Supplementary material for International Journal of Hydrogen Energy

Supplementary material:

"Chemical kinetic modeling of ammonia oxidation with improved reaction mechanism for ammonia/air and ammonia/hydrogen/air combustion"

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In Fig. S1, laminar flame speed was plotted as a function of fuel-air equivalence ratio using previous experimental [19, 48–51] and numerical calculation values [18, 21, 37, 40, 52, 53] in previous studies. The relevant references are listed in the main text. The fuel-air equivalence ratio was defined by overall of reaction, $NH_3 + 3/4O_2 \rightarrow 1/2N_2 + 3/2H_2O$.

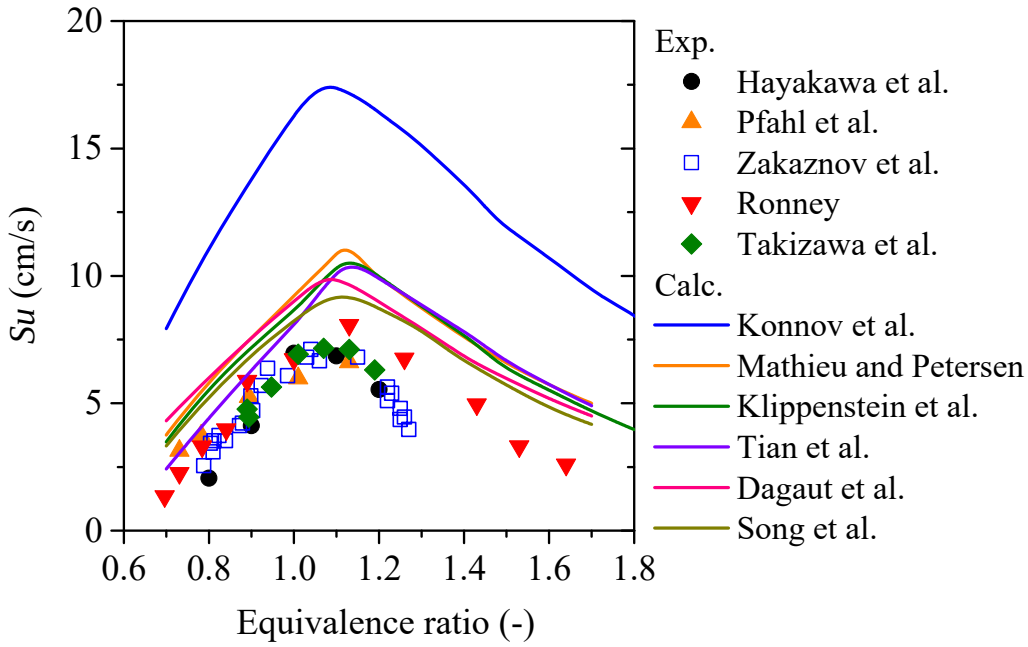

Fig. S1. Laminar flame speed *vs.* equivalence ratio at atmospheric pressure.

In Fig. S2, we also compared the shock tube ignition delay times of experimental value (Mathieu and Petersen [18]) and calculated values (Song et.al [40], Tian et.al [21], Dagaut [52], Klippenstein [53], and Mathieu and Petersen [18]).

