Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Ammonia Dynamic Modelling over Cu-SSZ-13 Catalyst for NOx Emission Control of Diesel Vehicles

Biao Liu[†,1], *Dongwei Yao*[†,1*], *Feng Wu*[†], *Xiaohan Hu*[†], *Yuxi Li*[†], *Xinlei Wang*[‡]

[†] College of Energy Engineering, Zhejiang University, Hangzhou 310027, China

[‡] Department of Agricultural and Biological Engineering, University of Illinois at Urbana-Champaign, Urbana 61801, USA

*Corresponding Author E-mail: dwyao@zju.edu.cn

[1] These authors are co-first authors of the article

1. The activation energy of ammonia desorption used in the reference

Table S1 The activation energy of ammonia desorption used in the reference

Reference	activation energy of S1 and S2/(kJ/mol)
L. Olsson, K. Wijayanti, K. Leistner, A. Kumar, S.Y. Joshi, K. Kamasamudram, N.W. Currier, A. Yezerets, A multi-site kinetic model for NH 3-SCR over Cu/SSZ-13, Applied Catalysis B: Environmental, 174 (2015) 212-224.	149.0/137.8
SR. Daya, S.Y. Joshi, J. Luo, R.K. Dadi, N.W. Currier, A. Yezerets, On kinetic modeling of change in active sites upon hydrothermal aging of Cu-SSZ-13, Applied Catalysis B: Environmental, 263 (2020) 118368	103/134
Y. Jangjou, C.S. Sampara, Y. Gu, D. Wang, A. Kumar, J. Li, W.S. Epling, Mechanism-based kinetic modeling of Cu-SSZ-13 sulfation and desulfation for NH3-SCR applications, Reaction Chemistry & Engineering, 4 (2019) 1038-1049.	82/82
X. Song, G. Parker, J.H. Johnson, J. Naber, J. Pihl, A Modeling Study of SCR Reaction Kinetics from Reactor Experiments, SAE International, 2013.	52.2/71.6
J. Gong, K. Narayanaswamy, C.J. Rutland, Heterogeneous Ammonia Storage Model for NH3–SCR Modeling, Ind Eng Chem Res, 55 (2016) 5874-5884.	43/88

