT} = \frac{kK_1K_2K_4K_7K_6K_3^{2}P_{CO}P_{H_2}}{P_{H_2O}\left(1+K1P_{CO}+\sqrt{K_3P_{H_2}}\right)^3}$	FT3 RDS-11	$r_{FT} = \frac{kK_1K_3K_{10}P_{CO}P_{H_2}}{(1+K_1P_{CO}+\sqrt{K_3P_{H_2}})^2}$
FT2 RDS-8	$r_{FT} = \frac{kK_1K_2K_6K_7K_3^{3/2}P_{CO}P_{H_2}^{5/2}}{P_{H_2O}\left(1+K_1P_{CO}+\sqrt{K_3P_{H_2}}\right)^{5/2}}$	FT4 RDS-13	$r_{FT} = \frac{kK_1K_{12}K_{10}K_3^{1/2}P_{CO}P_{H_2}^{1/2}}{(1+K_1P_{CO}+\sqrt{K_3P_{H_2}})}$
FT3RDS-4	$r_{FT} = \frac{kK_1K_3K_{10}K_{11}P_{CO}P_{H_2}}{K_{H_2O}(1+K_1P_{CO}+\sqrt{K_3P_{H_2}})^3}$	FT4 RDS-5	$r_{FT} = \frac{kK_1K_7K_{13}K_{12}K_{10}K_3^{\frac{3}{2}}P_{CO}P_{H_2}^{\frac{3}{2}}}{P_{H_2O}\left(1+K_1P_{CO}+\sqrt{K_3P_{H_2}}\right)}$
FT3 RDS-5	$r_{FT} = \frac{kK_4K_1K_{10}K_{11}K_3^{3/2}K_{H_2O}P_{CO}P_{H_2}^{\frac{3}{2}}}{P_{H_2O}\left(1+K_1P_{CO}+\sqrt{K_3P_{H_2}}\right)^3}$	FT5 RDS-14	$r_{FT} = \frac{kK_1P_{CO}P_{H_2}}{1+K_1P_{CO}+\sqrt{K_3P_{H2}}}$
		FT5 RDS-15	$r_{FT} = kK_1K_{14}P_{CO}P_{H_2}^2 = kP_{CO}P_{H_2}^2$

Table S2: Kinetic and adsorption parameter

Model no	k′	a	b
FT1RDS-4	$kK_1K_2K_7K_6K_3^{3/2}$	K_1	$K_3^{1/2}$
FT1RDS-5	$kK_2K_1K_4K_7K_6K_3^2$	K_1	$K_3^{1/2}$
FT2RDS-8	$kK_1K_2K_6K_7K_3^{3/2}$	K_1	$K_3^{1/2}$
FT3RDS-10	$kK_1K_3^{\frac{1}{2}}$	K_1	$K_3^{1/2}$
FT3RDS-11	$kK_1K_3K_{10}$	K_1	$K_3^{1/2}$
FT3RDS-4			
FT3 RDS-5	$kK_4K_1K_{10}K_{11}K_3^{3/2}K_{H_2O}$	K_1	$K_3^{1/2}$
FT4 RDS-13	$kK_1K_{12}K_{10}K_3^{1/2}$	K_1	$K_3^{1/2}$
FT4 RDS-5	$kK_1K_7K_{13}K_{12}K_{10}K_3^{\frac{3}{2}}$	K_1	$K_3^{1/2}$
FT5 RDS-14	kK_1	K_1	$K_3^{1/2}$
FT5 RDS-15	kK_1K_{14}	-	-

