Supplementary Materials

A simplified chemical kinetic model with a reaction mechanism based on multidimensional average error iteration method for ammonia and ammonia/hydrogen combustion

Daiyao Yue, Chongkai Zhao, Rui Sun, Jieyu Jiang, Chunjie Sui, Xin Zhong, Bin Zhang*

College of Electromechanical Engineering, Qingdao University of Science and Technology, Qingdao 266061, China

(*Corresponding author: zb-sh@163.com)

S1 Additional validations of the present model

1 Laminar flame speeds

1.1 H_2

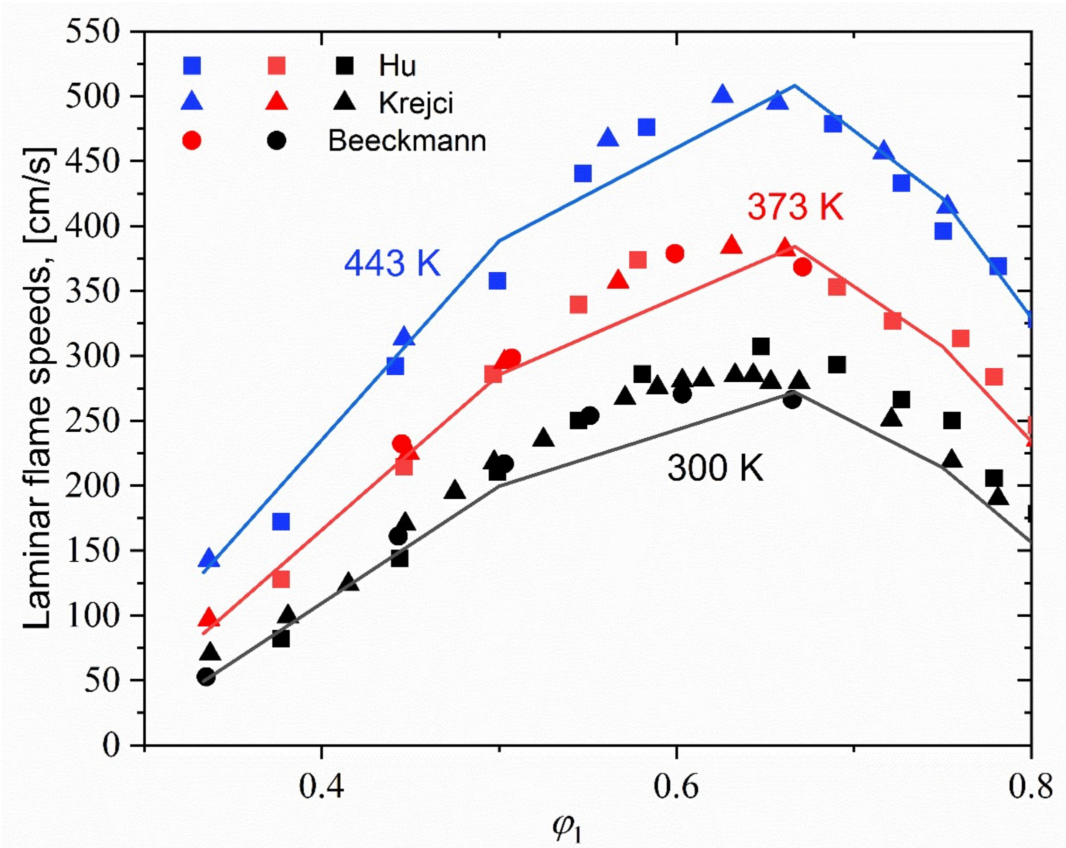


Fig. S1. Laminar flame speeds of H_2/air flame varying with normalized equivalence ratio, $\varphi_1 = \varphi\,(1 + \varphi)$, at standard pressure. Data sources of experiment: Hu (2009)[1]; Krejci (2013)[2]; Beeckmann (2016)[3].

1.2 Shrestha et al.[4]

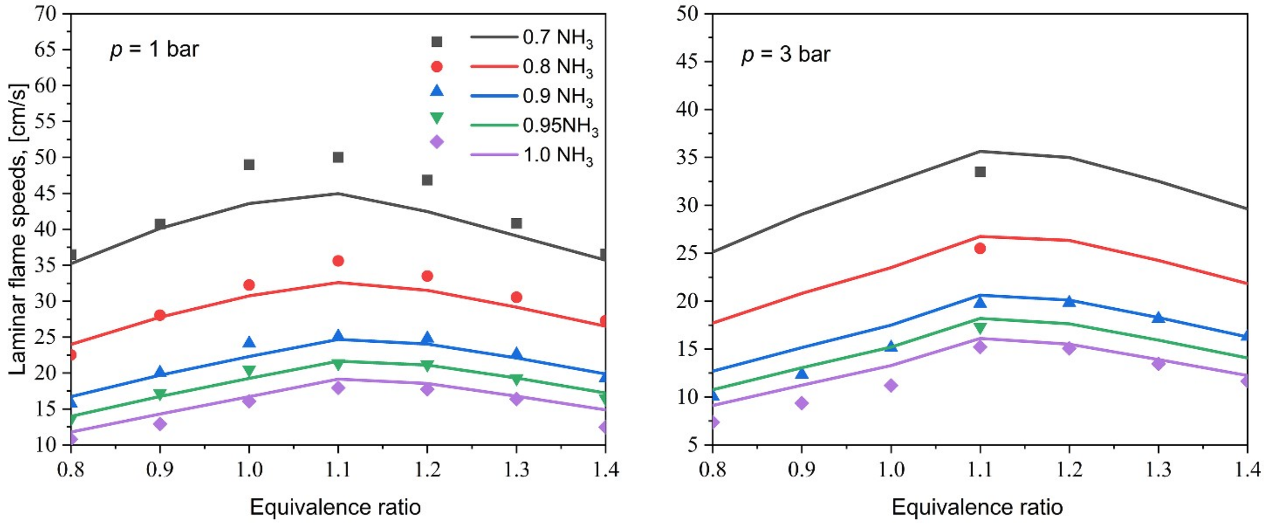


Fig. S2. Laminar flame speeds predictions for NH_3/H_2/air mixtures at variable pressure. T = 473 K.

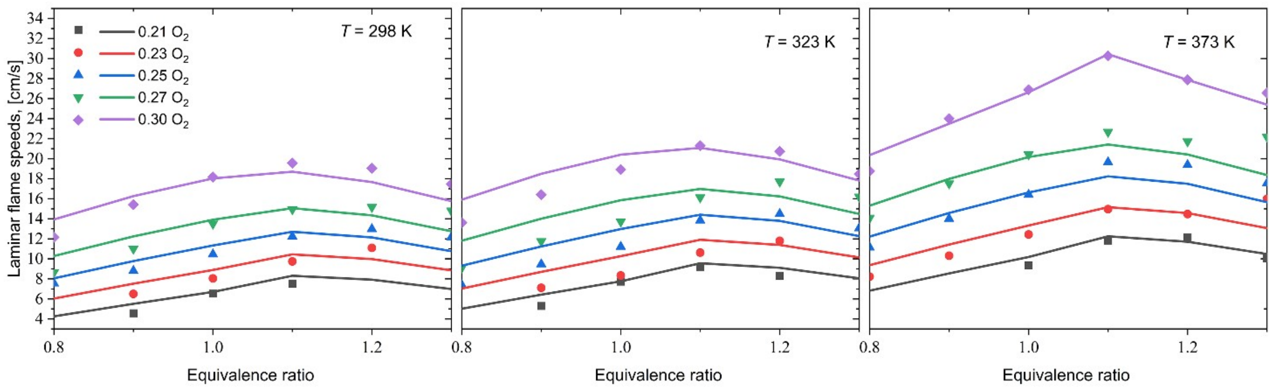


Fig. S3. Laminar flame speeds predictions for $NH_3/O_2/N_2$ mixtures at variable oxygen content. p = 1 bar.

1.3 Mei et al. [5]

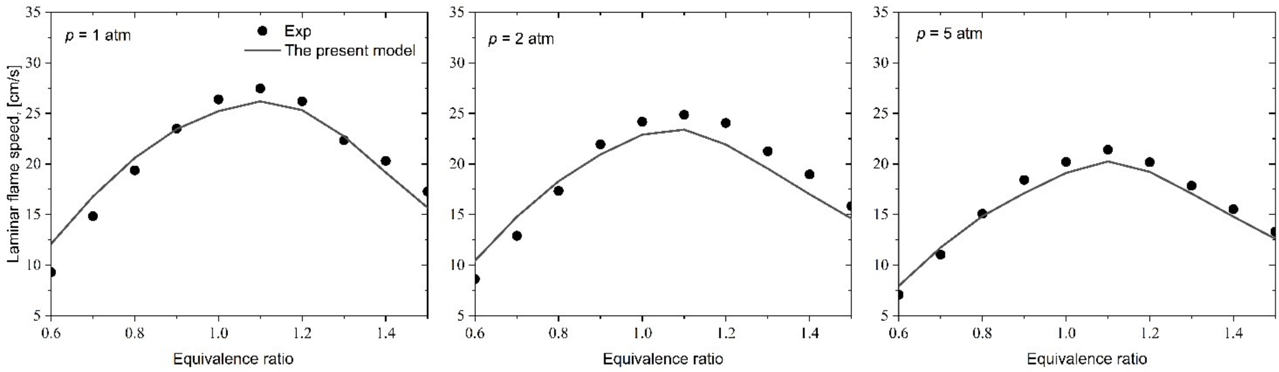


Fig. S4. Laminar flame speeds of NH_3/(35%O_2/65%N_2) mixtures at T = 298 K and p = 1–5 atm.