2. Identification results of modified dual-site model

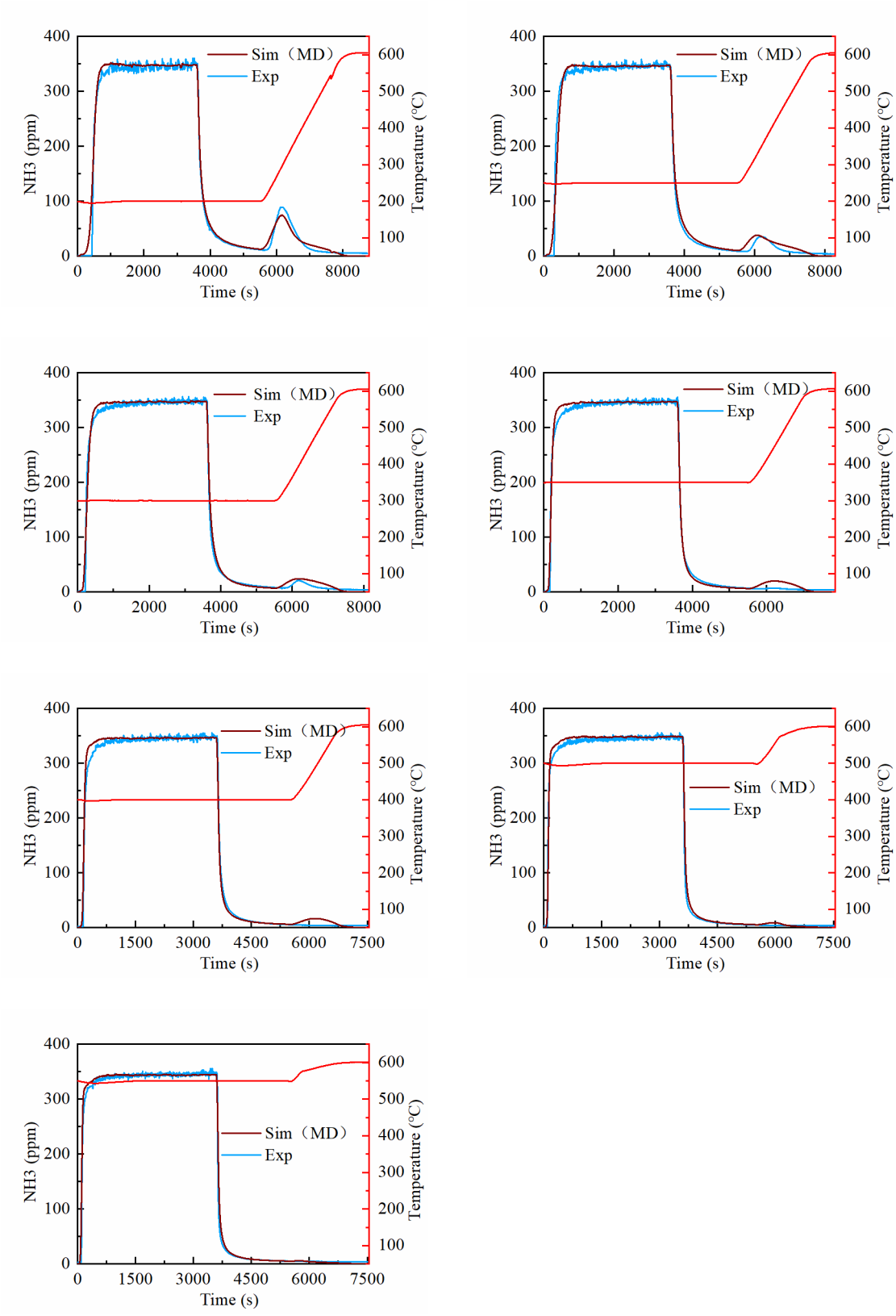

Figure S1 Experiment and kinetic modeling with modified dual-site model for NH_3-TPD over Cu-SSZ-13 catalysts at different temperatures (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 10 °C /min)

