THE JOURNAL OF Ammonia Energy

Cardiff University Press | Gwasg Prifysgol Caerdydd

2nd Symposium on Ammonia Energy

A Kinetic Modelling Study for Estimating Residual NH_3 Speciation at the Combustion Outlet in 70/30 vol% NH_3/H_2 Flames

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Topic: Reaction Modelling

Introduction

The development of new combustion systems for energy conversion is crucial due to recent constraints [1]. Global warming has highlighted the need for decarbonized fuels with zero carbon emissions. Hydrogen (H_2) and ammonia (NH_3) have emerged as promising alternatives, but their combustion characteristics, such as laminar flame speed, ignition delay times, and pollutant formation (e.g. NOx) must be understood. Kinetic reaction mechanisms are essential to comprehensively study the combustion chemistry of these fuels, including the breakdown of fuel molecules, formation of intermediate species, and production of combustion products like nitrogen and water when NH_3 is used as fuel.

Accurate speciation measurements of NH_3 and H_2 in the combustion system are of great importance as they directly impact combustion performance by providing crucial radicals that either accelerate or decelerate the combustion process. Ensuring a low level of residual NH_3 at the combustion exit is a crucial requirement to consider in the development of new combustion systems. A study conducted by Hayakawa et al. [2] determined that the optimal equivalence ratio for achieving a simultaneous reduction in unburned ammonia and NOx at the combustor exit is 1.2. Furthermore, when dealing with the fuel blend 70/30 vol% NH_3/H_2 in air, the ratio of final to initial mole fractions of $NH_3$is high, but this ratio decreases with increasing H_2 concentration [3]. Consequently, the primary objective of the present study is to analyse the performance of 70 different kinetic reaction mechanisms in estimating the mole fraction of unburned NH_3 at the combustion exit. Moreover, the study aims to identify the most accurate and reliable model by employing the symmetric mean absolute percentage error (SMAPE) formula as a quantitative metric. This evaluation will be conducted across various equivalence ratios (ϕ) to encompass a comprehensive range of operating conditions.

Kinetic modelling

In this study, 70 kinetic reaction mechanisms sourced from the literature were analyzed under atmospheric conditions to assess their performance in predicting the mole fraction of unburned NH_3 for a volumetric fuel mixture consisting of 70% NH_3 and 30% H_2 (Table 1). To conduct these analyses, a burner-stabilized stagnation flame model provided by ANSYS Chemkin-PRO 2022 R2 software was utilized. All numerical simulations were implemented in a one-dimensional computational model with a length of 2 cm, which closely mimicked the experimental setup used in previous studies (specifically, the distance between the nozzle burner and the top plate). Experimental measurements for validation purposes were obtained from [2], where identical fuel mixtures and operating conditions were employed. A stagnation flame configuration was chosen in the experimental setup to ensure accurate measurements and avoid issues with flame stabilization. To quantitatively determine the most accurate model that could faithfully reproduce the experimental measurements, a symmetric mean absolute percentage error (SMAPE) formula was employed as a metric. This formula allowed for a comprehensive evaluation of the models' performance and facilitated the identification of the model with the highest accuracy in predicting the mole fraction of unburned NH_3.

2nd symposium on AMMONIA ENERGY 11/13 July 2023 - Université d'Orléans | France

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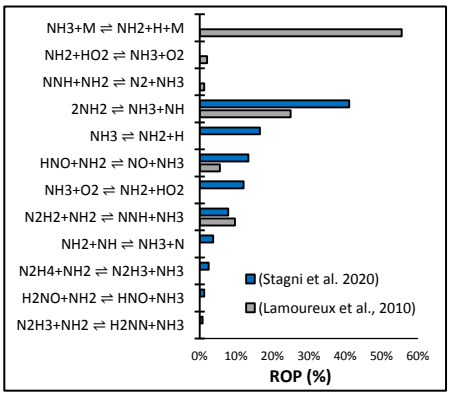
Table 1: Kinetic reaction mechanisms adopted in the present study.

