

Supplementary Materials: The Influence of Slight Protuberances in a Micro-Tube Reactor on Methane/Moist Air Catalytic Combustion

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Table S1. Mechanism of methane reactions on Pt surface ^a [1].

Rate constants are given in the form $k_{f,i} = A_i T^{\beta_i} \exp(-\frac{Ea}{RT_s}) \prod_{i=1}^n \Theta_s^{\mu_i} \exp(\frac{\epsilon_i \Theta_s}{RT_s})$					
Chemical Species					
Total number of species: 11 $\rightarrow$ C(s), CH(s), CH ₂ (s), CH ₃ (s), CO(s), CO ₂ (s), H(s), H ₂ O(s), O(s), OH(s), Pt(s)					
Label	Reactions	A_i (mol, cm, s)	β_i	Ea (kJ/mol)	ϵ_i, μ_i^b
(1)	H ₂ + 2Pt(s) $\rightarrow$ 2H(s)	4.60×10^{-2}			$\mu_{Pt(s)} = -1^c$
(2)	2H(s) $\rightarrow$ H ₂ + 2Pt(s)	3.70×10^{21}	0.0	67.4	$\mu_{H(s)} = 6$
(3)	H + Pt(s) $\rightarrow$ H(s)	1.00			c
(4)	O ₂ + 2Pt(s) $\rightarrow$ 2O(s)	1.80×10^{21}	-0.5	0.0	
(5)	O ₂ + 2Pt(s) $\rightarrow$ 2O(s)	0.023			c
(6)	2O(s) $\rightarrow$ O ₂ + 2Pt(s)	3.70×10^{21}	0.0	213.2	$\mu_{O(s)} = 60$
(7)	O + Pt(s) $\rightarrow$ O(s)	1.00			c
(8)	H ₂ O + Pt(s) $\rightarrow$ H ₂ O(s)	0.75			c
(9)	H ₂ O(s) $\rightarrow$ H ₂ O + Pt(s)	1.0×10^{13}	0.0	40.3	
(10)	OH + Pt(s) $\rightarrow$ OH(s)	1.00			c
(11)	OH(s) $\rightarrow$ OH + Pt(s)	1.0×10^{13}	0.0	192.8	
(12)	H(s) + O(s) $\rightarrow$ OH(s) + Pt(s)	3.70×10^{21}	0.0	11.5	
(13)	H(s) + OH(s) $\rightarrow$ H ₂ O(s) + Pt(s)	3.70×10^{21}	0.0	17.4	
(14)	OH(s) + OH(s) $\rightarrow$ H ₂ O(s) + O(s)	3.70×10^{21}	0.0	48.2	
(15)	CO + Pt(s) $\rightarrow$ CO(s)	8.40×10^{-1}			$\mu_{Pt(s)} = +1^c$
(16)	CO(s) $\rightarrow$ CO + Pt(s)	1.00×10^{13}	0.0	125.5	
(17)	CO ₂ (s) $\rightarrow$ CO ₂ + Pt(s)	1.00×10^{13}	0.0	20.5	
(18)	CO(s) + O(s) $\rightarrow$ CO ₂ (s) + Pt(s)	3.70×10^{21}	0.0	105.0	
(19)	CH ₄ + 2Pt(s) $\rightarrow$ CH ₃ (s) + H(s)	1.00×10^{-2}			$\mu_{Pt(s)} = +0.3^c$
(20)	CH ₃ (s) + Pt(s) $\rightarrow$ CH ₂ (s) + H(s)	3.70×10^{21}	0.0	20.0	
(21)	CH ₂ (s) + Pt(s) $\rightarrow$ CH(s) + H(s)	3.70×10^{21}	0.0	20.0	
(22)	CH(s) + Pt(s) $\rightarrow$ C(s) + H(s)	3.70×10^{21}	0.0	20.0	
(23)	C(s) + O(s) $\rightarrow$ CO(s) + Pt(s)	3.70×10^{21}	0.0	62.8	
(24)	CO(s) + Pt(s) $\rightarrow$ C(s) + O(s)	1.00×10^{18}	0.0	184.0	

^a The units of A are are (s⁻¹) for the first order reactions and (mol/(cm³·s)) or (mol·cm⁻³·s⁻¹) for the second order reactions; Ea and ϵ_i are in (kJ/mol). Reactions (4) and (5) represent alternative competing pathways; ^b According to Equation (2)—the rate coefficient of the forward reaction i [1]; ^c sticking coefficient.