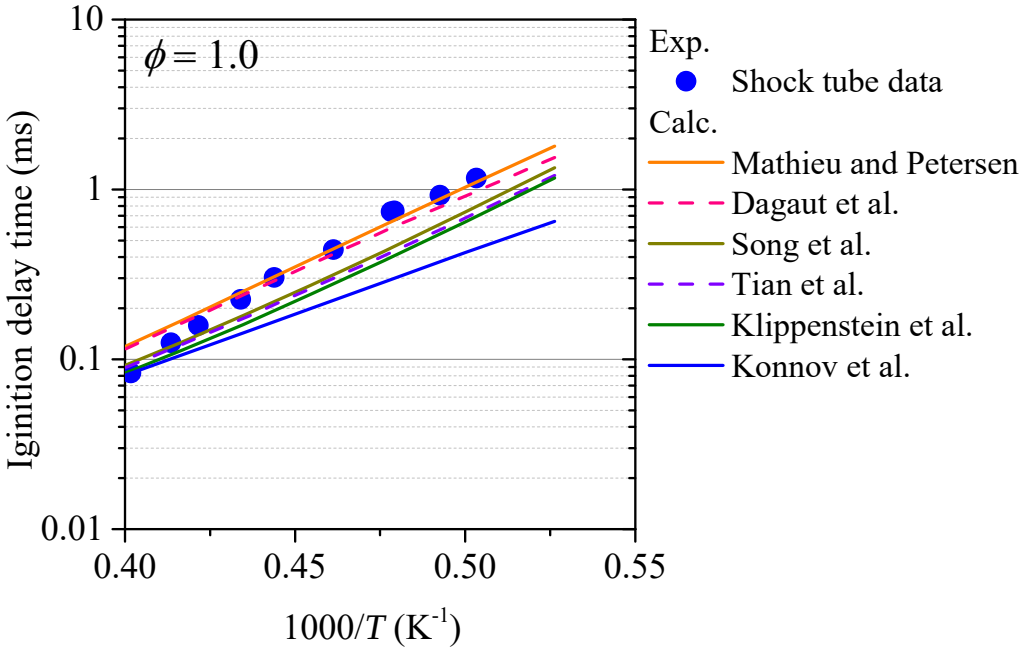

Fig. S2. Shock tube ignition delay time *vs.* equivalence ratio at atmospheric pressure.

Table S1 shows the sensitivity coefficients of laminar flame speed in ammonia combustion with equivalence ratio of 1.1 at 1 atm using the model reported in ref. [S1] (ref. [40] in the main text).

Table S1. Sensitivity coefficients (S_j) of laminar flame speed.

1. H+O2=O+OH	0.5279
3. O+H2=OH+H	0.0382
4. OH+H2=H+H2O	0.0305
5. OH+OH=O+H2O	0.0360
33. NH2+H=NH+H2	-0.0762
34. NH2+O=HNO+H	-0.0662
49. NH2+NO=N2+H2O	-0.0588
50. NH2+NO=N2+H2O	0.0285
51. NH2+NO=NNH+OH	0.0883
116. NO+H(+M)=HNO(+M)	0.0640
117. HNO+H=NO+H2	-0.0616
154. N2O(+M)=N2+O(+M)	0.0281
164. NH2+NH=N2H2+H	0.0627
173. N2H3=N2H2+H	-0.0441
186. N2H2+M=NNH+H+M	0.0820

Ref. [S1] (ref.40 in the main text) Y. Song, H. Hashemi, J. M. Christensen, C. Zou, P. Marshall, P. Glaborg, "Ammonia oxidation at high pressure and intermediate temperatures", Fuel, 181, 358-365, 2016.
(32 species, 204 reactions)

The sensitivity analysis for temperature has been performed. An example is shown in Fig. S3. Reactions (1) $NH_2 + H = NH + H_2$, (7) $NH_2 + NH = N_2H_2 + H$, (9) $N_2H_2 = NNH + H$, and (11) $NH + H = N + H_2$ in Table 1 (see main text) are sensitive to temperature.