3. Identification results of dual-site model

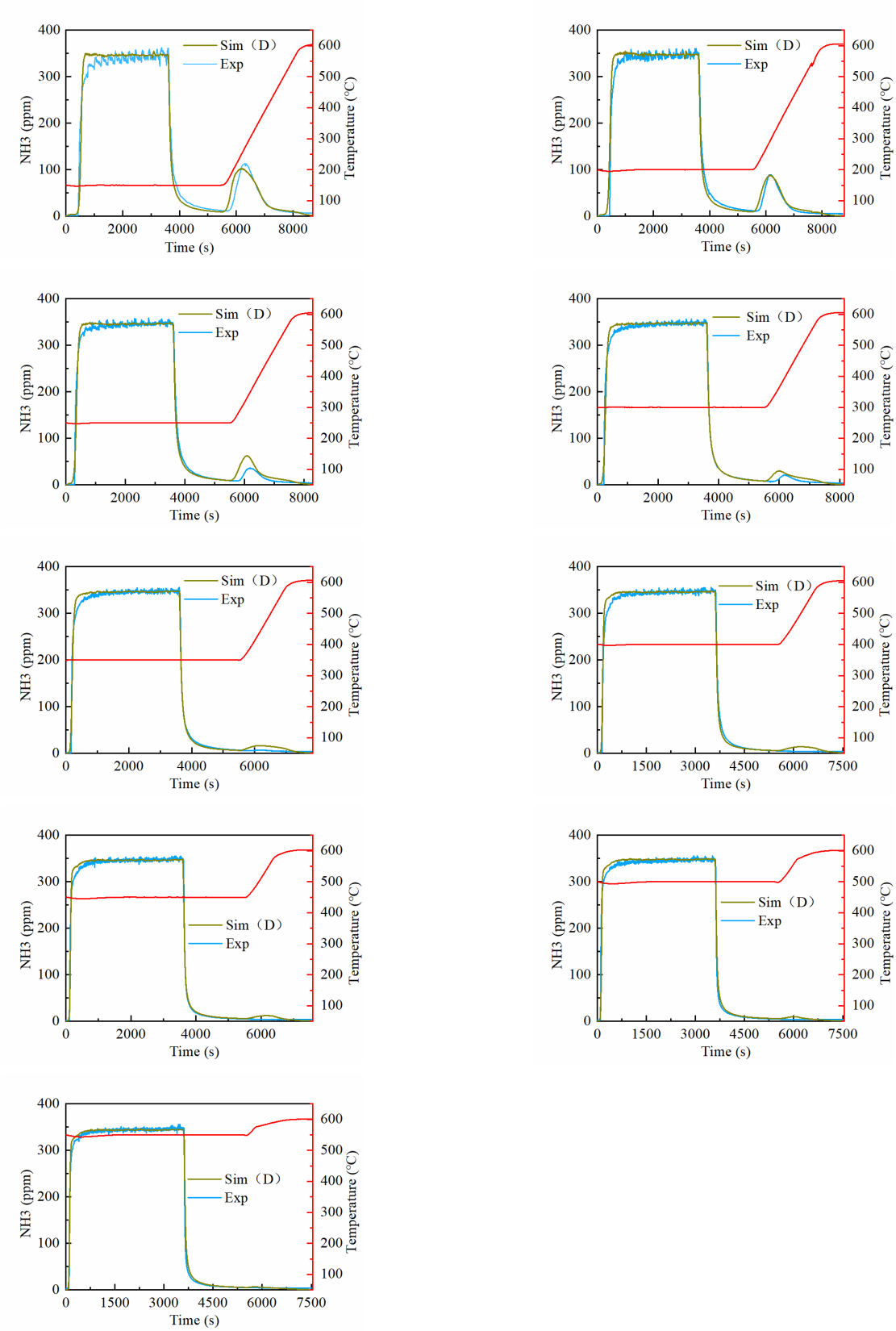

Figure S2 Experiment and kinetic modeling with dual-site model for NH_3-TPD over Cu-SSZ-13 catalysts at different temperatures (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 10 °C /min)