Table S3: Summary of experimental conditions

Sl No	Temp °C	Pressure bar	H_2/CO	GHSV ml/g-h	% CO Conversion	P_{H2}	P_{CO}
1	200	20	1.5	4200	7.2	10.00	6.67
2	200	20	1.5	5400	5.4	10.70	7.14
3	200	20	1.5	3000	10.3	10.00	6.67
4	200	20	1.5	6600	4.3	10.90	7.27
5	220	25	2	5400	16	14.81	7.41
6	220	15	2	3000	24	8.00	4.00
7	220	25	1	3000	22	10.00	10.00
8	220	15	1	5400	10	6.67	6.67
9	220	15	2	5400	13.5	8.89	4.44
10	220	25	1	5400	10	11.11	11.11
11	220	15	1	3000	18	6.00	6.00
12	220	25	2	3000	28	13.33	6.67
13	240	20	1.5	4200	20	10.00	6.67
14	240	20	1.5	4200	21.2	10.00	6.67
15	240	20	1.5	4200	22	10.00	6.67
16	240	20	1.5	4200	21	10.00	6.67
17	240	20	2.5	4200	23	11.90	4.76
18	240	10	1.5	4200	14.5	5.00	3.33
19	240	20	0.5	4200	14	5.71	11.43
20	240	20	1.5	6600	13	10.91	7.27
21	240	20	1.5	4200	21	10.00	6.67
22	240	30	1.5	4200	25	15.00	10.00
23	240	20	1.5	1800	46	10.00	6.67
24	240	20	1.5	4200	21	10.00	6.67
25	240	20	1.5	5400	16	10.71	7.14
26	240	20	1	4200	18	8.57	8.57
27	240	20	2	4200	22	11.43	5.71
28	240	15	1.5	4200	19	7.50	5.00
29	240	20	1.5	3000	29	10.00	6.67
30	260	25	1	5400	23.1	11.11	11.11
31	260	15	2	5400	18.5	8.89	4.44
32	260	25	2	3000	46	13.33	6.67
33	260	15	1	3000	30.5	6.00	6.00
34	260	25	1	3000	41.5	10.00	10.00
35	260	15	1	5400	16	6.67	6.67
36	260	15	2	3000	31.82	8.00	4.00
37	260	25	2	5400	26.5	14.81	7.41

Table S4: Literature model tested for the present study at 240 °C

Model	Rate Expression	Properties†	R^2	%MARR	Reference
FT6	$-r_{FT} = \frac{kP_{H2}^{0.75}P_{CO}^{0.5}}{(1+bP_{CO}^{0.5})^2}$	Co,(iii)	0.12	19.5	Botes et al.[44]
FT7	$-r_{FT} = \frac{kP_{H_2}P_{CO}}{(1+aP_{CO})^2}$	Co, (iii)	0.12	20.3	Yates & Satterfield[39]
FT8	$-r_{CO} = \frac{kP_{H_2}P_{CO}}{(1+bP_{CO}P_{H_2}^{0.5})^2}$	Co, (iii)	0.17	12.6	Fazlollahi et al.[27]
FT9[a]	$-r_{FT} = \frac{kP_{CO}^{0.5}P_{H_2}^{0.5}}{\left(1+cP_{CO}^{0.5}+bP_{H_2}^{0.5}\right)^2}$	Co,(iv)	0.94	3.8	B.W. Wojciechowski[74*-9]
FT10	$r_{FT} = \frac{kP_{H_2}P_{CO}}{P_{CO}+bP_{H2O}}$	Fe , (i),(iv)	0.06	19.7	M. E. Dry[1]
FT11	$-r_{FT} = \frac{kP_{H2}^{0.5}P_{CO}}{(1+bP_{CO})^2}$	Fe,(iv)	0.39	11.7	Botes and Breman[7]
FT12	$-r_{FT} = \frac{kP_{H_2}^2P_{CO}}{(P_{H_2}P_{CO}+bP_{H_2O})}$	Fe, (i),(iii),(iv)	0.06	19.7	Huff & Satterfield[12]
FT13A	$-r_{FT} = \frac{kP_{H_2}P_{CO}}{(1+aP_{CO}+bP_{H_2O})}$	Fe, (i),(iv)	0.11	20.23	Van der Laan & Beenackers[19]
FT13B	$-r_{FT} = \frac{kP_{H2}^{0.5}P_{CO}}{\left(1+aP_{CO}+bP_{H_2O}\right)^2}$	Fe,(i),(iv)	0.39	11.2	Van der Laan & Beenackers[19]
FT13C	$-r_{FT} = \frac{kP_{H_2}P_{CO}}{\left(1+aP_{CO}+bP_{H_2O}\right)^2}$	Fe,(i),(iv)	0.12	20.2	Van der Laan & Beenackers[19]
FT14	$r_{FT} = k_{FT}\frac{P_{H2}P_{CO}}{P_{CO}+aP_{CO2}}$	Fe, (ii),(iv)	0.06	19.7	Ledakowicz et al.[16]
FT15	$-r_{FT} = \frac{kP_{CO}P_{H_2}^{0.75}}{(1+aP_{CO})^2}$	Fe-Co	0.21	15.2	Mousavi et al.[71]
FT 16	$-r_{FT} = \frac{k*a*b*P_{CO}P_{H2}}{(1+2(aP_{CO})^{0.5})^2}$	Fe-Co,(iii)	0.12	26	Eshraghi et al.[58]
FT17[b]	$-r_{FT} = \frac{k*a*b*P_{CO}P_{H2}}{(1+2(aP_{CO})^{0.5}+bP_{H_2})^3}$	Fe-Co,(iii)	0.87	3.5	Mirzei et al.[56]
FT18[c]	$-r_{FT} = \frac{k*a*b*P_{CO}P_{H2}}{\left(1+aP_{CO}+bP_{H_2}\right)^2}$	Fe-Co,(iv)	0.87	3.9	Mirzei et al.[57]