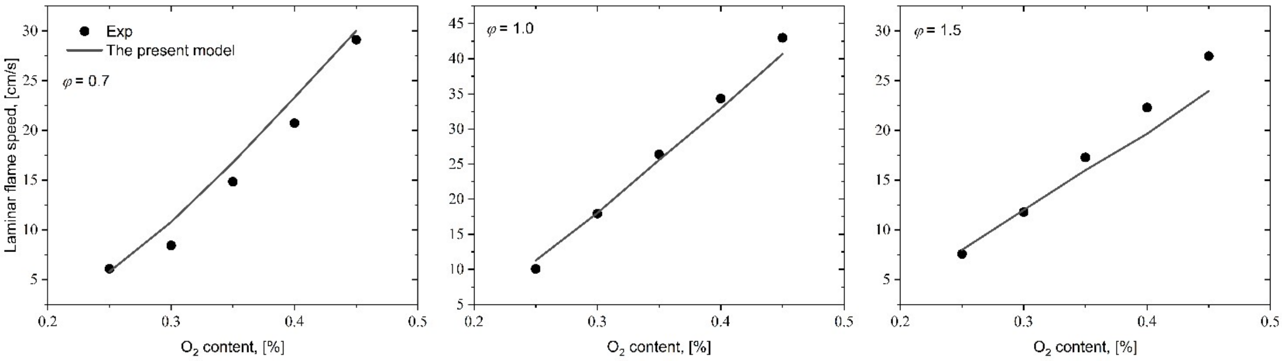
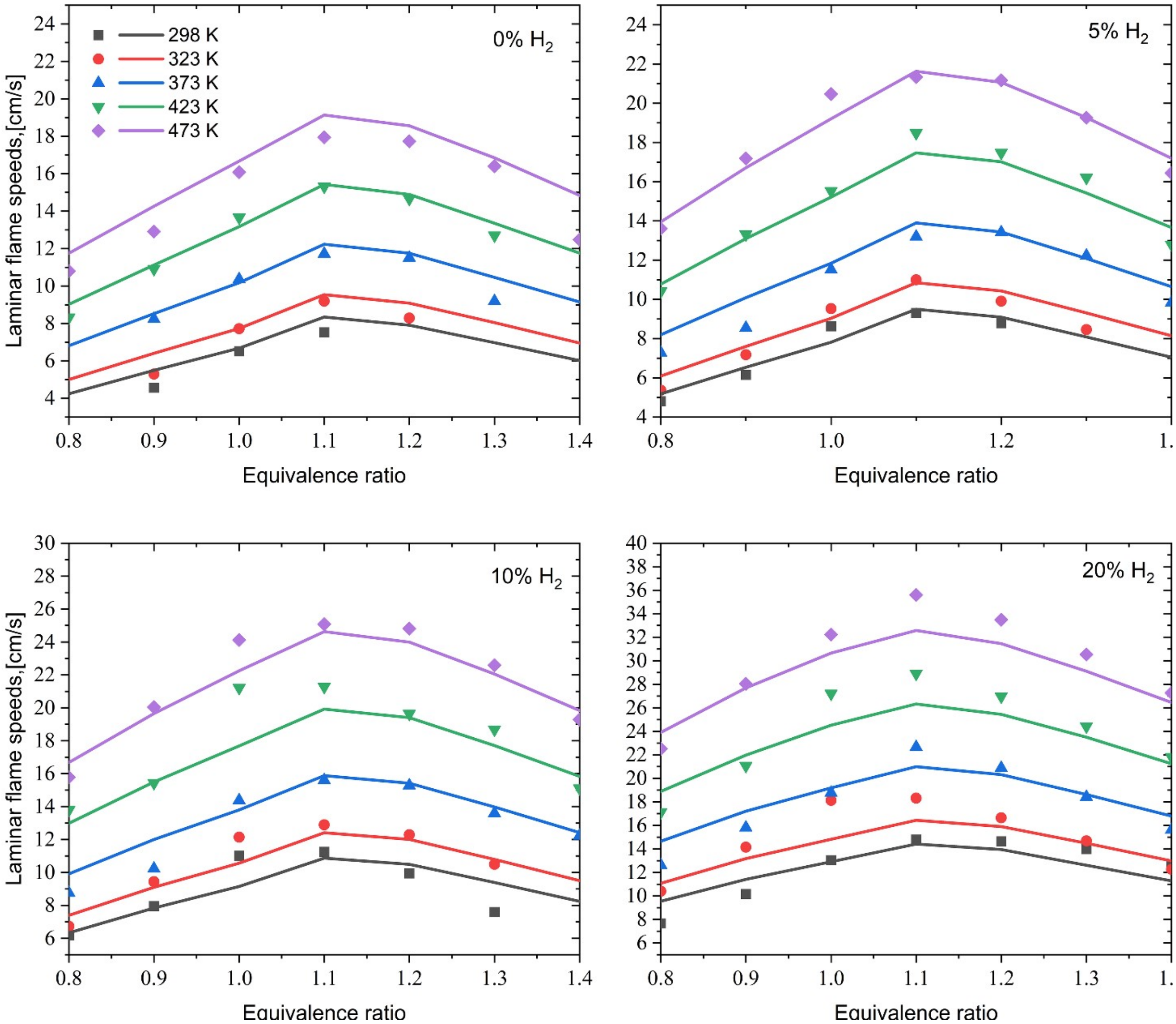


Fig. S5. Laminar flame speeds result of $NH_3/O_2/N_2$ mixtures at T = 298 K and p = 1 atm with different oxygen contents.

1.4 Lhuillier et al. [6]



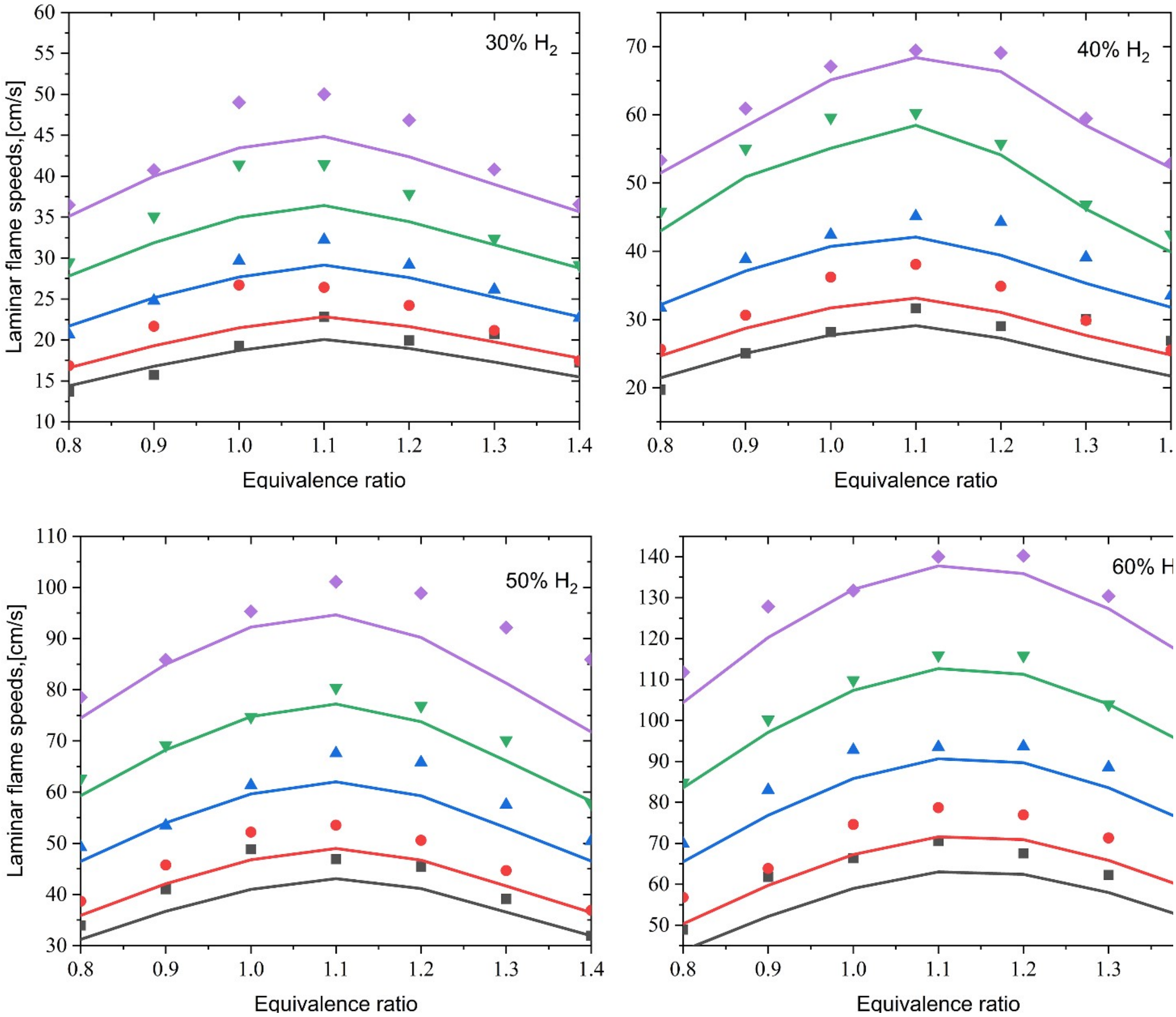


Fig. S6. Laminar flame speeds result of NH_3/H_2/air mixtures at T = 298–473 K, p = 1 atm and x_{H2} = 0–60%.

2 Ignition delay time

2.1 Dai et al. [7]

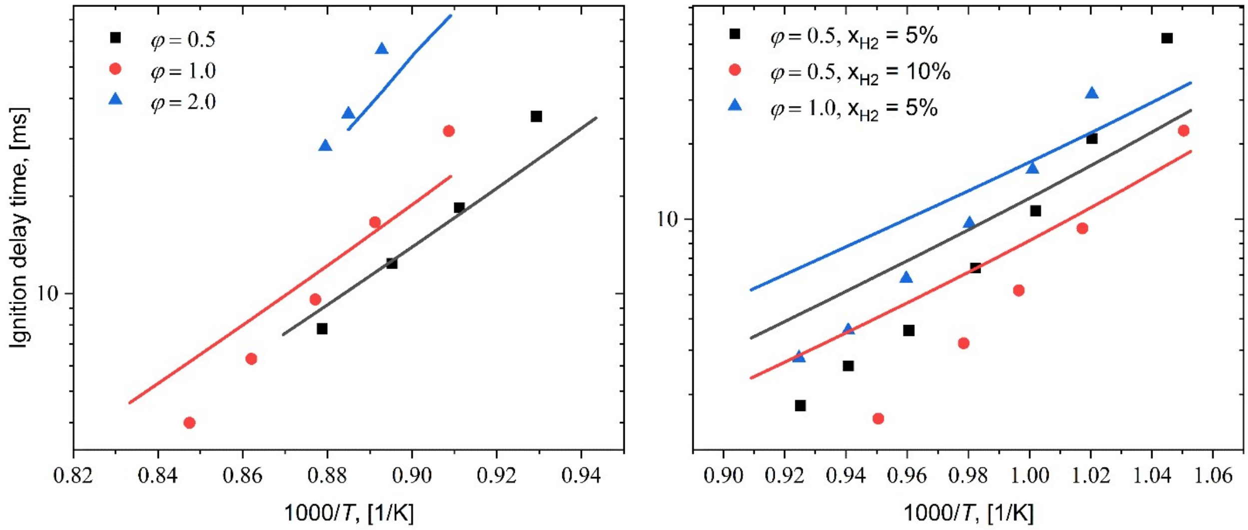


Fig. S7. Ignition delay times of NH_3/O_2 and $NH_3/O_2/H_2$ mixture measured in a rapid compression machines (RCM) at φ = 0.5–2.0, p = 60 bar.