4. Identification results of multi-site model

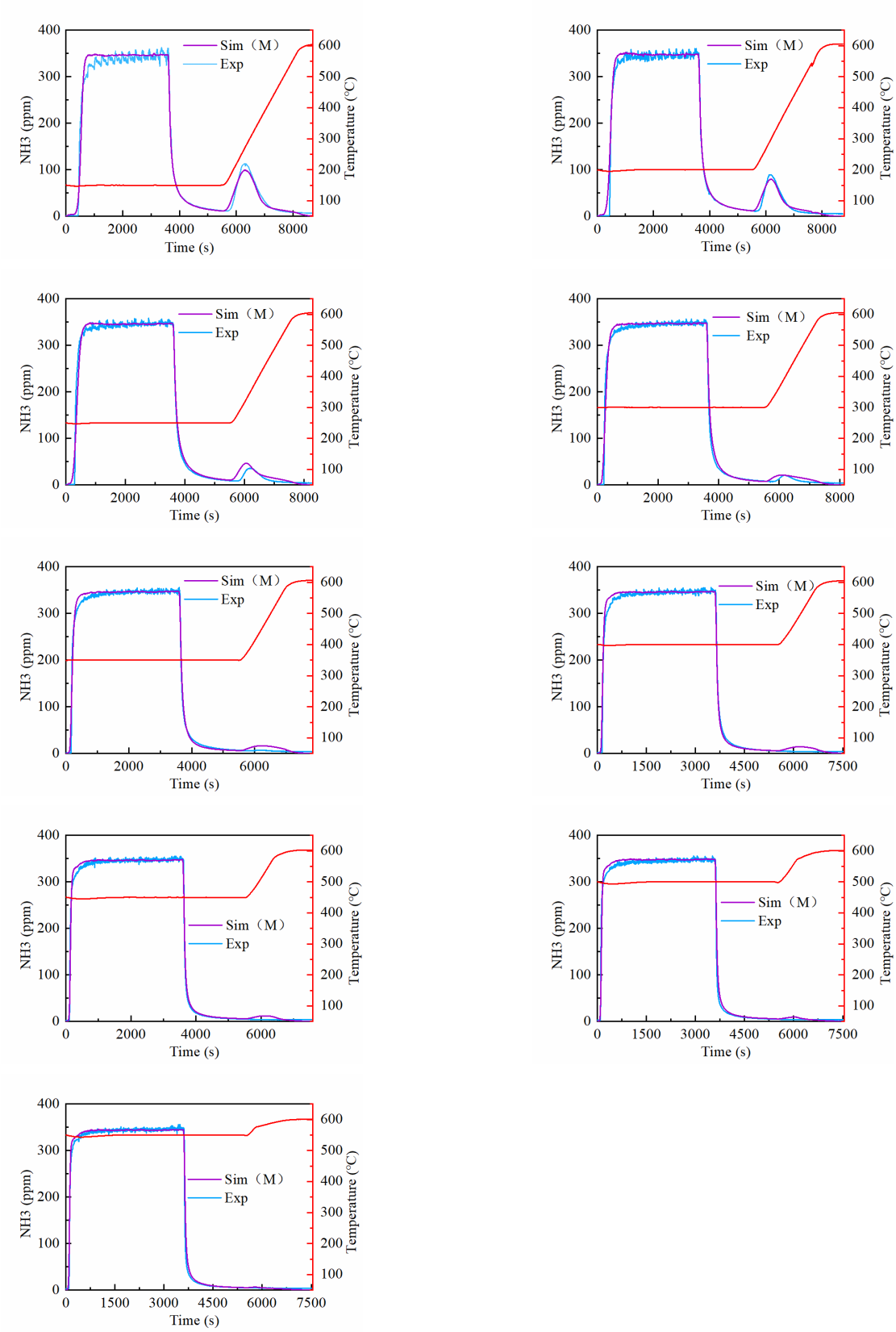

Figure S3 Experiment and kinetic modeling with multi-site model for NH_3-TPD over Cu-SSZ-13 catalysts at different temperatures (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 10 °C /min)

5. Ammonia storage in Figure 6 and Figure 7

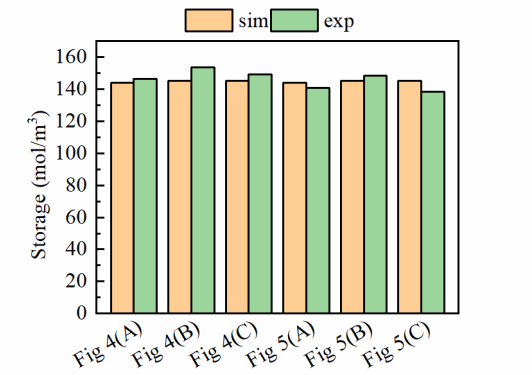

Figure S4 Ammonia storage in Figure 6 and Figure 7

6. Validation of dual-site model

6.1 validation with different adsorption NH_3 concentration

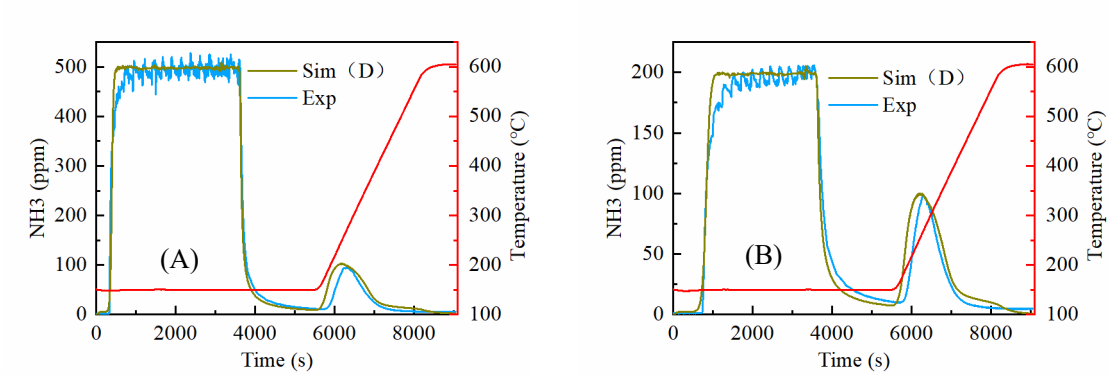

Figure S5 Validation of the dual-site model with different NH_3 concentration (Reaction conditions: NH_3 = 500 ppm (A) and 200 ppm (B), GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 10 °C /min)

