

Kinetics and computational fluid dynamics study for Fischer Tropsch synthesis in microchannel and fixed bed reactor

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Supporting Table 1: Hydrocarbon productivity and CO conversion during FTS in microchannel and fixed bed reactor.

Reactor	GHSV (mlg _{cat} ⁻¹ hr ⁻¹)	Hydrocarbon productivity (g.g _{cat} ⁻¹ .h ⁻¹)		CO conversion (%)
		CH ₄	C2+	
Microchannel	1500	0.022	0.136	92
Fixed-bed	1500	0.056	0.069	66.1
Microchannel	2080	0.027	0.163	60.9
Fixed-bed	2080	0.080	0.055	31.2

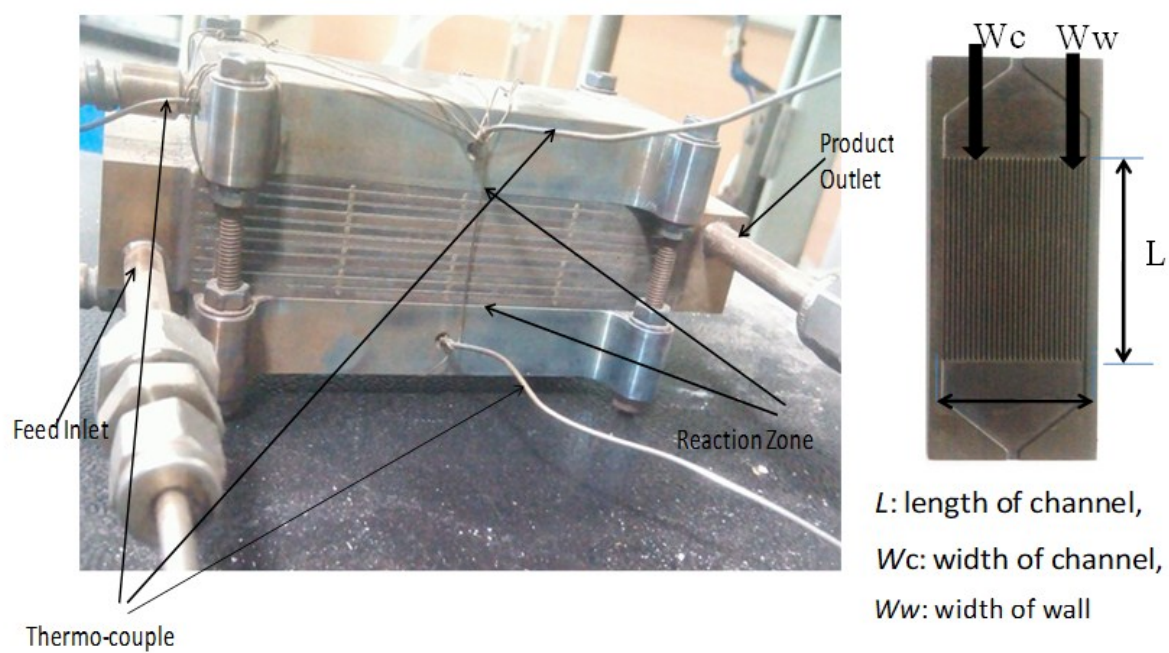
Temperature: 300 °C, H₂/CO: 1.5 ml/ml, pressure: 20 bar

Supporting Table 2: Thermodynamic and transport properties of species used for simulation in COMSOL.

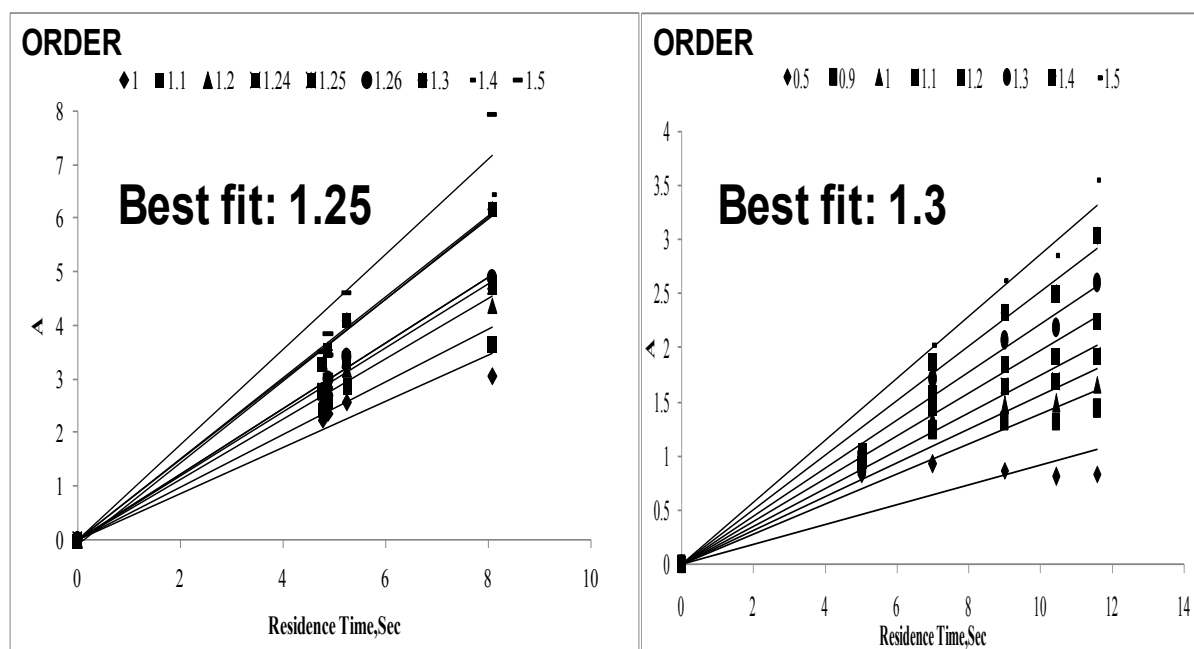
Species	Enthalpy H (J.mol ⁻¹)	Entropy S (J.mol ⁻¹ .K ⁻¹)	Sp. Heat (Cp) (J.mol ⁻¹ .K ⁻¹)	Thermal Cond. k (W.m ⁻¹ .K ⁻¹)	Diffusivity Di (m ² s ⁻¹)	Density ρ (kg.m ⁻³)
CO	12392	104.00	29.19	0.023	1.6*10 ⁻⁶	1.14
H₂	7926	107.71	28.84	0.168	6.9*10 ⁻⁶	0.08
CO₂	22263	120.56	37.44	0.015	1.2*10 ⁻⁶	1.80
CH₄	14598	107.19	35.80	0.034	1.4*10 ⁻⁶	0.67
C₂H₆	20057	102.19	52.85	0.021	9.2*10 ⁻⁷	1.23
C₃H₈	27999	125.56	74.45	0.018	2.7*10 ⁻⁶	1.83
C₃H₄	29723	126.90	62.12	0.017	7.3*10 ⁻⁷	1.70
C₄H₁₀	34477	148.97	100.62	0.017	2.3*10 ⁻⁶	2.45
C₄H₈	34762	146.04	98.34	0.016	5.8*10 ⁻⁷	2.40
C₅H₁₂	24557	82.49	122.96	0.014	2.3*10 ⁻⁶	2.94
C₅H₁₀	24557	82.49	120.71	0.013	4.5*10 ⁻⁷	2.86
C₈H₂₀O₄	-27953	83.00	563.00	0.144	1.5*10 ⁻⁷	698.39
H₂O	1878	6.61	75.33	0.609	7.6*10 ⁻⁷	997.09