2.2 Pochet et al. [8]

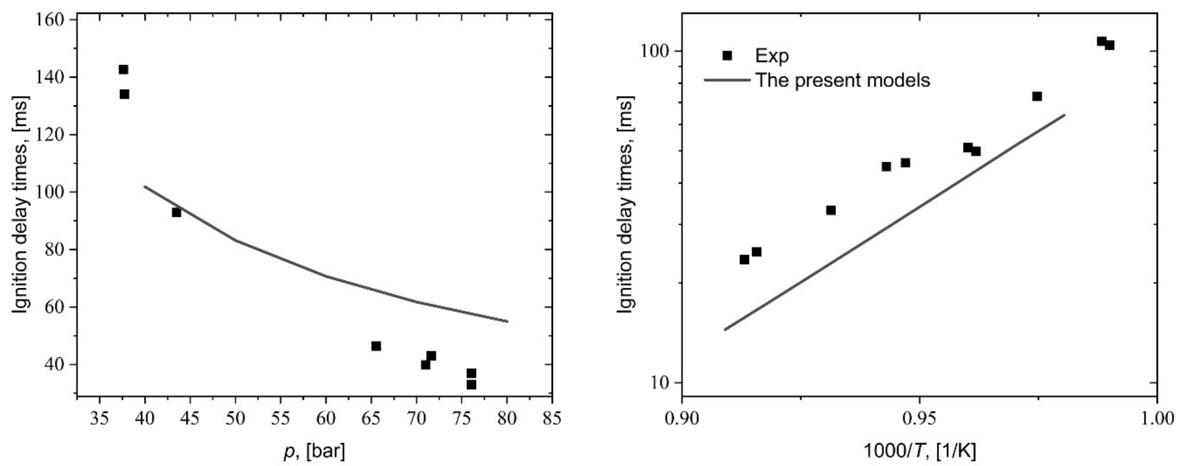


Fig. S8. Ignition delay times of NH_3/O_2 mixture measured in a rapid compression machines (RCM) at different T and p. φ = 0.35.

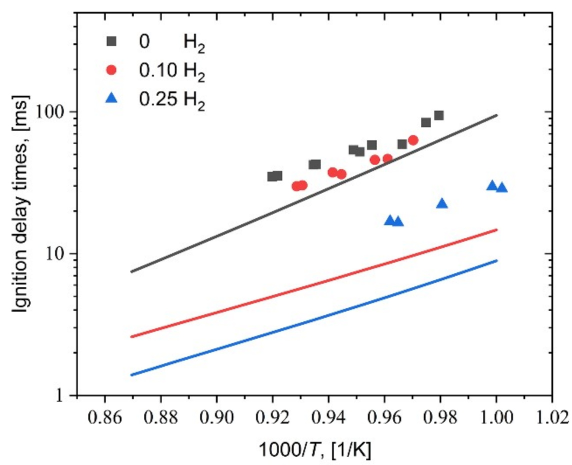


Figure. S9. Ignition delay times of $NH_3/O_2/H_2$ mixture measured in a rapid compression machines (RCM) at different T. x_{H2} = 0–25%, φ = 0.35, p = 43.5 bar

3 species concentration

3.1 Stagni et al.[9]

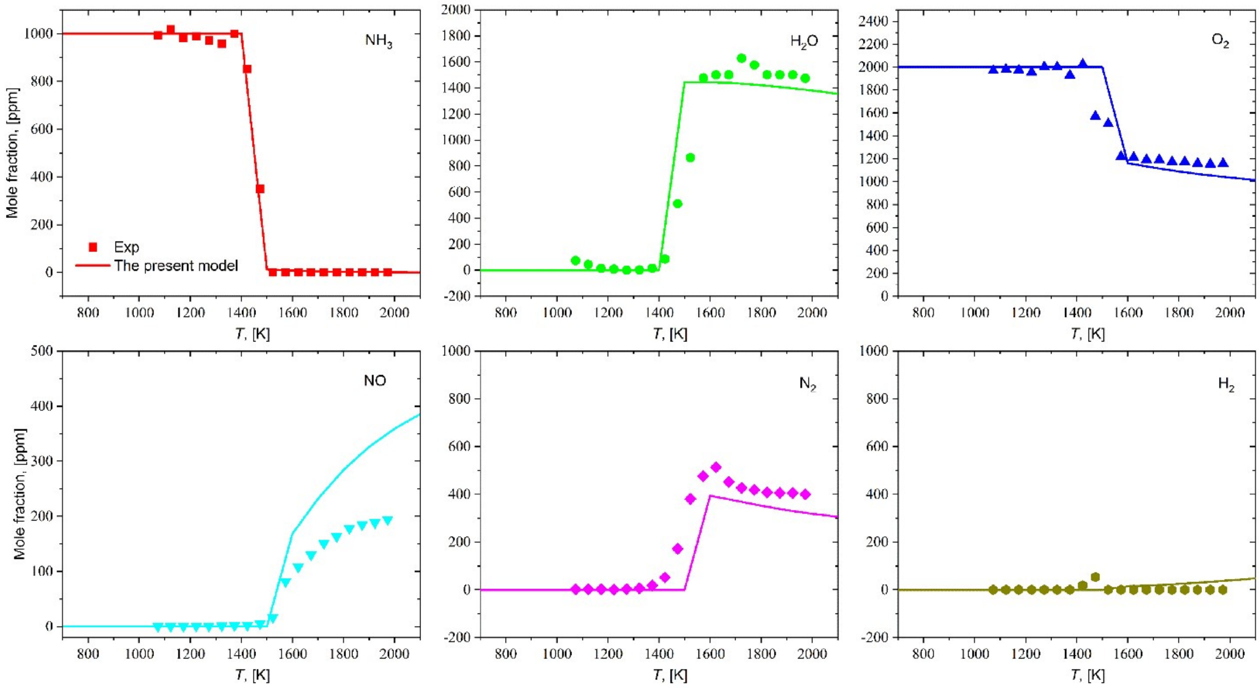
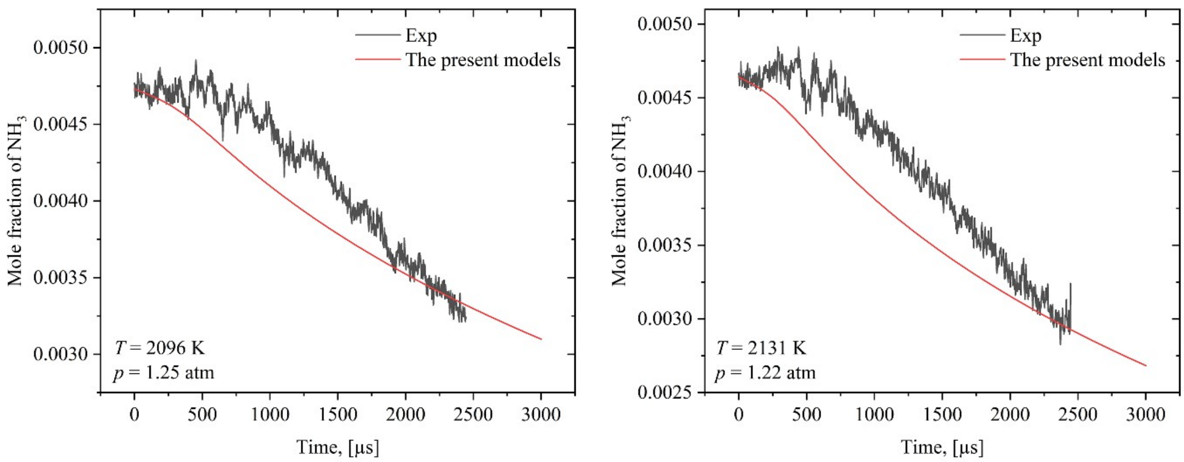
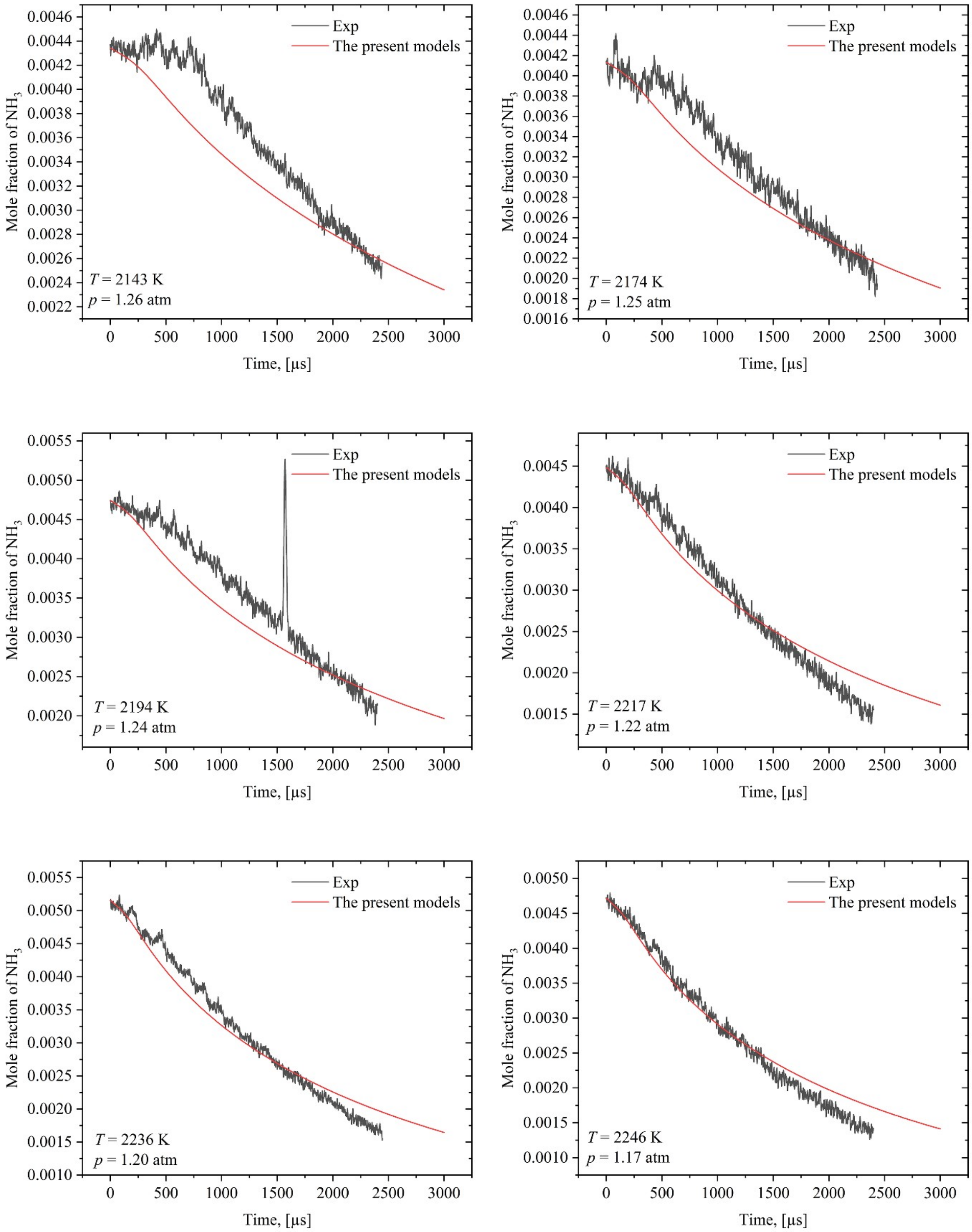