NO.	Kinetic mechanism	No. of Reactions	No. of species	Ref	NO.	Kinetic mechanism	No. of Reactions	No. of species	Ref
1	(Bertolino et al., 2021)	264	38	[4]	36	(Dagaut et al., 2008)	250	41	[5]
2	(Mei, Ma, et al., 2021)	264	38	[6]	37	(Gregory P. Smith et al., 2000)	325	53	[7]
3	(Han et al., 2021)	298	36	[8]	38	(Coda Zabetta & Hupa, 2008)	371	60	[9]
4	(Mei, Zhang, et al., 2021)	257	40	[10]	39	(Alzueta MU, 2016)	654	131	[11]
5	(Gotama et al., 2022)	119	26	[12]	40	(Shmakov et al., 2010)	1207	127	[13]
6	(Shrestha et al., 2021)	1099	125	[14]	41	(Esarte et al., 2011)	536	79	[15]
7	(Z. Wang et al., 2021)	444	91	[16]	42	(Abian et al., 2015)	201	31	[17]
8	(X. Zhang et al., 2021)	263	38	[18]	43	(T. Wang et al., 2018)	925	81	[19]
9	(Arunthanayothin et al., 2021)	2444	157	[20]	44	(T. Faravelli, 2017)	158	29	[21]
10	(Stagni et al., 2020)	203	31	[22]	45	(POLIMI, 2014)	155	29	[23]
11	(Han et al., 2019)	177	35	[24]	46	(Marques et al., 2073)	318	61	[25]
12	(De Persis et al., 2020)	647	103	[26]	47	(Aranda et al., 2013)	566	95	[27]
13	(Mei et al., 2019)	265	38	[28]	48	(Jiang et al., 2020)	60	19	[29]
14	(Li et al., 2019)	957	128	[30]	49	(Sun et al., 2022)	486	66	[31]
15	(Okafor et al., 2019)	356	59	[32]	50	(Song et al., 2019)	158	29	[33]
16	(Glarborg et al., 2018)	231	39	[34]	51	(Mével et al., 2009)	203	32	[35]
17	(Shrestha et al., 2018)	1081	124	[36]	52	(Da Rocha-Mathiue et al., 2019)	66	22	[37]
18	(Otomo et al., 2018)	213	32	[3]	53	(Da Rocha-Otomoet al., 2019)	51	21	[37]
19	(U. Mechanism, 2018)	41	20	[38]	54	(Da Rocha-Okafor et al., 2019)	70	24	[37]
20	(Klippenstein et al., 2018)	211	33	[39]	55	(Kovaleva et al., 2022)	354	59	[40]
21	(Nakamura et al., 2017)	232	33	[41]	56	(Houshfar et al., 2012) Midd temp	91	26	[42]
22	(Y. Zhang et al., 2017)	251	44	[43]	57	(Houshfar et al., 2012) High temp	430	52	[42]
23	(Lamoureux et al., 2016)	934	123	[44]	58	(Houshfar et al., 2012) Low temp	198	35	[42]
24	(Xiao et al., 2017)	276	55	[45]	59	(Capriolo et al., 2021)	2300	201	[46]
25	(Song et al., 2016)	204	32	[47]	60	(Xu et al., 2023)	389	69	[48]
26	(Nozari & Karabeyoğlu, 2015)	91	21	[49]	61	(Thomas et al., 2022)	1099	125	[50]
27	(Mathieu & Petersen, 2015)	278	54	[51]	62	(Kovács et al., 2020)	214	34	[52]
28	(Duynslaegher et al., 2012)	80	19	[53]	63	(Kovács et al., 2021)	537	70	[54]
29	(Klippenstein et al., 2011)	202	31	[55]	64	(Saxena & Williams, 2007)	288	59	[56]
30	(K. Zhang et al., 2011)	701	88	[57]	65	(Valkó et al., 2022)	537	70	[58]
31	(Lamoureux et al., 2010)	883	119	[59]	66	(Alzueta et al., 2001)	464	65	[60]
32	(Konnov, 2009)	1207	127	[61]	67	(Nakamura & Shindo, 2019)	485	66	[62]
33	(Mendiara & Glarborg, 2009)	779	79	[63]	68	(Glarborg, 2022)	270	41	[64]
34	(Tian et al., 2009)	703	84	[65]	69	(Tang et al. 2022)	211	35	[66]
35	(Singh et al. 2022)	259	32	[67]	70	(Marshall et al. 2023)	228	34	[68]

Results and Discussions

The primary findings of the SMAPE investigations reveal that the performance of the Lamoureux et al. mechanism [59] is satisfactory, displaying an error estimation range of 4% to 7% when considering the ϕ values between 1 and 1.2. However, its accuracy diminishes when estimating the mole fraction of NH_3 at ϕ of 1.4, resulting in underestimation. In contrast, the Stagni et al. mechanism [22] proves to be more precise in predicting the mole fraction of unburned NH_3 under highly rich conditions (ϕ=1.4).