† (i) H_2O inhibition, (ii) CO_2 inhibition, (iii) unassisted CO dissociation, (iv) H_2 assisted CO dissociation

a-Fvalue-86.7, RMSE-3.13×10^{-4}; b-Fvalue-37.5, RMSE-5.2×10^{-4}; c-Fvalue-38.17, RMSE-5.38×10^{-4}

$F_{(0.05,3,14)} = 3.34$

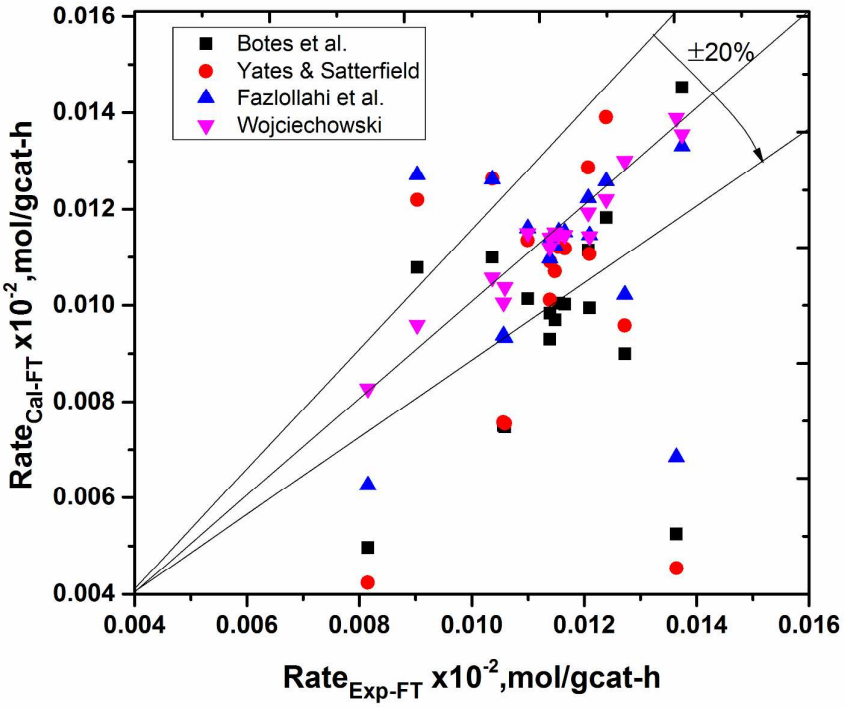


