Table SI-1 Thermodynamics parameters of the gas species [1]

Species .	$\Delta_f H_m^{\theta} \times 10^{-5}$	a_{cp}	b_{cp}	$c_{cp} \times 10^3$	$d_{cp} \times 10^7$	$\lambda_{To} \times 10^2$	$k_{\lambda} \times 10^4$
	J/kg	J/kg/K	J/kg/K	J/kg/K	J/kg/K	K/m	1/m
C ₂ H ₄	18.68	135.93	5.59	-2.98	6.27	-1.90	1.41
C_3H_6	4.86	88.33	5.58	-2.76	5.25	-2.02	1.31
C_4H_8	0.02	-53.46	6.31	-3.55	7.97	-2.22	1.27
C_5H_{10}	-3.48	-1.91	6.18	-3.31	6.69	-2.02	1.00
CH ₄	-46.81	1203.13	3.26	0.75	-7.08	-2.46	1.92
C_3H_8	-23.61	-96.00	6.96	-3.60	7.31	-2.31	1.44
CH ₃ OH	-62.91	660.94	2.22	0.81	-8.91	-2.38	1.08
H ₂ O	-134.44	1791.11	0.11	0.59	-2.00	0.80	1.26

Table SI-2 Dual-cycle reaction kinetics for the DMTO [1]

Classification	Reaction equation	Reaction rate
Olefins-based cycle		
(Happened on active site <i>S</i>)		
	$MeOH \xrightarrow{s} CH_4 + H_2O$	$r_1 = k_1 \rho_{MeOH} Y_S \Phi$
	$MeOH \xrightarrow{s} C_2H_4 + H_2O$	$r_2=k_2 \rho_{MeOH} Y_S \Phi$
	$MeOH \xrightarrow{s} C_3H_6+H_2O$	$r_3=k_3 ho_{MeOH}Ysoldsymbol{\Phi}$
	$MeOH \xrightarrow{s} C_3H_8+H_2O$	$r_4=k_4 ho_{MeOH}Ysoldsymbol{\Phi}$
	$MeOH \xrightarrow{s} C_4H_8+H_2O$	$r_5=k_5 ho_{MeOH}Ysoldsymbol{\Phi}$
	$MeOH \xrightarrow{s} C_{5+} + H_2O$	r_6 = $k_6 ho_{MeOH} Ys oldsymbol{\Phi}$
	$MeOH+C_2H_4 \xrightarrow{s} C_3H_6+H_2O$	r_7 = $k_7 ho_{MeOH} ho_{C2H4} Ys oldsymbol{\Phi}$

Transformation

Classification	Reaction equation	Reaction rate
	$MeOH+S \rightarrow R+H_2O$	$r_8 = k_8 ho_{ m MeOH}^{0.3} Y_S$
	$C_2H_4+S \rightarrow R$	$r_9 = k_9 \rho_{{}_{{}^{\!$
	$C_3H_6+S \rightarrow R$	$r_{10}=k_{10}\rho_{_{{\rm C3H6}}}^{_{0.3}}Y_{S}$
	$C_4H_8+S \rightarrow R$	$r_{11} = k_{11} \rho_{\text{C4H8}}^{0.3} Y_S$
	$C_{5+}+S\rightarrow R$	$r_{12} = k_{12} \rho_{\text{CS+}}^{0.3} Y_S$
Aromatics-based cycle		
(Happened on protonated		
aromatics R)		
	$MeOH \xrightarrow{R} CH_4 + H_2O$	$r_{13}=k_{13} ho_{MeOH}Y_R oldsymbol{\Phi}$
	$MeOH \xrightarrow{R} C_2H_4 + H_2O$	$r_{14}\!\!=\!\!k_{14} ho_{MeOH}Y_{R}oldsymbol{\Phi}$
	$MeOH \xrightarrow{R} C_3H_6 + H_2O$	$r_{15}\!\!=\!\!k_{15} ho_{MeOH}Y_Roldsymbol{\Phi}$
	$MeOH \xrightarrow{R} C_3H_8+H_2O$	$r_{16}\!\!=\!\!k_{16} ho_{MeOH}Y_{R}oldsymbol{\Phi}$
	$MeOH \xrightarrow{R} C_4H_8+H_2O$	$r_{17}\!\!=\!\!k_{17} ho_{MeOH}Y_Roldsymbol{\Phi}$

 k_i (i=1, 2, ..., 17) is the reaction rate constant of reaction i, which is obtained from the Arrhenius equation:

$$k_i = k_{0i} \exp\left[-\frac{E_{ai}}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right],$$
 (1)

where T_0 is the reference and is 723 K in this study, and k_{0i} and E_{ai} are the reaction rate coefficient and activation energy of reaction i at T_0 . R is the molar gas constant, and T is the temperature of the reaction. The detailed values of the k_{0i} and E_{ai} of the reaction network are listed in Table SI-3.

Table SI-3 Kinetic parameters of dual-cycle reaction model[2]

k_i	k_{i0}	E_{ai}	k_i	k_{i0}	E_{ai}
k_{I}	0.013	-0.04	k_{10}	0.00020	35.05
k_2	0.17	0.78	k_{II}	0.00073	35.03
k_3	0.24	1.23.	k_{12}	0.00073	35.06
k_4	0.032	-0.78	k_{13}	0.011	-10.13
k_5	0.12	0.82	k_{14}	0.77	28.23
k_6	0.10	-1.11	k_{15}	0.61	-17.82
k_7	0.41	1.97	k_{16}	0.019	1.20
k_8	0.00028	-1.47	k_{17}	0.11	-18.39
<i>k</i> ₉	0.00012	35.02			

Table SI-4 Reaction network of dual-cycle reaction model for each specie [2]

Species	Reaction
МеОН	$R_{MeOH} = -\left(\sum_{i=1}^{6} r_i + \frac{8}{15}r_7 + r_8 + \sum_{i=13}^{17} r_i\right) m_{cat}$
Coke	$R_{coke} = \frac{14}{32}r_8 + r_9 + r_{10} + r_{11} + r_{12}$
CH ₄	$R_{CH_4} = \frac{14}{32} (r_1 + r_{13}) m_{cat}$
C_2H_4	$R_{C_2H_4} = \left[\frac{14}{32}(r_2 + r_{14}) - \left(\frac{7}{15}r_7 + r_9\right)\right] m_{cat}$
C ₃ H ₆	$R_{C_3H_6} = \left[\frac{14}{32}(r_3 + r_{15}) + \frac{7}{10}r_7 - r_{10}\right]m_{cat}$
C ₃ H ₈	$R_{C_3H_8} = \frac{14}{32} (r_4 + r_{16}) m_{cat}$

Species	Reaction
C ₄	$R_{C_4} = \left[\frac{14}{32}(r_5 + r_{17}) - r_{11}\right] m_{cat}$
C ₅₊	$R_{C_5^+} = (\frac{14}{32}r_6 - r_{12})m_{cat}$
H ₂ O	$R_{H_2O} = \frac{18}{32} \left(\sum_{i=1}^{6} r_i + \frac{8}{15} r_7 + r_8 + \sum_{i=13}^{17} r_i \right) m_{cat}$

- [1] B.E. Poling, J.M. Prausnitz, J.P. O'Connell, The properties of gases and liquids, Mcgraw-hill New York 2001.
- [2] X. Yuan, H. Li, M. Ye, Z. Liu, Kinetic modeling of methanol to olefins process over SAPO-34 catalyst based on the dual-cycle reaction mechanism, AlChE J. 65(2) (2019) 662-674.