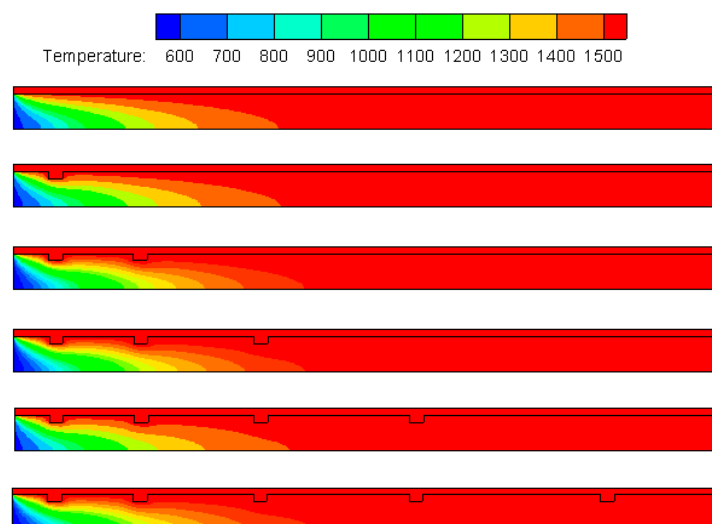


Figure S1. The contours of temperature (K) in the micro-tubes with 0–5 rectangular protuberances ($0.2 \text{ mm} \times 0.1 \text{ mm}$).

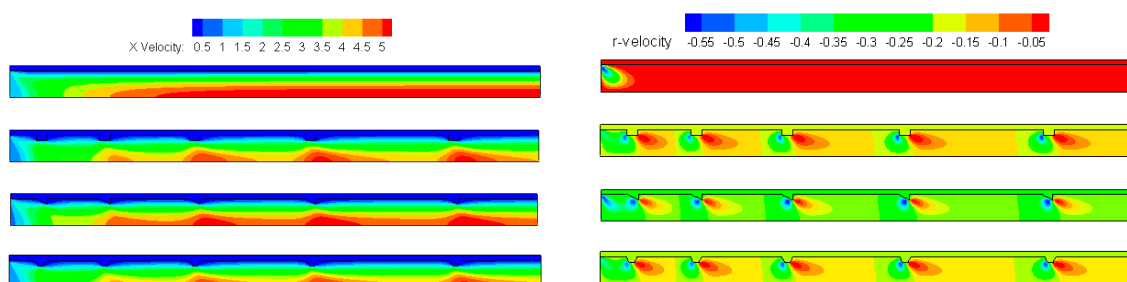


Figure S2. The x-velocity and r-velocity (m/s) contours in the micro-tubes with different protuberance shapes.

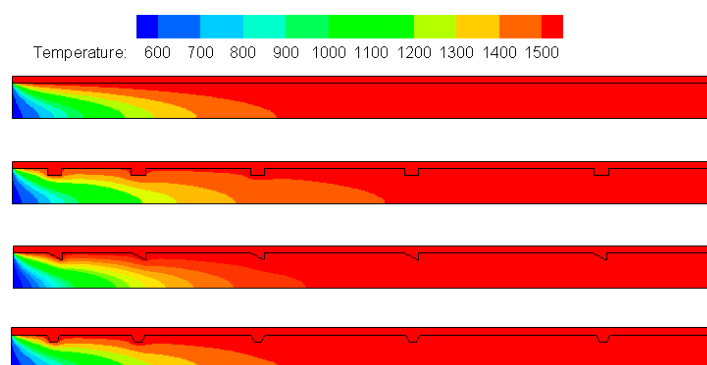


Figure S3. The contours of temperature (K) in the micro tubes with different protuberance shapes.

Reference

1. Deutschmann, O.; Maier, L.I.; Riedel, U.; Stroemman, A.H.; Dibble, R.W. Hydrogen assisted catalytic combustion of methane on platinum. *Catal. Today* **2000**, *59*, 141–150.