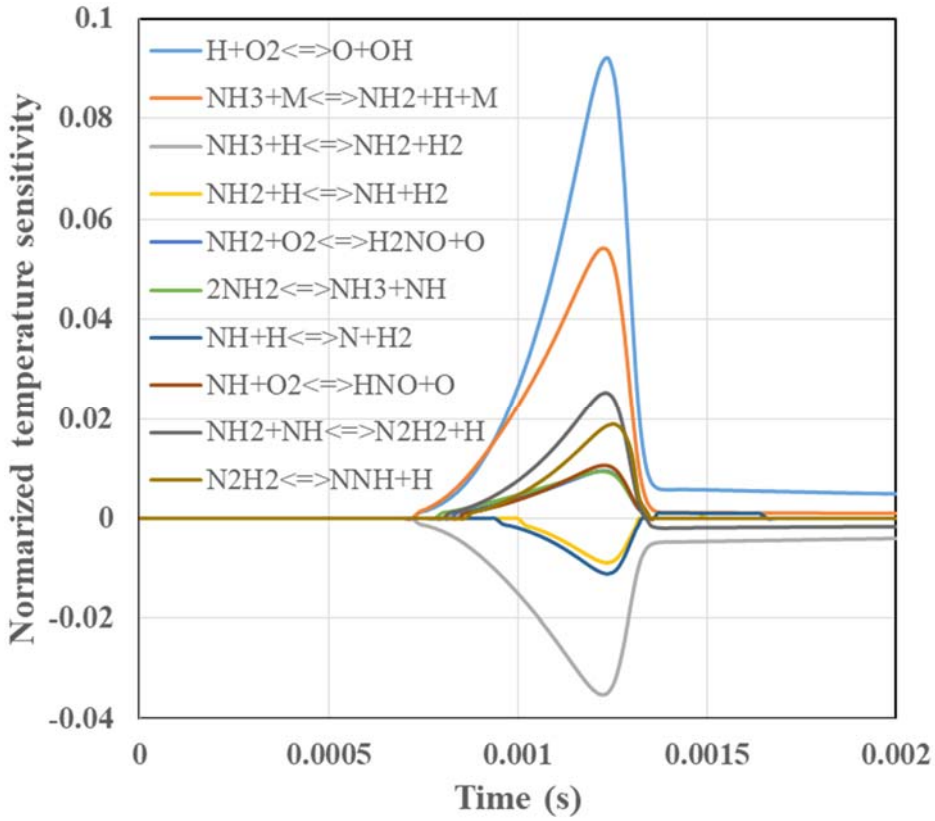

Fig. S3. Normalized temperature sensitivity.
T_0 = 2000 K, P_0=1.4 atm, $NH_3/O_2/Ar$ = 0.00572/0.00429/0.99 (ϕ = 1).

Simulations of atmospheric stagnation flame structures were performed, based on the experimental work of Brackmann et al. [46]. Experimental temperature profiles are included in the simulations, and (a) NH, (b) OH, and (c) NO profiles are compared (Fig. S4).