Figure S1: Parity plot for literature model on cobalt catalyst

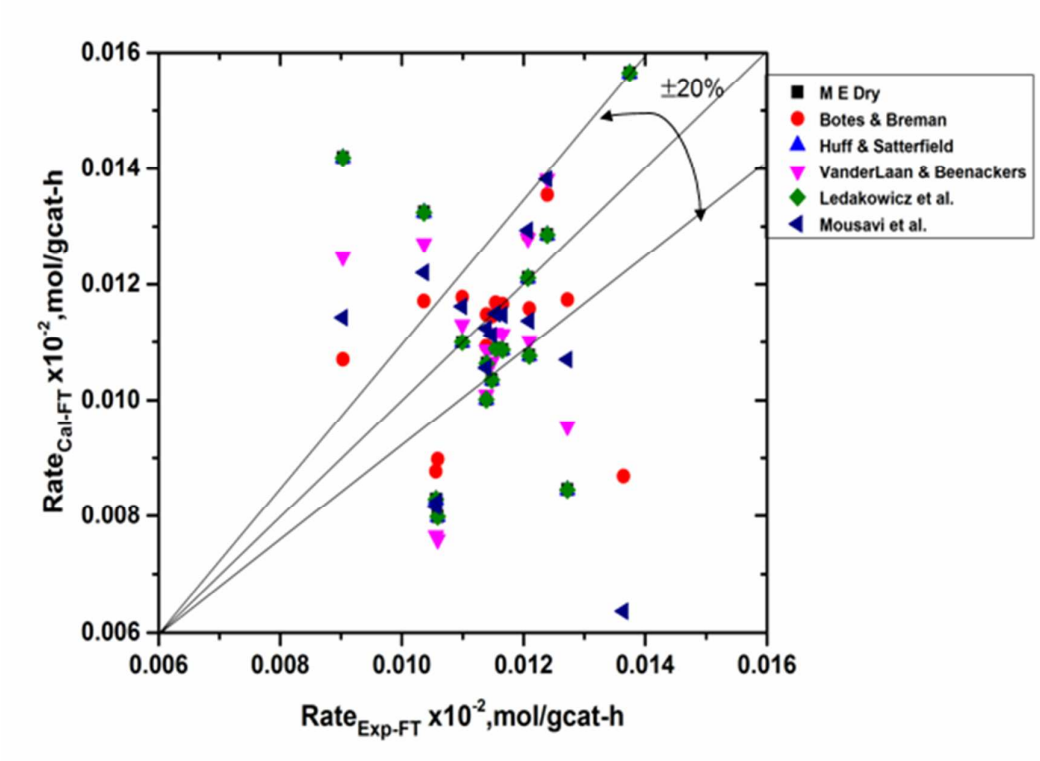


Figure S2: Parity plot for literature model on iron catalyst

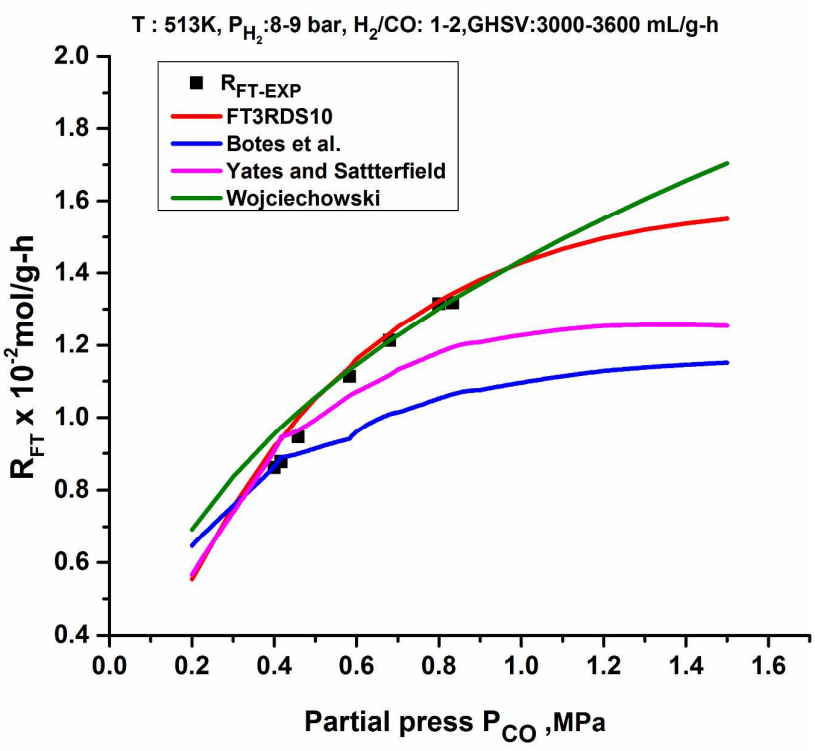


Figure S3: Effect of partial pressure of CO on rate

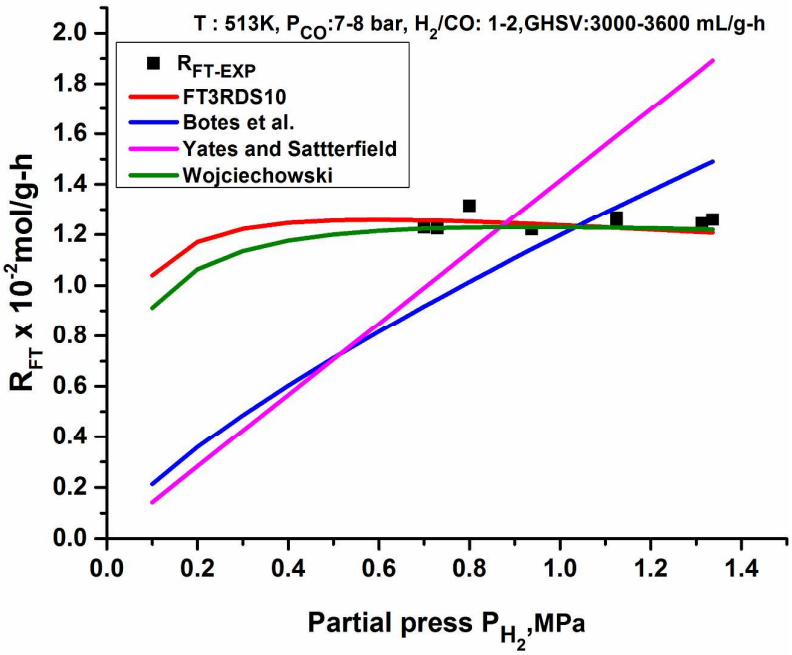