6.2 Validation with different flushing duration

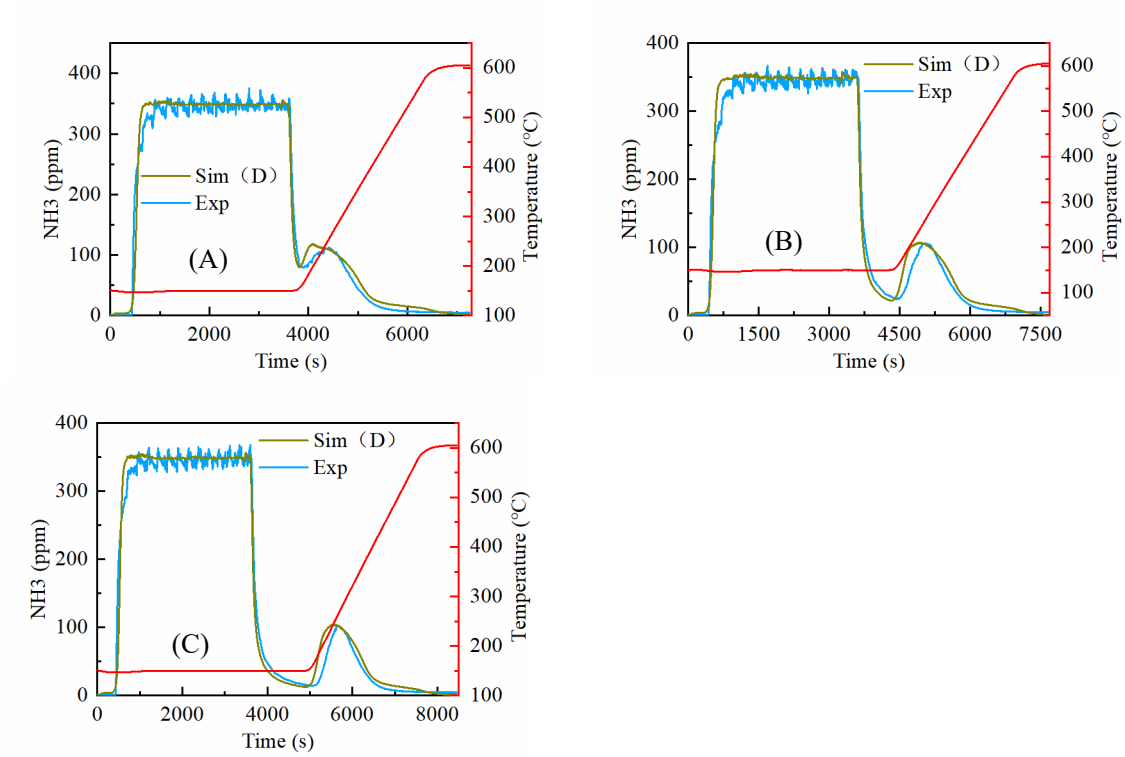

Figure S6 Validation of the dual-site model with different flushing duration (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 0 min(A), 10 min(B), 20 min(C), heating rate = 10 °C /min)

