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CaRMeN: A tool for analysing and deriving kinetics in the real world

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Supplemental material

Table S1: Selection of experimental literature data [Ref.] for CH_4 conversion over Rh and surface reaction mechanisms [Mechanism] used for modeling these experiments.

	CH_4/Ox	P (bar)	Temp (K)	GHSV/τ/Flow/U	Catalyst	Reactor type	Mechanism	Remarks	Ref.
CPO	CH_4/O_2=0.8-2.2	1.42	600 -1500	U_o(298K)=20.6 cm/s	Rh/ Al_2O_3	monolith	Hickman – Schmidt 1993[1]		Hickman and Schmidt[1]
	CH_4/O_2 = 1.8	1.10	T_o=300	flow=7 slpm	Rh/ Al_2O_3	monolith	Maier – Deutschmann 2001[2]		Deutschmann et al. [2]
	CH_4/O_2=1-1.78	1.10	573-1123	GHSV= 8×10^5- 4.5×10^6 Nl kg^{-1} h^{-1}	Rh or Rh/γ-Al_2O_3 coated α-Al_2O_3 foam	annular reactor	Maestri-Vlachos 2009[3]	H_2O, CO_2, CO co-feed=1–2 %	Maestri et al.[3]
	CH_4/O_2=1-4	1.40-8.00	1060-1400	τ=1-75 × 10^{-3} s	Rh/α-Al_2O_3	fixed bed	Hickman – Schmidt 1993[1]	industrially relevant conditions	Slaa et al.[4]
	CH_4/O_2=1.4, 2.0, 2.6	1.00	300-1500	flow=5 slpm	Rh-coated foam monoliths	monolith	Maier - Deutschmann 2001[2], Maestri-Vlachos 2009 [3]	spatially-resolved data	Williams et al.[5]

	CH_4/Ox	P (bar)	Temp (K)	GHSV/τ/Flow/U	Catalyst	Reactor type	Mechanism	Remarks	Ref.
	CH_4/O_2=1.4, 2.0, 2.8	1.00	300-1500	flow=5 slpm or 10 slpm	Rh-coated foam monoliths	monolith	Maier – Deutschmann 2001[2]	spatially-resolved data	Horn et al.[6]
	CH_4/O_2=2.0	1.32-1.52	T_o=300	GHSV=200-500 $Nm^3\ kg^{-1}\ h^{-1}$	Rh/ Al_2O_3 spheres	fixed bed	Maier – Deutschmann 2001[2]	integral conversion and selectivity	Bizzi et al.[7]
	CH_4/O_2=3.0	1.32-1.52	T_o=300	GHSV=200-500 $Nm^3\ kg^{-1}\ h^{-1}$	Rh/ Al_2O_3 spheres	fixed bed	Maier – Deutschmann 2001[2]		Bizzi et al.[8]
	CH_4/O_2=1.7	1.10	385-1000	$\tau=20\times10^{-3}$ s	Rh/α-Al_2O_3	honeycomb monolith	Maier – Deutschmann 2001[2, 9]	transient light-off experiments	Schwiedernoch et al.[9]
	CH_4/O_2 = 2, 1.7	1.10	T_o=298	GHSV=$1.0 \times 10^5\ h^{-1}$	Rh/α-Al_2O_3	foam monolith	Maier – Deutschmann 2001[2]	Effect of He, H_2O, and CO_2 addition	Ding et al.[10]
	CH_4/O_2 = 2.0	1.10	T_o=ambient	GHSV=$4.0 \times 10^5\ h^{-1}$	Rh/γ-Al_2O_3	monolith	Maier – Deutschmann 2001[9]	Transient species profiles	Williams et al.[11]
	CH_4/O_2 = 0.9–1.75	5.00	T_o=429-457	U_{in}=0.28-0.57 m/s	Rh/Al_2O_3 ceramic plates	coated channel flow reactor	Maier – Deutschmann 2001[9], Kraus - Lindstedt 2017[12]	optically accessible channel flow reactor-Raman-LIF	Sui et al.[13]
	CH_4/O_2 = 0.15-0.2	2.00-12.00	T_o =377-476	U_{in}=0.21-1.25 m/s	Rh/Al_2O_3 coated ceramic plates	coated channel flow reactor	Karakaya - Deutschmann 2016[14], Deshmuhk - Vlachos 2007[15], Kraus - Lindstedt 2017[12]	in situ Raman	Sui et al.[16]
	CH_4/O_2 = 2.5-4	4.00-6.00	T_o =385-673	U_{in}=0.19-13.20 m/s	Rh/ZrO_2 coated ceramic plates	coated channel flow reactor	Maier – Deutschmann 2001[9], Kraus - Lindstedt 2017[12]	in situ Raman	Appel et al.[17]