Supporting Table 3: Inlet boundary conditions of reactants used for simulation in microchannel reactor and fixed bed reactor.

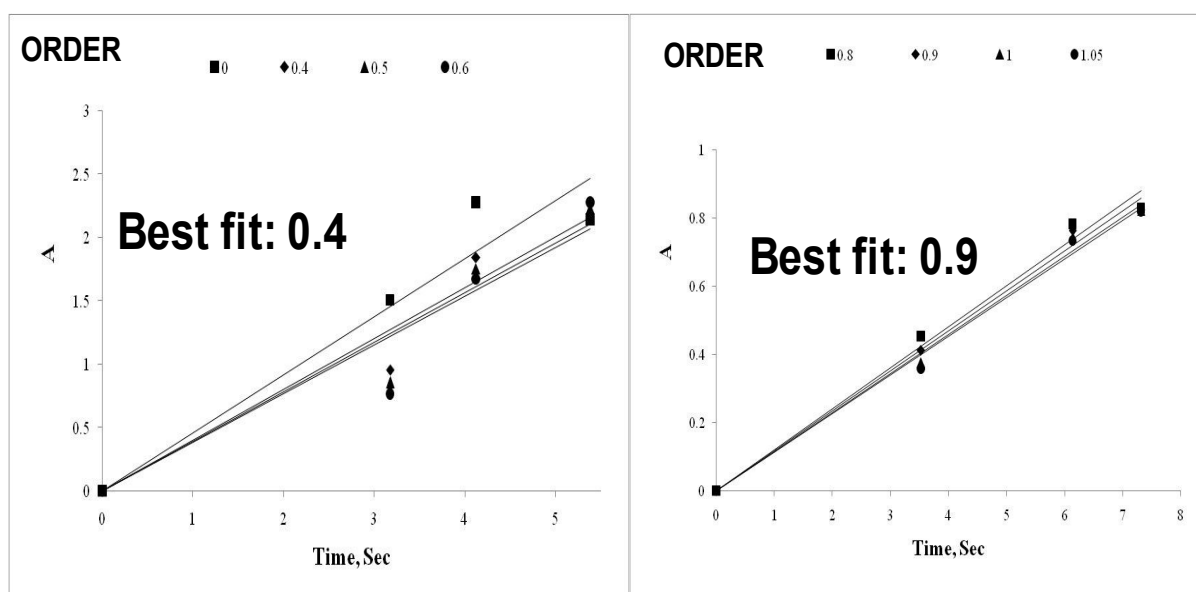
Boundary Conditions	(microchannel reactor)	(fixed bed reactor)
Inlet Flow Rate (m ³ /s)	5.75*10 ⁻⁸	1.67*10 ⁻⁷
Inlet velocity (m/s)	0.0164	0.04
Inlet CO Molar Flow Rate (mol/s)	9.4*10 ⁻⁷	2.72*10 ⁻⁶
Inlet H ₂ Molar Flow Rate (mol/s)	1.41*10 ⁻⁶	4.08*10 ⁻⁶
Inlet Temperature (K)	598	598
Inlet Pressure (bar)	20	20



Supporting Figure 1: Microchannel reactor experimental set-up and microchannel plate.



Supporting Figure 2: Rate constant and order calculation for H₂ and CO in microchannel reactor at 300 °C, H₂/CO 1.5 and 20 bars (for H₂ & CO)



Supporting Figure 3: Rate constant and order calculation for H_2 and CO in microchannel reactor at 300 °C, H_2/CO 1.5 and 20 bars (for H_2 & CO)