6.3 Validation with different heating rate

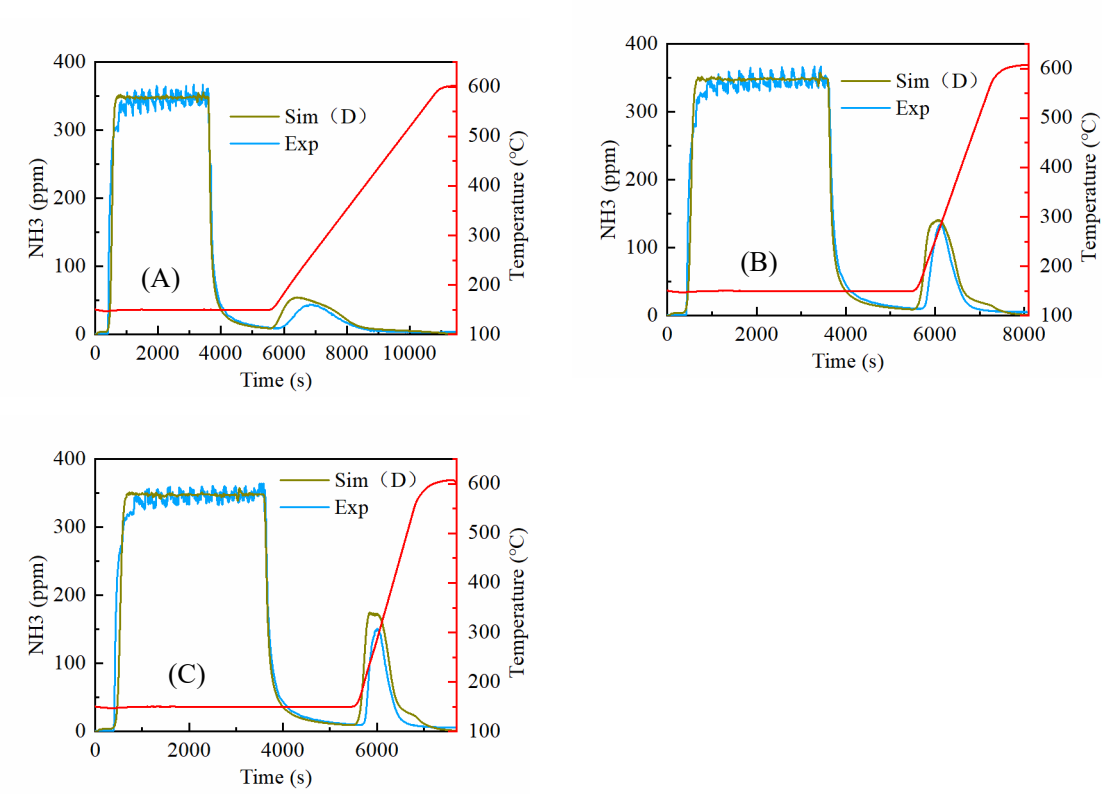

Figure S7 Validation of the dual-site model with different heating rate (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 5 °C /min(A), 15 °C /min(B), 20 °C /min(C))

7. Validation of multi-site model

7.1 Validation with different NH_3 adsorption concentration

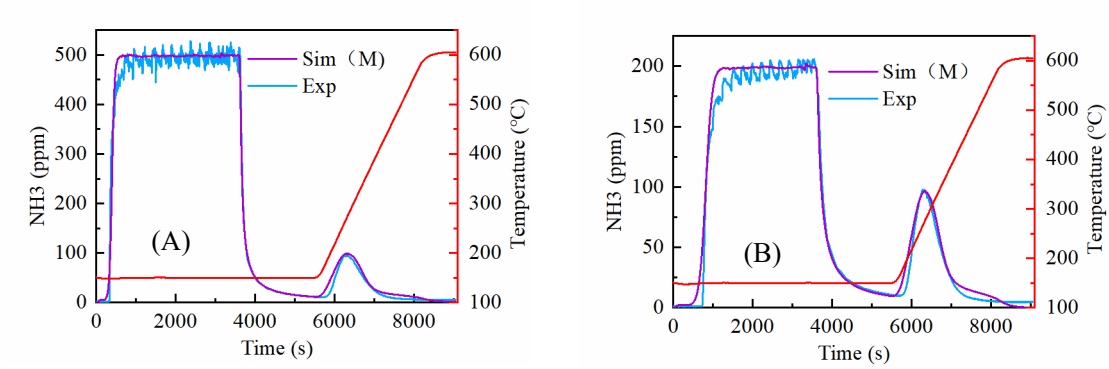

Figure S8 Validation of the multi-site model with different NH_3 concentration (Reaction conditions: NH_3 = 500 ppm (A) and 200 ppm (B), GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 10 °C /min)