Fig. S10. Oxidation of 1000 ppm NH_3 with 2000 ppm O_2 in a FR. Experimental and modeling results. p = 950 torr. τ = 0.05 s.

3.2 Alturaifi et al. [10]





Exp
The present models
Mole fraction of NH_3
Time, [μs]
T = 2143 K
p = 1.26 atm
T = 2174 K
p = 1.25 atm
T = 2194 K
p = 1.24 atm
T = 2217 K
p = 1.22 atm
T = 2236 K
p = 1.20 atm
T = 2246 K
p = 1.17 atm

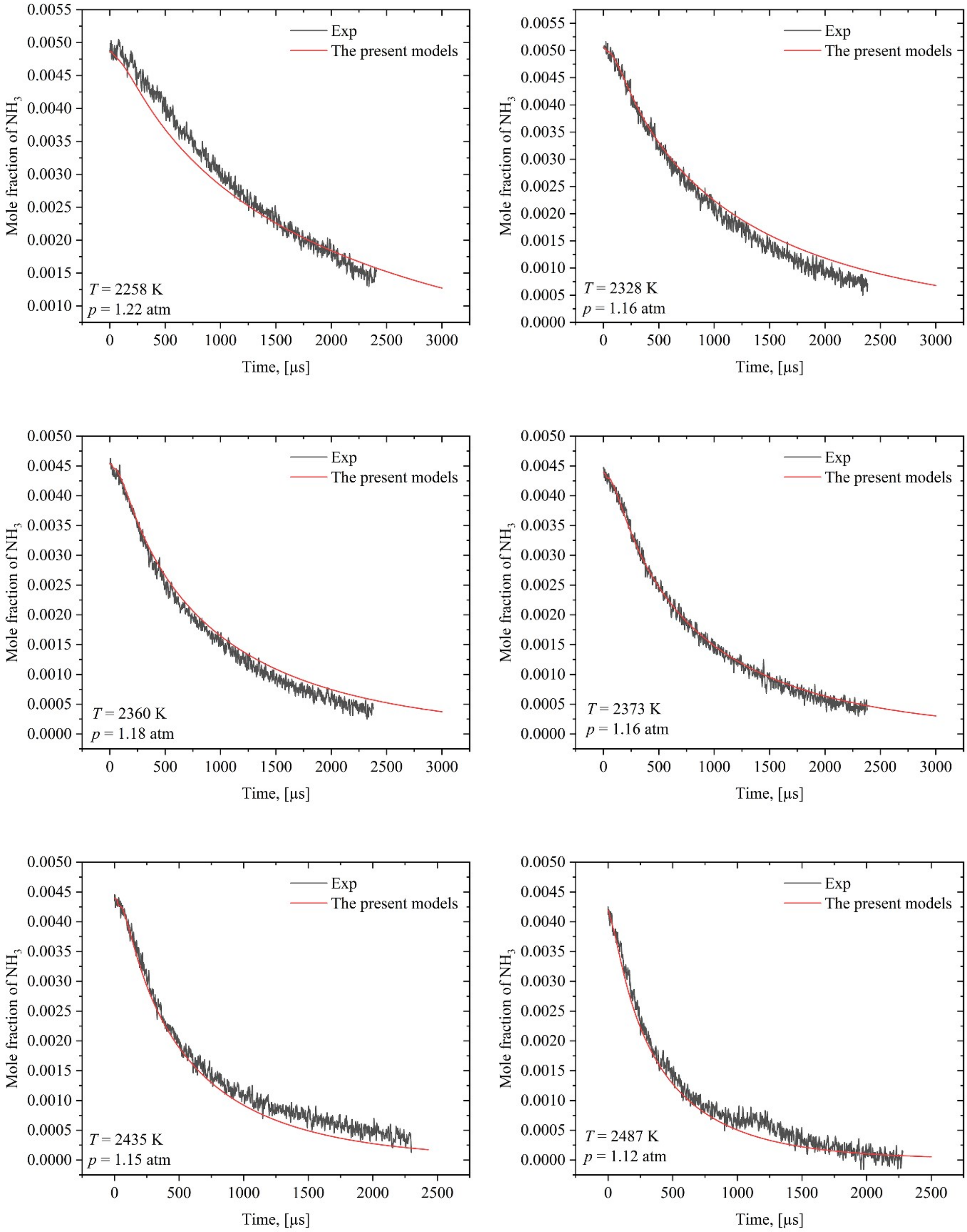
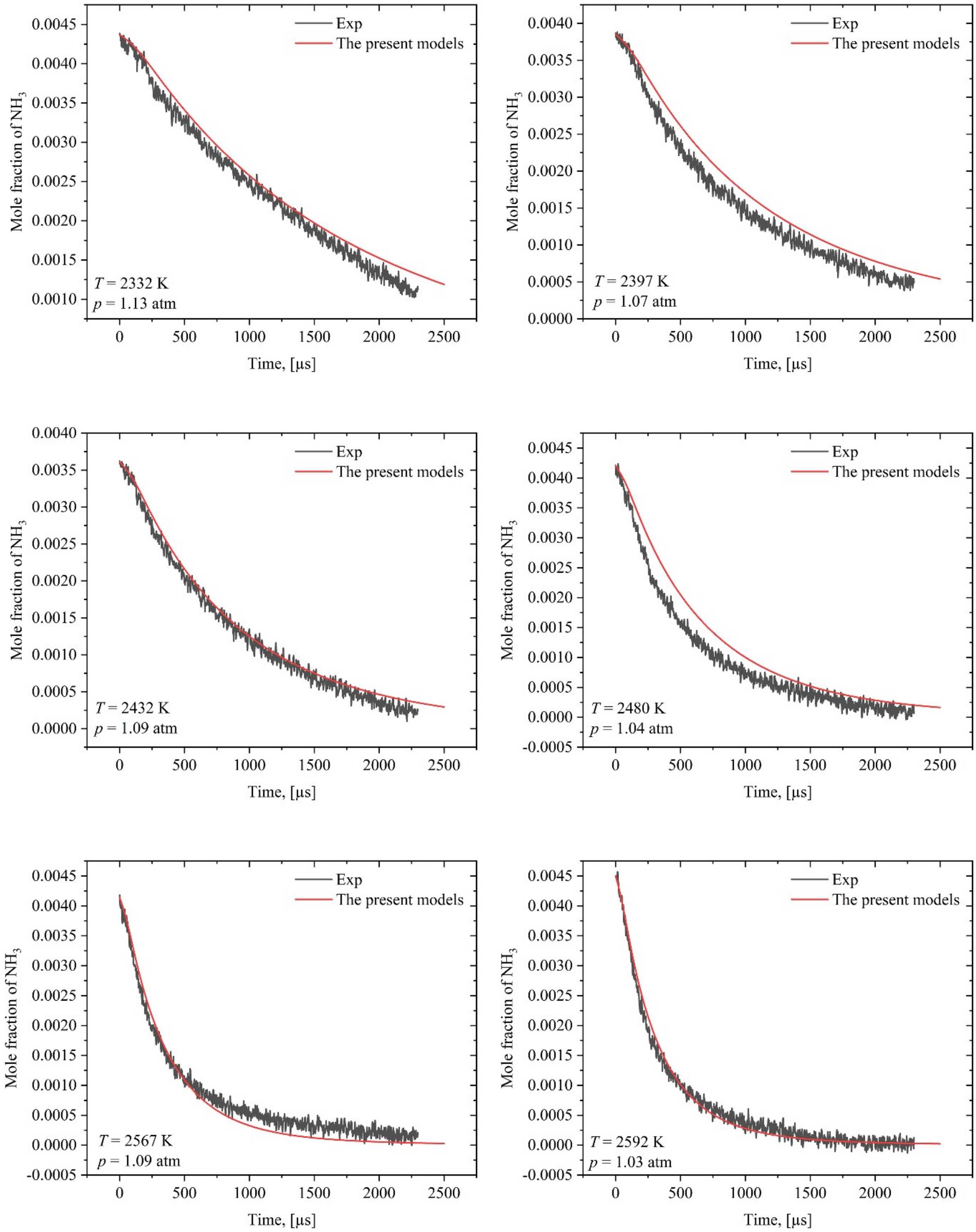


Fig. S11. Experiments and modeling results for NH_3 speciation profiles for a mixture of 0.5% NH_3 in shock tube.