(a) NH

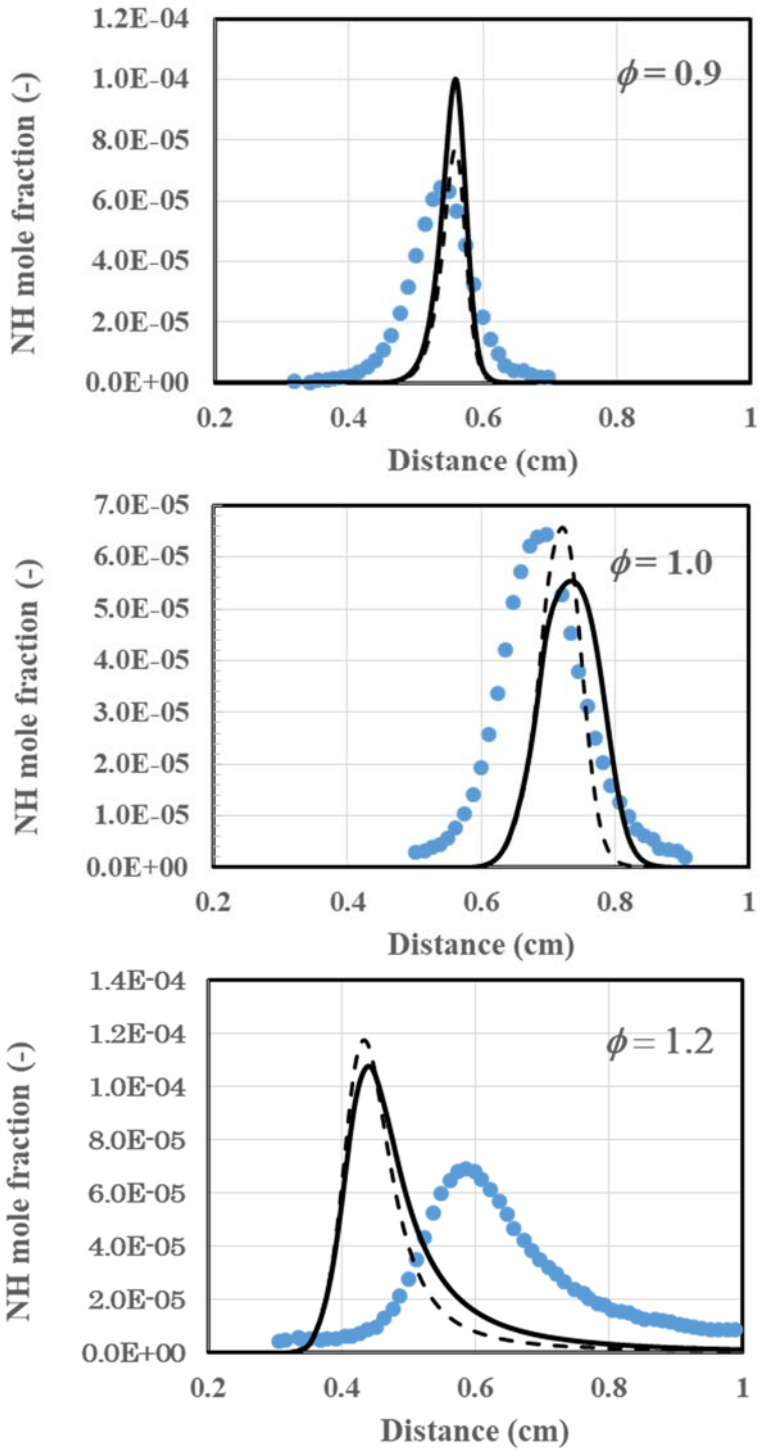

Fig. S4. (a) NH mole fraction profiles. Filled circle: experimental value [46], solid line: UT-LCS model, broken line: base model (Song et al., [40]).

(b) OH

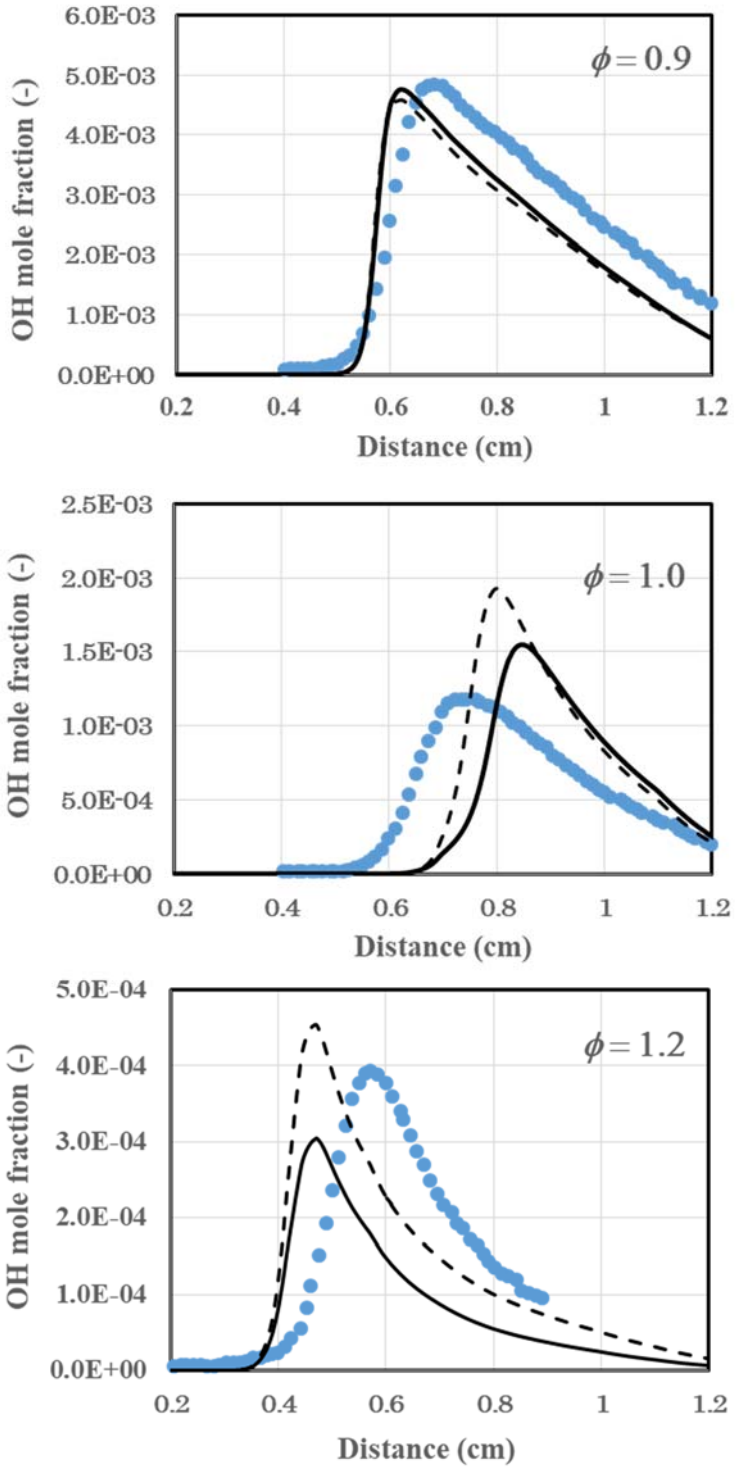

Fig. S4. (b) OH mole fraction profiles. Filled circle: experimental value [46], solid line: UT-LCS model, broken line: base model (Song et al., [40]).