7.2 Validation with different flushing duration

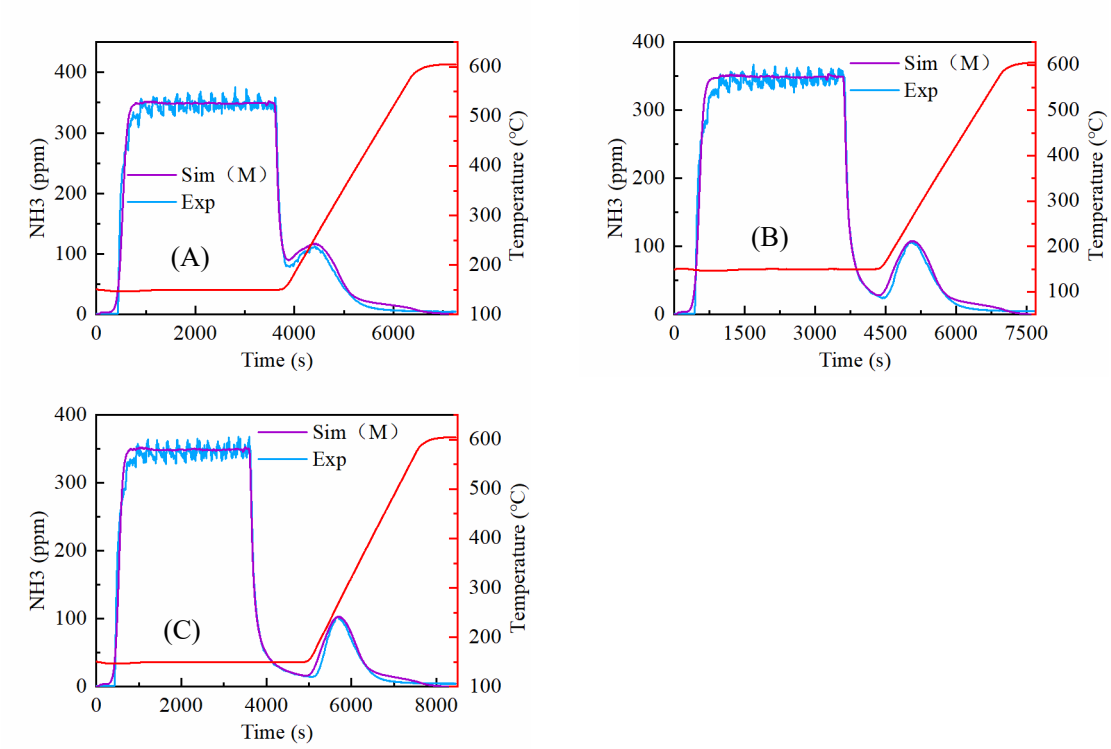

Figure S9 Validation of the dual-site model with different flushing duration (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 0 min(A), 10 min(B), 20 min(C), heating rate = 10 °C /min)

7.3 Validation with different heating rate

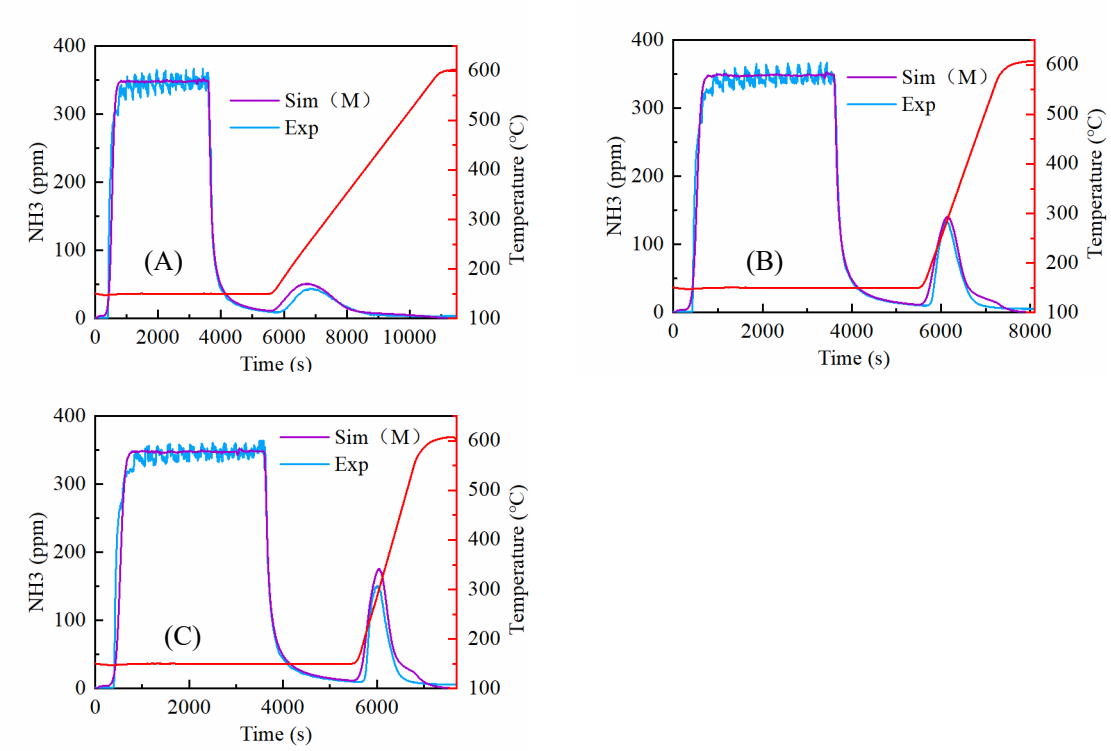

Figure S10 Validation of the modified dual-site model with different heating rate (Reaction conditions: NH_3 = 350 ppm, GHSV = 60000h^{-1}, flushing duration = 30 min, heating rate = 5 °C /min(A), 15 °C /min(B), 20 °C /min(C))