Exp
The present models
Mole fraction of NH3
Time, [μs]
T = 2332 K
p = 1.13 atm
T = 2397 K
p = 1.07 atm
T = 2432 K
p = 1.09 atm
T = 2480 K
p = 1.04 atm
T = 2567 K
p = 1.09 atm
T = 2592 K
p = 1.03 atm

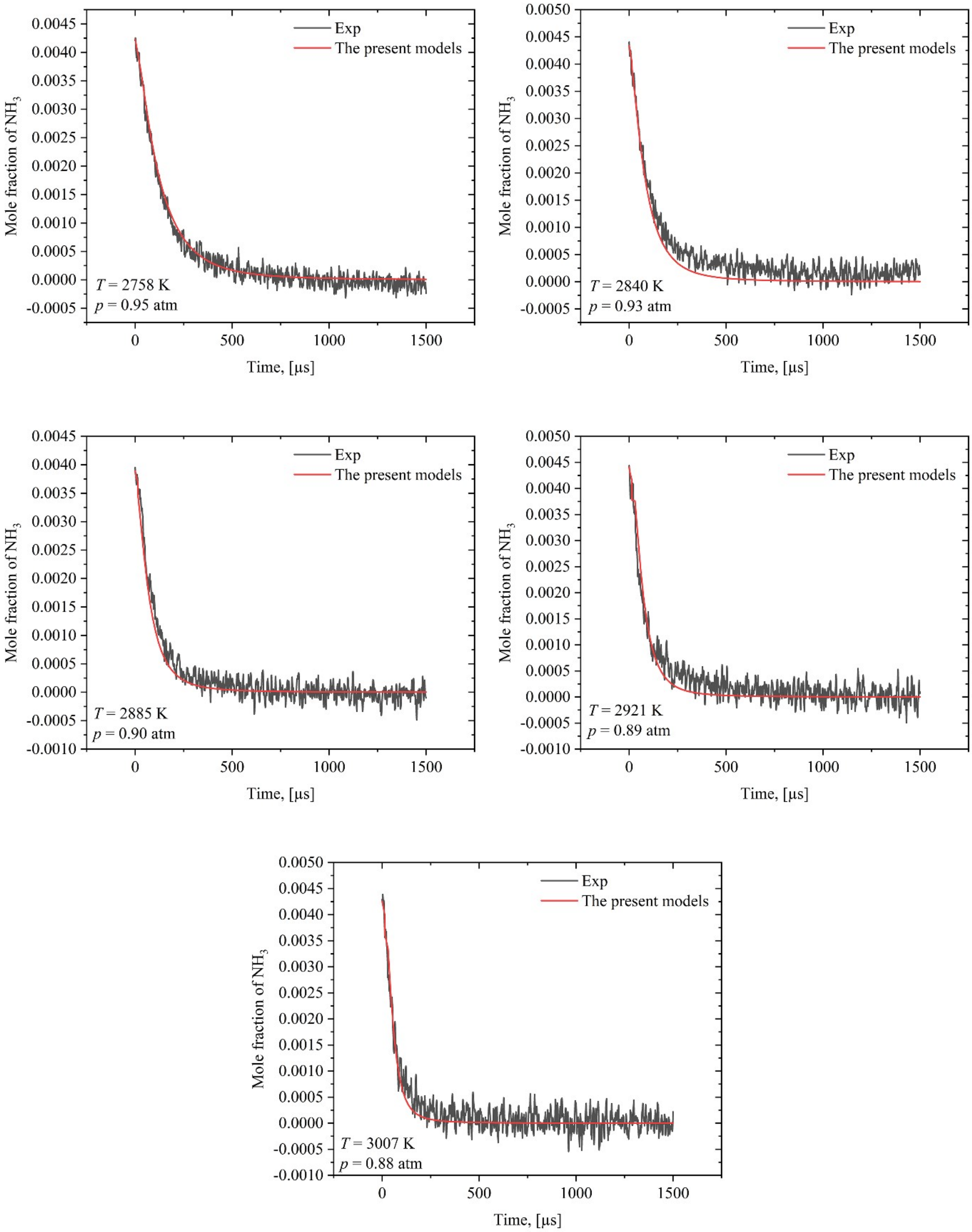
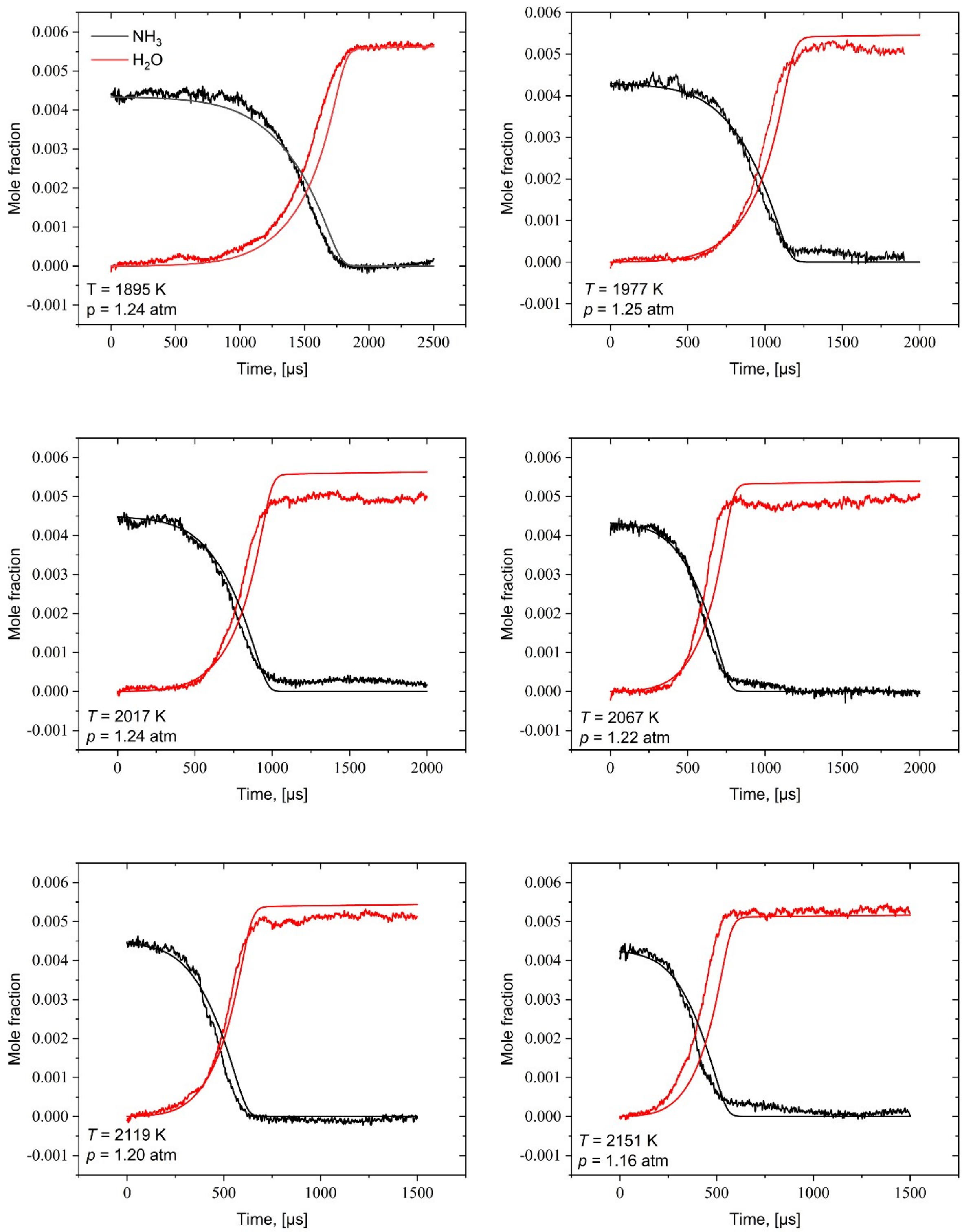


Fig. S12. Experiments and modeling results for NH_3 speciation profiles for a mixture of 0.42% NH_3/2% H_2 in shock tube.

3.3 Alturaifi et al. [11]


NH3
H2O
Mole fraction
Time, [µs]
T = 1895 K
p = 1.24 atm
T = 1977 K
p = 1.25 atm
T = 2017 K
p = 1.24 atm
T = 2067 K
p = 1.22 atm
T = 2119 K
p = 1.20 atm
T = 2151 K
p = 1.16 atm

