

Table S1: The main reactions and the reaction rate expression for methanol synthesis (the adsorption expression is the dominator of the rate expression) [1-2]

Step Definition	Reaction	Rate of Reaction	Kinetic Factor	Driving Force
CO Hydrogenation	$CO + 2H_2 \leftrightarrow CH_3OH$	r_1 $= \frac{k_1 K_{CO} \left[f_{CO} f_{H_2}^{1.5} - \frac{f_{CH_3OH}}{f_{H_2}^{0.5} K_{P1}} \right]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) \left[f_{H_2}^{0.5} + \left(\frac{K_{H_2O}}{K_{H_2}^{0.5}} \right) f_{H_2O} \right]}$	$k_1 K_{CO}$	$\left[f_{CO} f_{H_2}^{1.5} - \frac{f_{CH_3OH}}{f_{H_2}^{0.5} K_{P1}} \right]$
CO ₂ Hydrogenation	$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$	r_2 $= \frac{k_2 K_{CO_2} \left[f_{CO_2} f_{H_2}^{1.5} - \frac{f_{CH_3OH} f_{H_2O}}{f_{H_2}^{1.5} K_{P2}} \right]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) \left[f_{H_2}^{0.5} + \left(\frac{K_{H_2O}}{K_{H_2}^{0.5}} \right) f_{H_2O} \right]}$	$k_2 K_{CO_2}$	$\left[f_{CO_2} f_{H_2}^{1.5} - \frac{f_{CH_3OH} f_{H_2O}}{f_{H_2}^{1.5} K_{P2}} \right]$
Reverse Water Gas-Shift	$CO_2 + H_2 \leftrightarrow CO + H_2O$	r_3 $= \frac{k_3 K_{CO_2} \left[f_{CO_2} f_{H_2} - \frac{f_{H_2O} f_{CO}}{K_{P3}} \right]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) \left[f_{H_2}^{0.5} + \left(\frac{K_{H_2O}}{K_{H_2}^{0.5}} \right) f_{H_2O} \right]}$	$k_3 K_{CO_2}$	$\left[f_{CO_2} f_{H_2} - \frac{f_{H_2O} f_{CO}}{K_{P3}} \right]$

Table S2: Reaction constants for Methanol Synthesis (Graaf et al, 1-2)

Reaction rate constants		
$k = A e^{\frac{B}{RT}}$	A	B
k_1	4.89×10^7	-113,000
k_2	1.09×10^5	-87,500
k_3	9.64×10^{11}	-152,900
Adsorption equilibrium constants		
$K = A e^{\frac{B}{RT}}$	A	B
K_{CO}	2.16×10^{-5}	46,800
K_{CO_2}	7.05×10^{-7}	61,700

$\frac{K_{H_2O}}{K_{H_2}^{0.5}}$	6.37×10^{-9}	84,000
Reaction equilibrium constants		
$K_P = 10^{\frac{A}{T}-B}$	A	B
K_{P1}	5,139	12.621
K_{P2}	3,066	10.592
K_{P3}	-2,073	-2.029

Table S3: Kinetic factors and driving forces parameters input to the Aspen Plus interphase for Methanol Synthesis

Kinetic Factor reaction 1		Driving Force reaction 1		
k (A)	1056.24	Constant	Term1	Term2
E (-B)	66200	A	0	29.06
n	0	B	0	-11833
Kinetic Factor reaction 2		Driving Force reaction 2		
k (A)	0.076	Constant	Term1	Term2
E (-B)	25800	A	0	24.39
n	0	B	0	-7059.73
Kinetic Factor reaction 3		Driving Force reaction 3		
k (A)	679620	Constant	Term1	Term2
E (-B)	91200	A	0	-4.67
n	0	B	0	4773.259

Table S4: Adsorption constant input to the Aspen Plus interphase

Adsorption reaction						
Coefficient /Term no.	1	2	3	4	5	6
Coefficient A	0	-10.74	-14.17	-18.87	-29.61	-33.04
Coefficient B	0	5629.06	7421.22	10103.44	15732.50	17524.66
Coefficient C	0	0	0	0	0	0
Coefficient D	0	0	0	0	0	0

References

- [1] Graaf GH, Scholtens + H, Stamhuis EJ, Beenackers AACM. INTRA-PARTICLE DIFFUSION LIMITATIONS IN LOW-PRESSURE METHANOL SYNTHESIS. vol. 45. 1990.
- [2] Graaf GH, Sijtsema PJM, Stamhuis EJ, Joosten GEH. CHEMICAL EQUILIBRIA IN METHANOL SYNTHESIS. vol. 41. 1986.