(c) NO

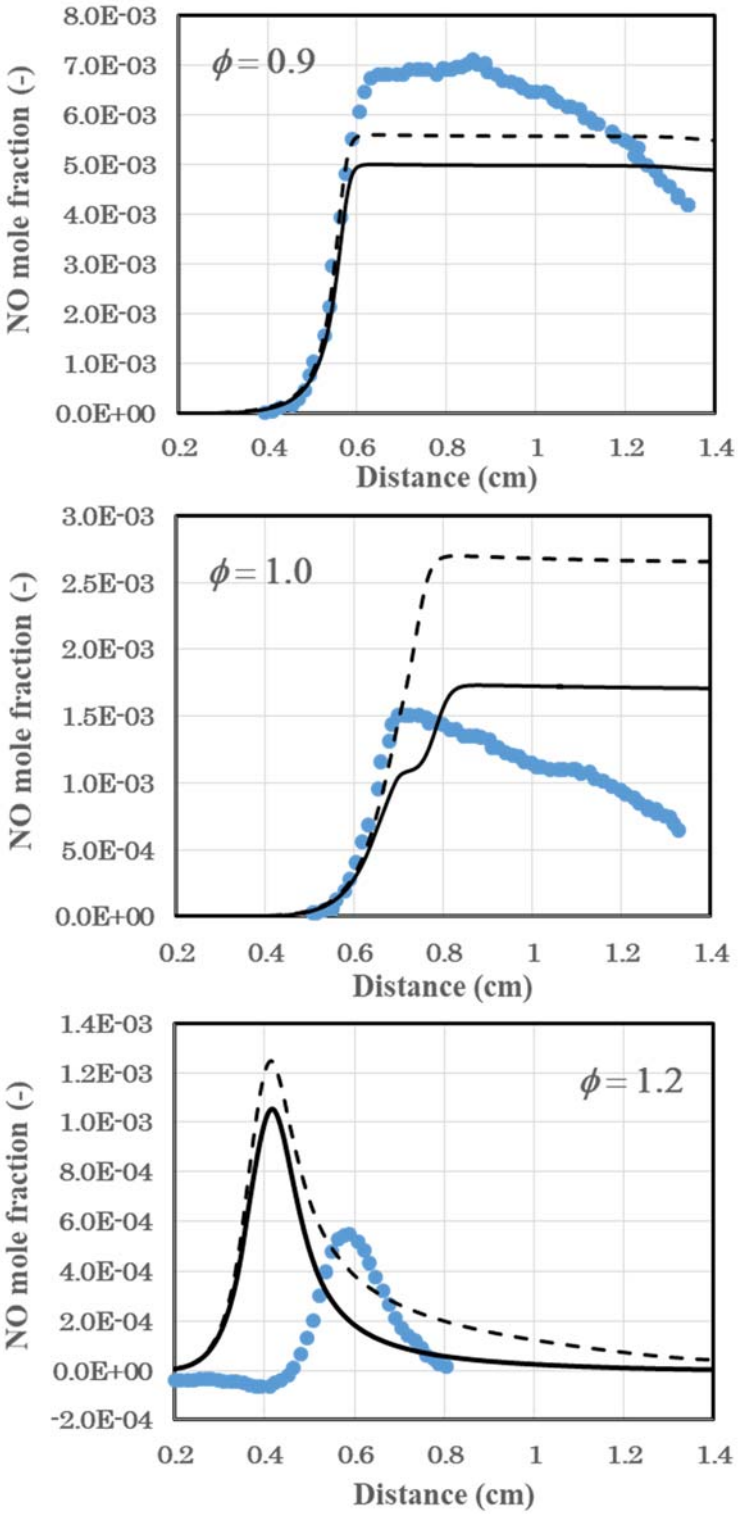

Fig. S4. (c) NO mole fraction profiles. Filled circle: experimental value [46], solid line: UT-LCS model, broken line: base model (Song et al., [40]).