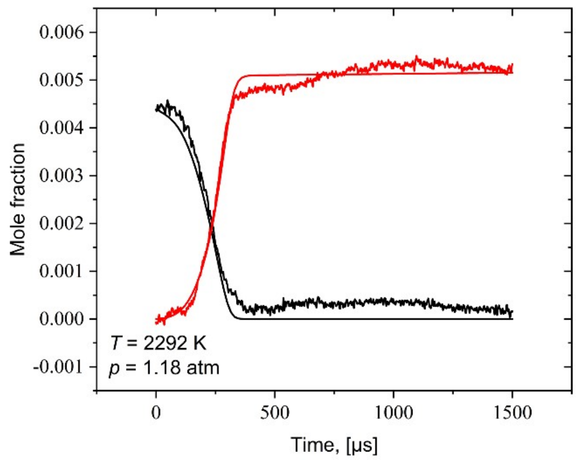
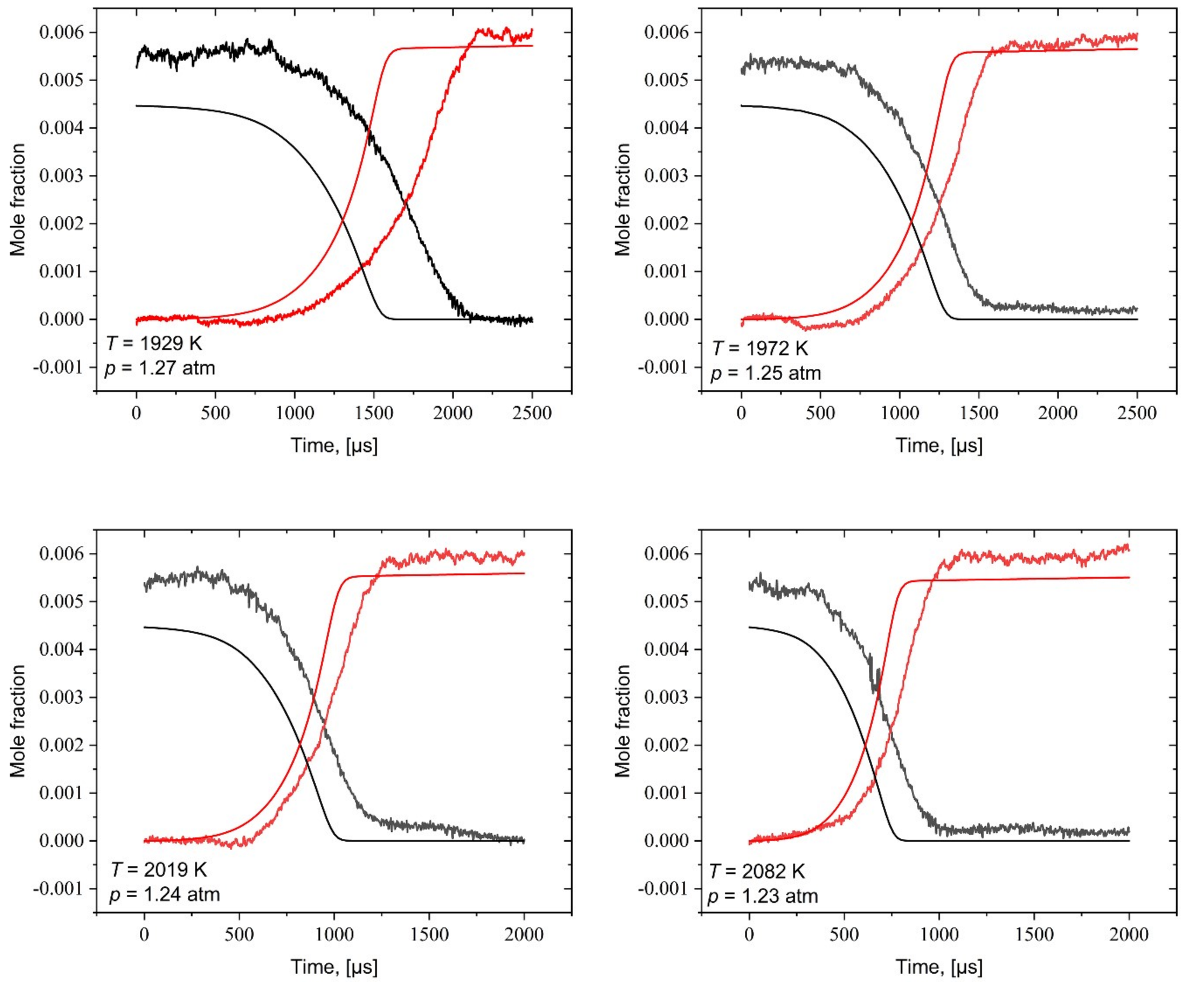


Fig. S13. NH_3 and H_2O speciation profiles in the oxidation of NH_3 in ~99% Ar. φ = 0.58.



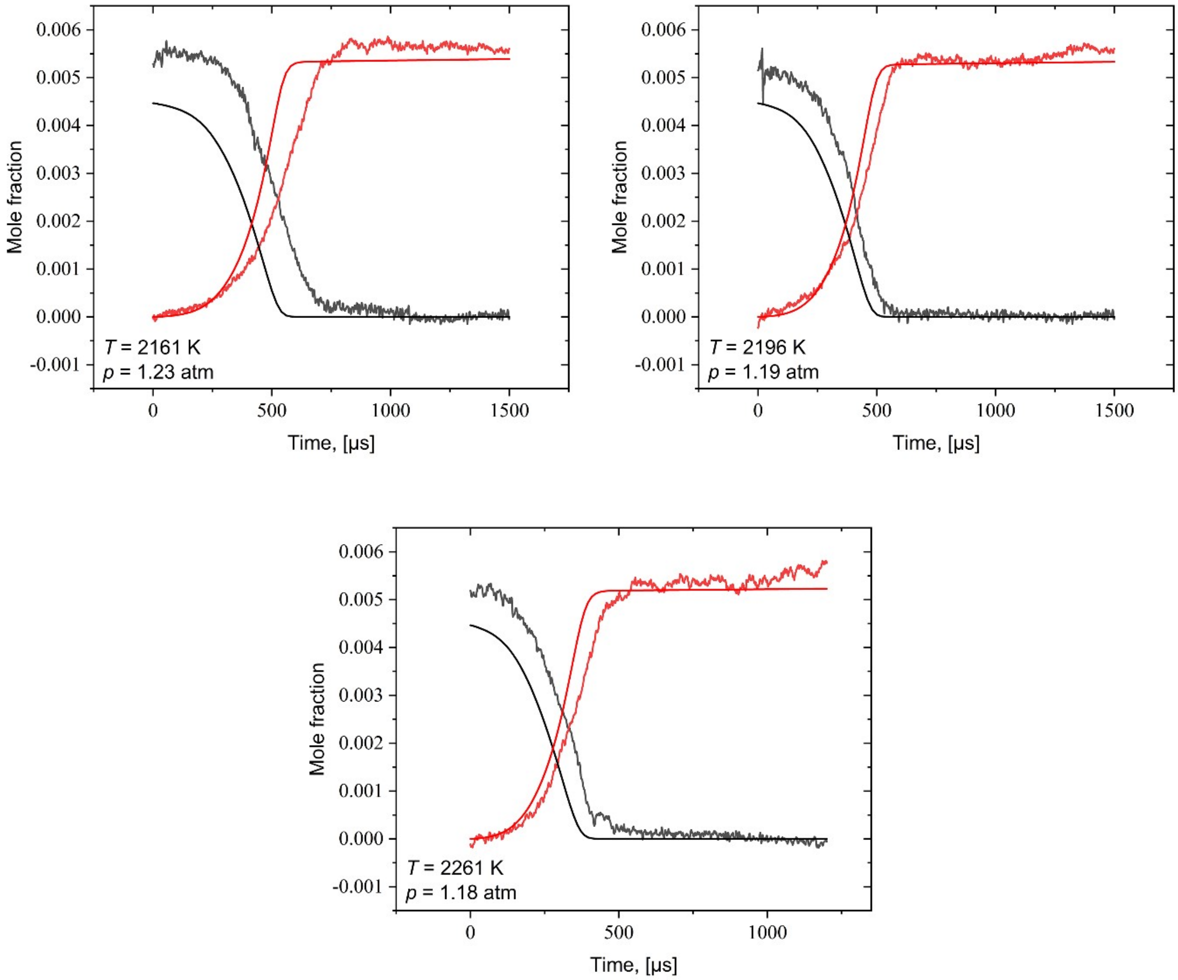
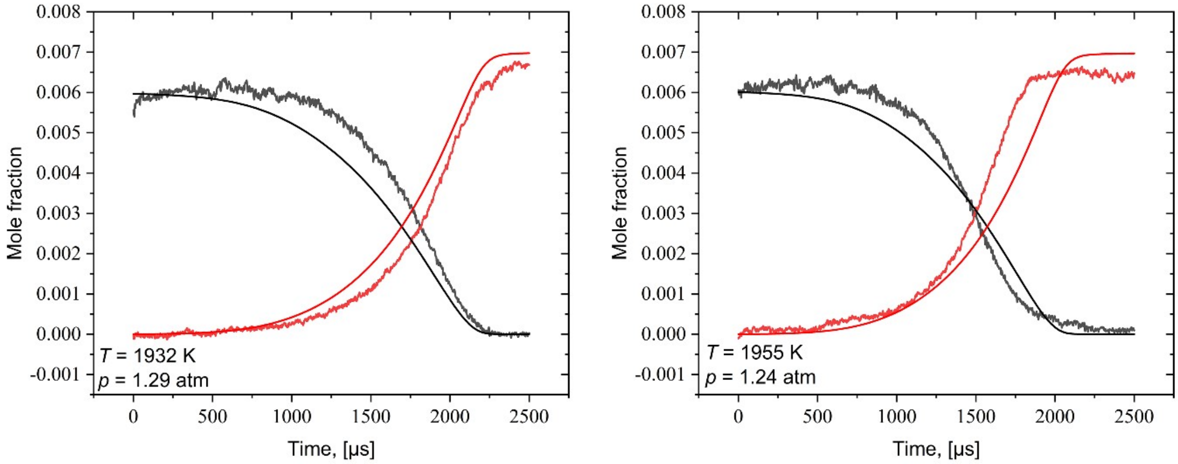


Fig. S14. NH_3 and H_2O speciation profiles in the oxidation of NH_3 in ~99% Ar. φ = 0.90.



