

Supplementary Information

Table S1. Graaf et al. original (Graaf et al., 1988) vs Fitted.

Kinetic parameter	Original	Units	Estimated with CO in the feed	Units
k_{CO}	$4.89 \times 10^7 \cdot \exp\left(\frac{-113000}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$8.15 \times 10^{-2} \cdot \exp\left(\frac{-20300}{R \cdot T}\right)$	mol/h/g/bar ²
k_{CO_2}	$1.09 \times 10^5 \cdot \exp\left(\frac{-87500}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$4.66 \times 10^8 \cdot \exp\left(\frac{-111600}{R \cdot T}\right)$	mol/h/g/bar ²
k_{RWGS}	$9.64 \times 10^{11} \cdot \exp\left(\frac{-152900}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-0.5}$	$1.29 \times 10^{16} \cdot \exp\left(\frac{-173019}{R \cdot T}\right)$	mol/h/g/bar ²
K_{CO}	$2.16 \times 10^{-5} \cdot \exp\left(\frac{46800}{R \cdot T}\right)$	bar ⁻¹	-	-
K_{CO_2}	$7.05 \times 10^{-7} \cdot \exp\left(\frac{61700}{R \cdot T}\right)$	bar ⁻¹	-	-
			$K_{H_2O} = 1.5510$	
	$\frac{K_{H_2O}}{K_{H_2}^{0.5}} = 6.37 \times 10^{-9} \cdot \exp\left(\frac{84000}{R \cdot T}\right)$	bar ^{-0.5}	$K_{H_2} = 7.65 \times 10^9 \cdot \exp\left(\frac{-109626.2}{R \cdot T}\right)$	bar ⁻¹

Table S2. Vanden Bussche and Froment original (van den Bussche & Froment, 1996) vs fitted.

Kinetic parameter	Original	Units	Estimated with CO in the feed	Units
k_{CO_2}	$1.07 \times 10^{-10} \cdot \exp\left(\frac{36696}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot Pa^{-2}$	$20.86 \cdot \exp\left(\frac{-23908.8}{R \cdot T}\right)$	mol/h/g/bar ²
k_{RWGS}	$1.22 \times 10^5 \cdot \exp\left(\frac{-94765}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot Pa^{-1}$	$6.8 \times 10^8 \cdot \exp\left(\frac{-94381.3}{R \cdot T}\right)$	mol/h/g/bar ²
	$\sqrt{K_{H_2}} = 1.578 \times 10^{-3} \cdot \exp\left(\frac{17197}{R \cdot T}\right)$	Pa ^{-0.5}	$K_{H_2} = 1.41 \cdot \exp\left(\frac{-2689.8}{R \cdot T}\right)$	bar ⁻¹
K_{H_2O}	$6.62 \times 10^{-16} \cdot \exp\left(\frac{124119}{R \cdot T}\right)$	Pa ⁻¹	$1.20 \cdot \exp\left(\frac{-5435.5}{R \cdot T}\right)$	bar ⁻¹
	$\frac{K_{H_2O}}{K_8 K_9 K_{H_2}} = 3.45338$	-	$K_8 K_9 = 30.03 \cdot \exp\left(\frac{-8959.6}{R \cdot T}\right)$	-

Table S3. Slotboom et al original 6 parameter model (Slotboom et al., 2020) vs fitted.

Kinetic parameter	Original	Units	Estimated with CO in the feed	Units
k_{CO_2}	$7.414 \times 10^{14} \cdot \exp\left(\frac{-166000}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$2.19 \times 10^2 \cdot \exp\left(\frac{-43921.4}{R \cdot T}\right)$	mol/h/g/bar ²
k_{RWGS}	$1.111 \times 10^{19} \cdot \exp\left(\frac{-203700}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$2.75 \times 10^{10} \cdot \exp\left(\frac{-110563}{R \cdot T}\right)$	mol/h/g/bar ²
K_{H_2}	1.099	bar ^{-0.5}	13.62	bar ^{-0.5}
$K_{H_2O/9}$	126.4	bar ⁻¹	41.55	bar ⁻¹

Table S4. Seidel et al original (Seidel et al., 2018; Seidel et al., 2020) vs fitted.

Kinetic parameter	Original	Units	Estimated with CO in the feed	Units
ΔG_1	-1134.8	J/mol	-	-
ΔG_2	-769.3	J/mol	-	-
ΔG_3	-365.5	J/mol	-	-
k_{CO}	$3.074 \times 10^{12} \cdot \exp\left(\frac{-154400}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$1.99 \times 10^{-2} \cdot \exp\left(\frac{-12024.4}{R \cdot T}\right)$	mol/h/g/bar ²
k_{CO_2}	$4.613 \times 10^7 \cdot \exp\left(\frac{-96820}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$9.14 \cdot \exp\left(\frac{-5406.3}{R \cdot T}\right)$	mol/h/g/bar ²
k_{RWGS}	$6.107 \times 10^{13} \cdot \exp\left(\frac{-161000}{R \cdot T}\right)$	$mol \cdot kg_{cat}^{-1} \cdot s^{-1} \cdot bar^{-1}$	$1.56 \times 10^6 \cdot \exp\left(\frac{-76382}{R \cdot T}\right)$	mol/h/g/bar ²
K_{CO}	0.1470	bar ⁻¹	$1.87 \times 10^{33} \cdot \exp\left(\frac{-309237.6}{R \cdot T}\right)$	bar ⁻¹
$K_{CH_3OH}^{\ominus}$	0	-	0	-
$K_{CO_2}^{\ominus}$	0	-	0	-
$\frac{K_{H_2O}K_O}{K_{H_2}} = 34.9226$		-	$K_O = 1.79 \times 10^{-1} \cdot \exp\left(\frac{-5000.9}{R \cdot T}\right)$	-
K_{CO_2}	0.04712	bar ⁻¹	0	-
$K_{CH_3OH}^*$	0	-	0	-
K_{H_2O}	0.0297	bar ⁻¹	$2.34 \cdot \exp\left(\frac{-10922.9}{R \cdot T}\right)$	bar ⁻¹
	$\sqrt{K_{H_2}} = 1.1665$	bar ^{-0.5}	$K_{H_2} = 1.96 \times 10^1 \cdot \exp\left(\frac{-4086.1}{R \cdot T}\right)$	bar ^{-0.5}

Table S5. MOD parameters.

Kinetic parameter	Estimated with CO in the feed	Units
ΔG_1	-	-
ΔG_2	-	-
ΔG_3	-	-
k_{CO_2}	$3.77 \times 10^2 \cdot \exp\left(\frac{-25000}{R \cdot T}\right)$	mol/h/g/bar ²
k_{RWGS}	$3.60 \times 10^8 \cdot \exp\left(\frac{-98200}{R \cdot T}\right)$	mol/h/g/bar ²
K_{CO}	$1.87 \times 10^7 \cdot \exp\left(\frac{-68434.8}{R \cdot T}\right)$	bar ⁻¹
$K_{CH_3OH}^{\ominus}$	0	-
$K_{CO_2}^{\ominus}$	0	-
K_O	178.17	-
K_{CO_2}	0	-
$K_{CH_3OH}^*$	0	-
K_{H_2O}	0.0581	bar ⁻¹
K_{H_2}	3.786	bar ^{-0.5}

Table S6. Plug flow calculation, this follows the criteria discussed in reference (Ertl et al., 1997; Delgado, 2006).

Geometrical Characteristics			
d_t (mm)	10.1	d_t/d_p	107.4
h_{bed} (mm)	3.82	h_{bed}/d_p	40.7
d_p (μ m)	94		

References

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