	CH_4/Ox	P (bar)	Temp (K)	GHSV/τ/Flow/U	Catalyst	Reactor type	Mechanism	Remarks	Ref.
	CH_4/O_2 = 2.0	5.00	T_o =473, 573, 623 K	U_{in}=3.90-5.10 m/s	Rh/Al_2O_3, Rh/ZrO_2, Rh/CeO_2-ZrO_2	coated channel flow reactor	Maier – Deutschmann 2001[9]	*in situ* Raman, H_2O and CO_2 co-feed	Ericksson et al.[18]
	CH_4/O_2=0.56-2.06	0.50	873-1023	flow=15.5 slpm	Rh/ Al_2O_3	stagnation flow	Karakaya – Deutschmann 2016[14]		Karakaya et al.[14]
	CH_4/O_2=2	1.10	T_o =423, T_{cat}<673	flow=5 slpm	Rh or Rh/γ-Al_2O_3 coated α-Al_2O_3 foam	annular reactor	Maestri - Vlachos 2009[3]	spatially resolved autothermal experiments - effect of washcoat addition	Donazzi et al.[19]
	CH_4/O_2=1.78	1.10	T_o =533-623	flow=10 Nl/m	Rh/ α-Al_2O_3 monolith	adiabatic lab scale reactor	Maestri - Vlachos 2009[3]	spatially resolved CPO experiments - CO_2 addition	Donazzi et al.[20]
	CH_4/O_2=1-1.78	1.10	623-1123	GHSV= 8×10^5- 4.5×10^6 Nl/ kg^{-1} h^{-1}	Rh/ α-Al_2O_3	annular reactor	Maestri - Vlachos 2009[3]	H_2O, CO_2, CO, H_2 co-feed=1–2%	Donazzi et al.[21]
	CH_4/O_2=1.75	1.00-4.00	T_o =623	flow=10 Nl/m	Rh/Al_2O_3	honeycomb monolith	Maestri - Vlachos 2009[3]	spatially resolved temperature and concentration profiles	Donazzi et al.[22]
SR	S/C = 1-3	1.10	673–823	GHSV=30000-70000 h^{-1}	Rh/CeO_2-ZrO_2-La_2O_3	fixed bed	Kechagiopoulos – Lemonidou 2017[23]	low temperature SR	Kechagiopoulos et al.[23]
	S/C =1.5, 2, 2.5	1.10	623-1123	GHSV= 2×10^6 Nl kg^{-1} h^{-1}	Rh/α-Al_2O_3	annular reactor	Maestri - Vlachos 2009[3]		Donazzi et al.[21]

	CH_4/Ox	P (bar)	Temp (K)	GHSV/τ/Flow/U	Catalyst	Reactor type	Mechanism	Remarks	Ref.
	S/C =1.04-1.06	0.50	973, 1008	flow=17.2 slpm	Rh/ Al_2O_3	stagnation flow	Karakaya – Deutschmann 2016 [14]		Karakaya et al.[14]
	S/C =2.2-4	1.10	673-1123	GHSV= 40000 h^{-1}	Rh/ Al_2O_3	honeycomb monolith	Schädel - Deutschmann 2009 [24]	Exp. also with C_2H_6, C_3H_8, C_4H_{10}	Schädel et al. [24]
	S/C=4	1.10	973	GHSV= 48000 h^{-1}	Rh/CeO_2	Microchannel reactor	Thormann - Deutschmann 2009 [25]	Exp. also with propane and hexadecane	Thormann et al. [25]
ATR	16.7% CH_4, 0–40.0% H_2O, 1.7–16.7% O_2	1.00	573-1073	GHSV=7200 h^{-1}	Rh/ Al_2O_3	fixed bed	Maier - Deutschmann 2001[2]	Exp. data taken from Ayabe et al.[26]	Dixit et al.[27]
DR	CO_2=1–4%, CH_4=1–2%, O_2 co-feed=0.1%, H_2 co-feed=0.1–1%	1.10	623-1123	GHSV= 2 × 10^6 Nl kg_{cat}^{-1} h^{-1}	Rh/a-Al_2O_3	annular reactor	Maestri-Vlachos 2009[3]		Donazzi et al.[28]
	CH_4/CO_2=1.1	0.50	973	Flow=15.5 slpm	Rh/ Al_2O_3	stagnation flow	Karakaya – Deutschmann 2016 [14]		Karakaya et al.[14]
WGS	$CO/H_2O/N_2$ = 4/2.7/93.3, 1.5/2.3/96.2, 1.5/3.5/95.	1.10	623-546	GHSV= 2 × 10^6 Nl kg_{cat}^{-1} h^{-1}	Rh/ Al_2O_3	annular reactor	Maestri - Vlachos 2009[3]		Donazzi et al.[21]
RWGS	CO=1–2%, H_2O=1–4%	1.10	623-546	GHSV= 2 × 10^6 Nl kg_{cat}^{-1} h^{-1}	Rh/ Al_2O_3	annular reactor	Maestri-Vlachos 2009[3]	Also CO & H_2-rich combustion tests	Donazzi et al.[28]

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