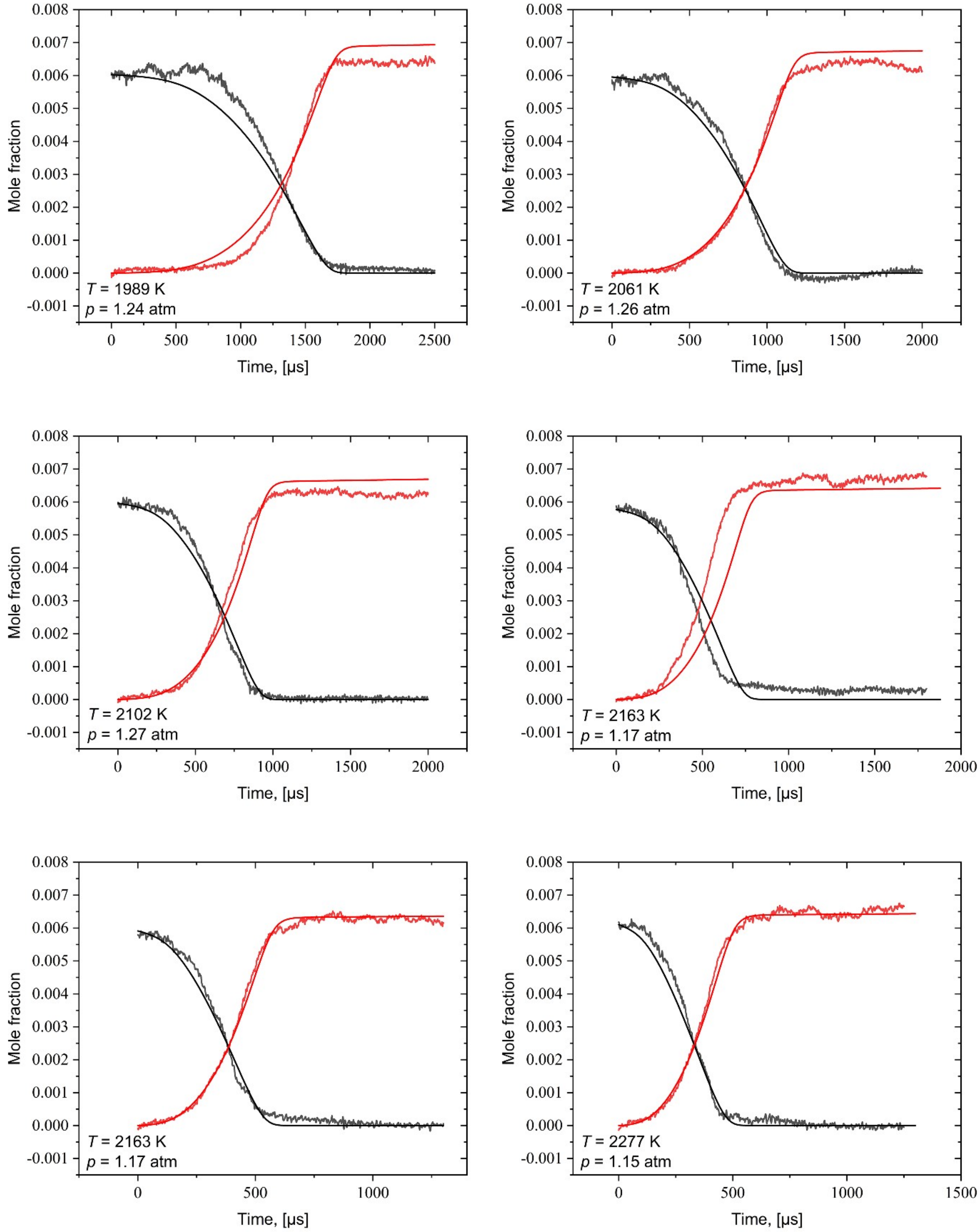
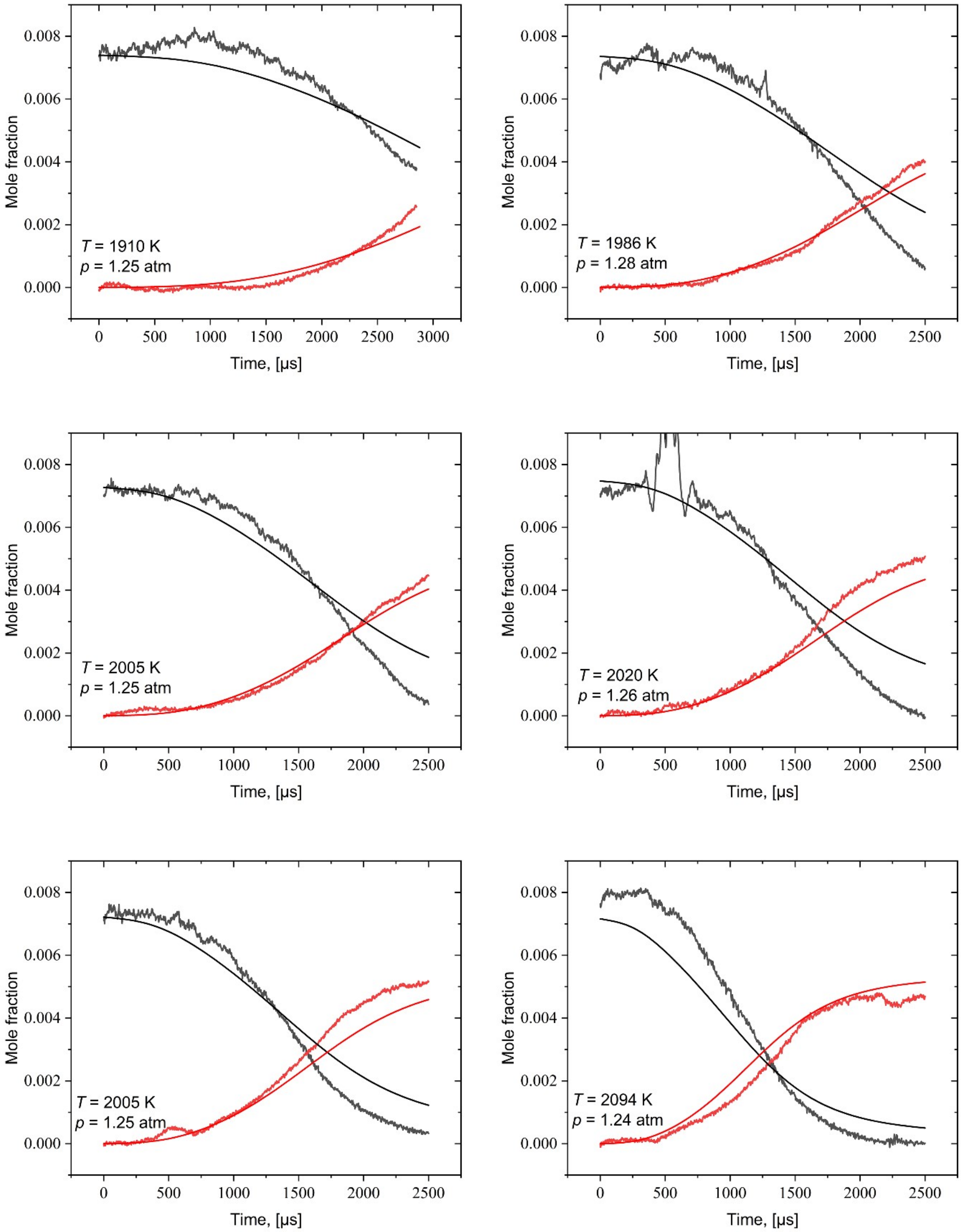


Fig. S15. NH_3 and H_2O speciation profiles in the oxidation of NH_3 in ~99% Ar. φ = 1.06.



Mole fraction
Time, [µs]
T = 1910 K
p = 1.25 atm
T = 1986 K
p = 1.28 atm
T = 2005 K
p = 1.25 atm
T = 2020 K
p = 1.26 atm
T = 2005 K
p = 1.25 atm
T = 2094 K
p = 1.24 atm

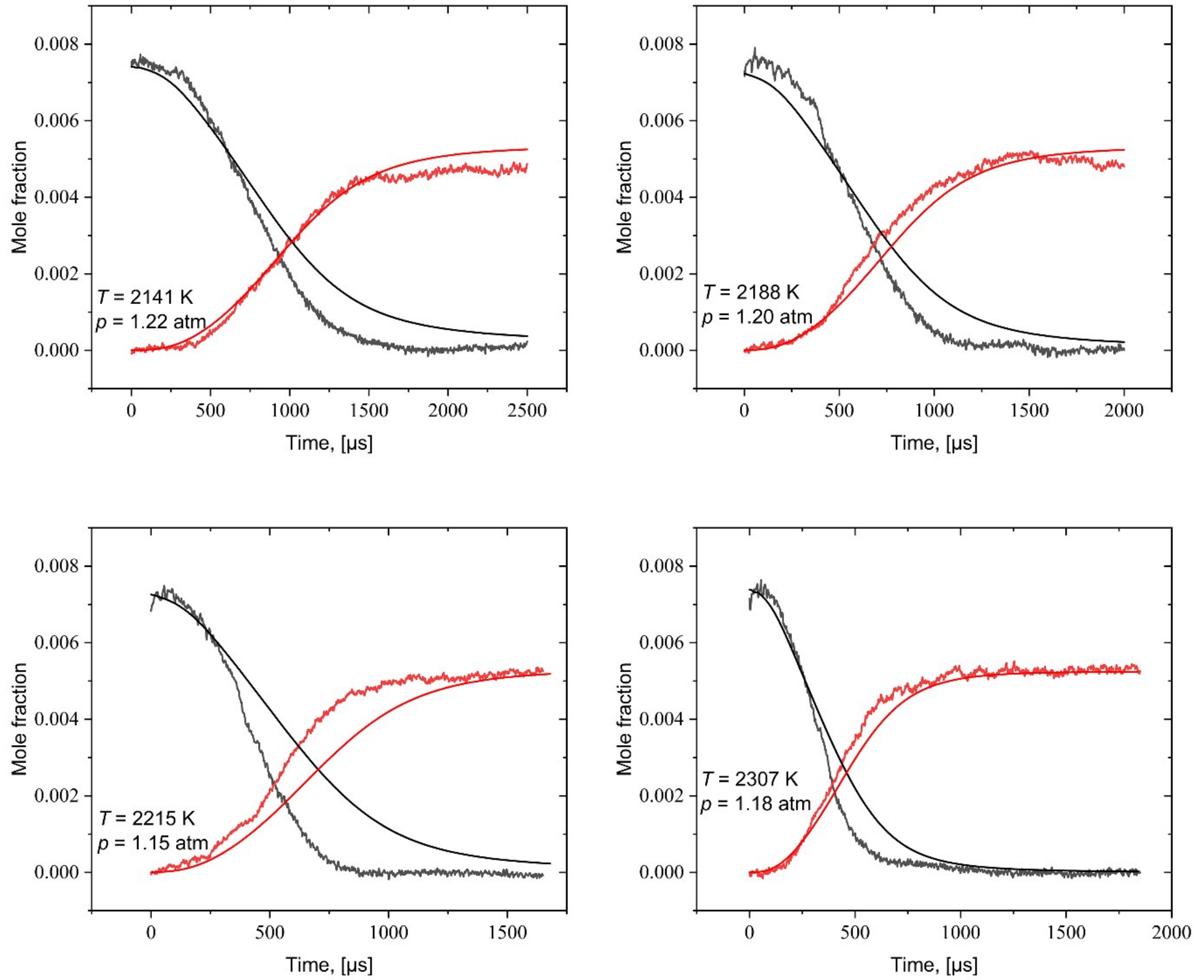
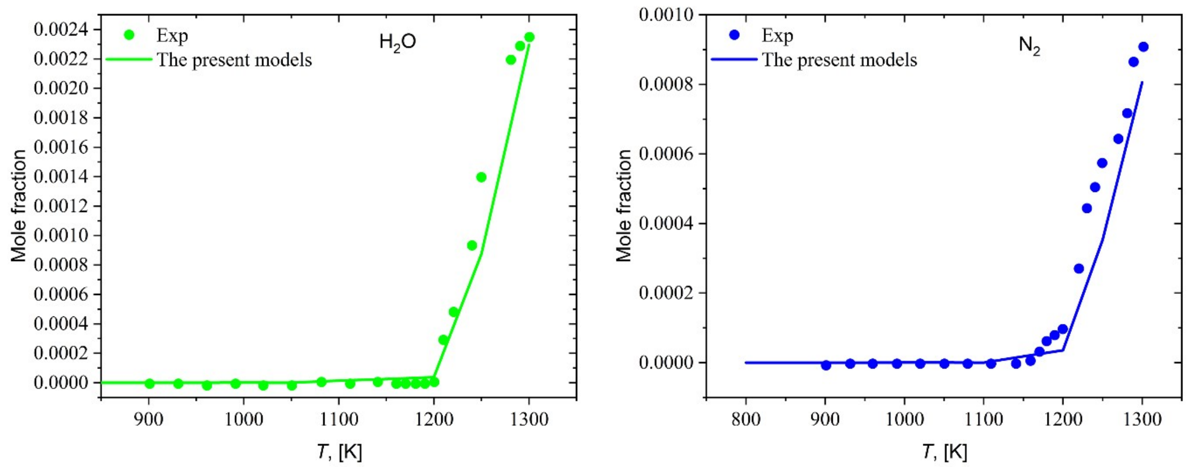


Fig. S16. NH_3 and H_2O speciation profiles in the oxidation of NH_3 in ~99% Ar. φ =2.03.