Figure S4: Effect of partial pressure of H_2 on rate

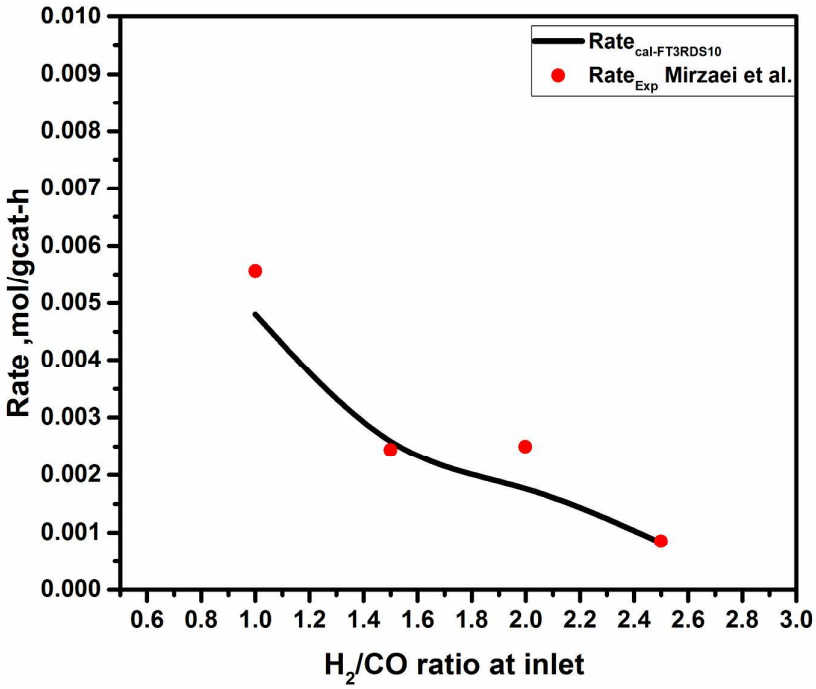


Figure S5: Effect of H_2/CO ratio on the rate at 260 °C (Exp data by Mirzaei et al.)

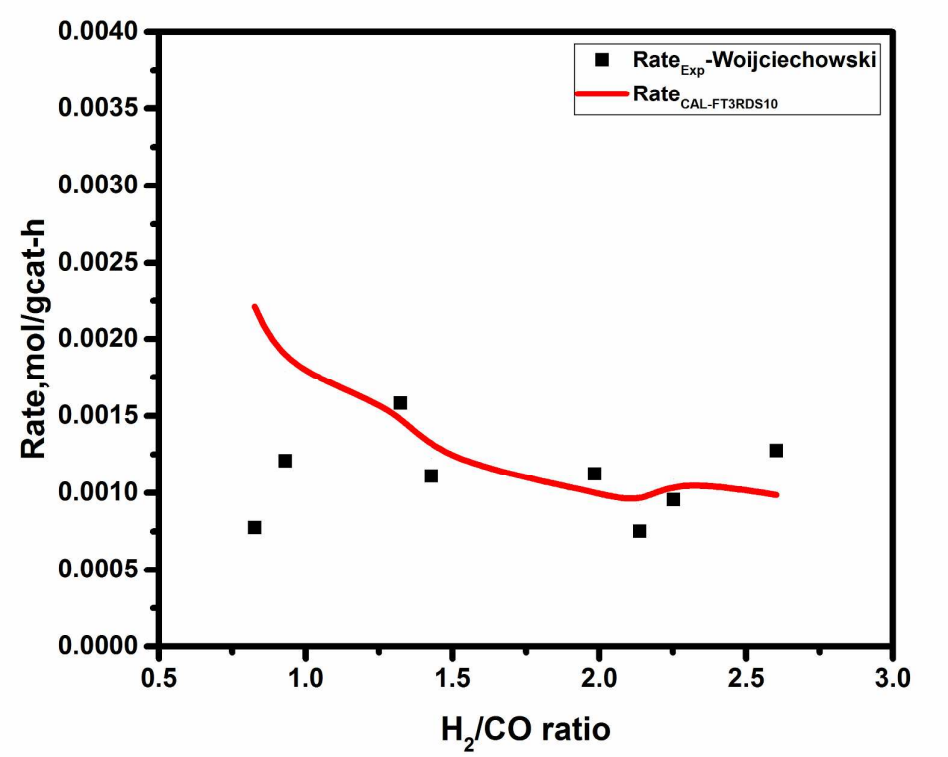


Figure S6: Effect of H_2/CO ratio on the rate (Exp data by Wojciechowski) at 190 °C