3.4 Osipova et al. [12]



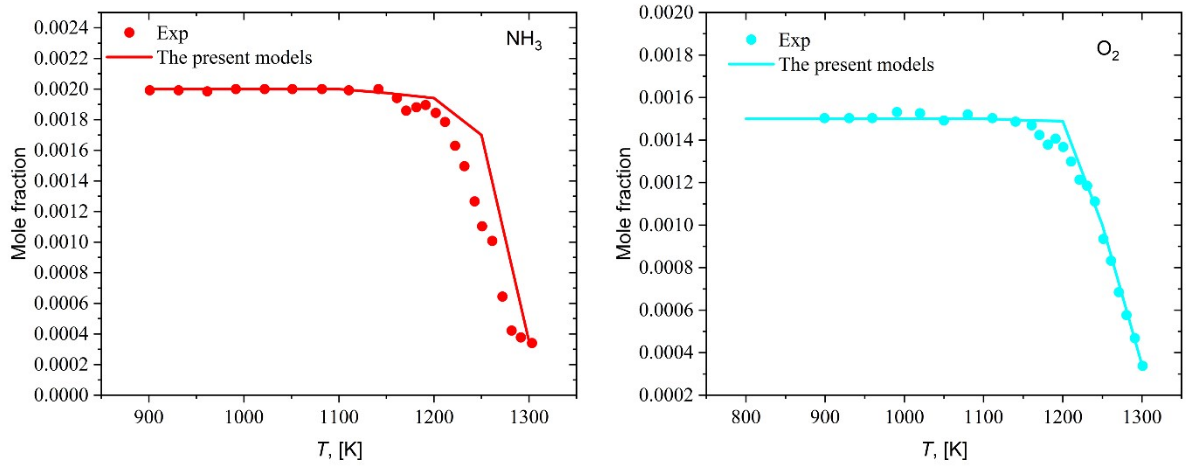
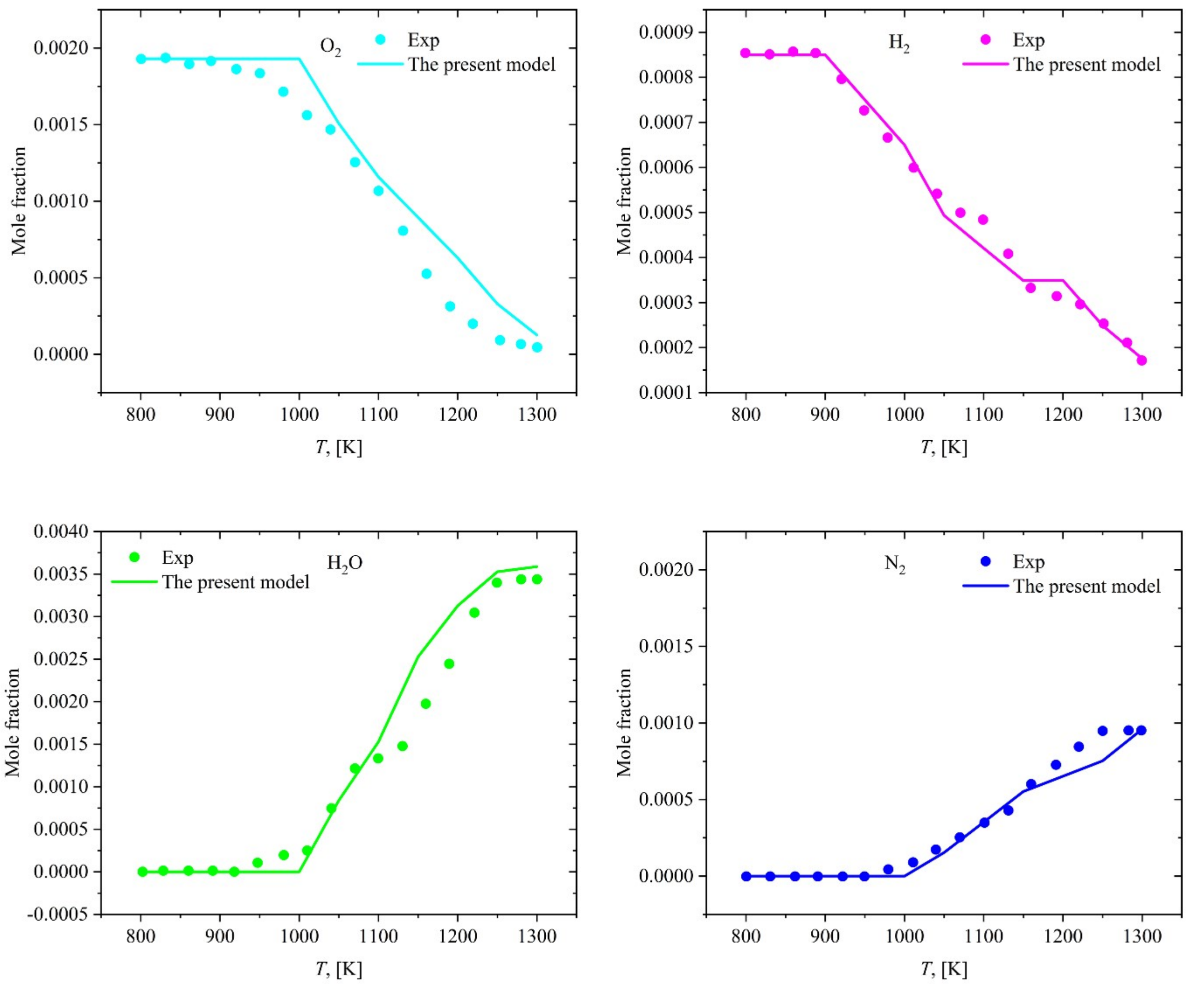


Fig. S17. Mole fraction profiles of reagents and main oxidation products in the stoichiometric $NH_3/O_2/Ar$ blend (p = 1 atm, T = 900–1300 K, τ = 1 s, NH_3 = 2000 ppm).



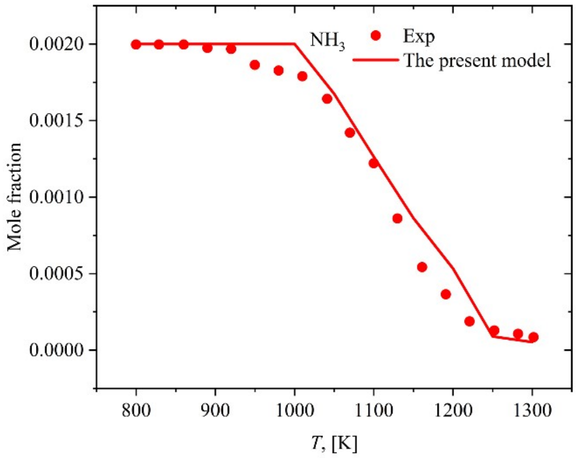


Fig. S18. Mole fractions profiles of reagents and main oxidation products in the stoichiometric $NH_3/H_2/O_2/Ar$ blend (p = 1 atm, T = 800–1300 K, τ = 1 s, NH_3 = 2000 ppm, NH_3/H_2 = 7/3 by volume).

References:

1 E. Hu, Z. Huang, J. He, C. Jin and J. Zheng, *International Journal of Hydrogen Energy*, 2009, **34**, 4876–4888.

2 M. C. Krejci, O. Mathieu, A. J. Vissotski, S. Ravi, T. G. Sikes, E. L. Petersen, W. Metcalfe, A. Keromnes and H. J. Curran, .

3 J. Beeckmann, R. Hesse, S. Kruse, A. Berens, N. Peters, H. Pitsch and M. Matalon, *Proceedings of the Combustion Institute*, 2017, **36**, 1531–1538.

4 K. P. Shrestha, C. Lhuillier, A. A. Barbosa, P. Brequigny, F. Contino, C. Mounaïm-Rousselle, L. Seidel and F. Mauss, *Proceedings of the Combustion Institute*, 2021, **38**, 2163–2174.

5 B. Mei, X. Zhang, S. Ma, M. Cui, H. Guo, Z. Cao and Y. Li, *Combustion and Flame*, 2019, **210**, 236–246.

6 C. Lhuillier, P. Brequigny, N. Lamoureux, F. Contino and C. Mounaïm-Rousselle, *Fuel*, 2020, **263**, 116653.

7 L. Dai, S. Gersen, P. Glarborg, H. Levinsky and A. Mokhov, *Combustion and Flame*, 2020, **215**, 134–144.

8 M. Pochet, V. Dias, B. Moreau, F. Foucher, H. Jeanmart and F. Contino, *Proceedings of the Combustion Institute*, 2019, **37**, 621–629.

9 A. Stagni, C. Cavallotti, S. Arunthanayothin, Y. Song, O. Herbinet, F. Battin-Leclerc and T. Faravelli, *React. Chem. Eng.*, 2020, **5**, 696–711.

10 S. A. Alturaifi, O. Mathieu and E. L. Petersen, *Combustion and Flame*, 2022, **235**, 111694.

11 S. A. Alturaifi, O. Mathieu and E. L. Petersen, *Proceedings of the Combustion Institute*, 2023, **39**, 233–241.

12 K. N. Osipova, X. Zhang, S. M. Sarathy, O. P. Korobeinichev and A. G. Shmakov, *Fuel*, 2022, **310**, 122202.