The conducted sensitivity analysis underscores the significance of specific reaction steps, such as NH+O ⇌ NO+H, NH_3+M ⇌ NH_2+H+M, and NH+OH ⇌ HNO+H, in enhancing the reactivity of the system by facilitating the production of crucial radicals, notably H, which play a vital role in sustaining the reaction process. Moreover, the reaction flow analysis highlights the importance of reactions including HNO+NH_2 ⇌ NO+NH_3, 2NH_2 ⇌ NH_3+NH, and NH_3+M ⇌ NH_2+H+M, as they contribute significantly to the formation of NH_3, Fig.1. Notably, the reactivity of reaction steps 2NH_2 ⇌ NH_3+N and NH_3+M ⇌ NH_2+H+M demonstrates an increase with higher ϕ values, while reaction HNO+NH_2 ⇌ NO+NH_3 exhibits a decrease. Furthermore, the consumption of NH_3 is predominantly governed by reaction steps NH_3+OH ⇌ NH_2+H_2O, NH_3+H ⇌ NH_2+H_2, and NH_3+O ⇌ NH_2+OH, which are the reactions of NH_3 with the most reactive radicals such as OH, H, and O, Fig.2. These reactions heavily influence the depletion of NH_3 within the system.

Fig. 1. Rate of formation of NH_3 at ϕ =1.4

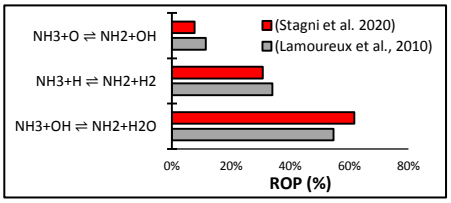


Fig. 2. Rate of consumption of NH_3 at ϕ =1.4

Conclusions

This study investigated 70 kinetic reaction models to assess their accuracy in reproducing NH_3 speciation at the combustion exit zone. Differences in reaction steps and rate parameters were observed among the tested mechanisms. The Lamoureux model provided reliable estimates of unburned NH_3 within the ϕ range of 1-1.2, but its accuracy declined near 1.4. NH_3 was primarily converted to NH_2 radicals through OH reactions across all temperatures, with secondary involvement of O radicals at low-intermediate temperatures. NH_3 dehydrogenation also occurred via H radicals through the NH_3+H ⇌ NH_2+H_2 reaction at higher temperatures. Additionally, NH_3 regeneration at the combustion exit was predominantly driven by the NH_3 ⇌ NH_2+H reaction at T=504 K.

References

[1] Paris Agreement, Https://Climate.Ec.Europa.Eu/Index_en. [accessed 18 May 2023].
[2] A. Hayakawa, M. Hayashi, M. Kovaleva, G.J. Gotama, E.C. Okafor, S. Colson, S. Mashruk, A. Valera-Medina, T. Kudo, H. Kobayashi, Experimental and numerical study of product gas and N2O emission characteristics of ammonia/hydrogen/air premixed laminar flames stabilized in a stagnation flow, Proceedings of the Combustion Institute. (2022). https://doi.org/10.1016/j.proci.2022.08.124.
[3] J. Otomo, M. Koshi, T. Mitsumori, H. Iwasaki, K. Yamada, Chemical kinetic modeling of ammonia oxidation with improved reaction mechanism for ammonia/air and ammonia/hydrogen/air combustion, Int J Hydrogen Energy. 43 (2018) 3004–3014. https://doi.org/10.1016/j.ijhydene.2017.12.066.
[4] A. Bertolino, M. Fürst, A. Stagni, A. Frassoldati, M. Pelucchi, C. Cavallotti, T. Faravelli, A. Parente, An evolutionary, data-driven approach for mechanism optimization: theory and application to ammonia combustion, Combust Flame. 229 (2021). https://doi.org/10.1016/j.combustflame.2021.02.012.
[5] P. Dagaut, P. Glarborg, M.U. Alzueta, The oxidation of hydrogen cyanide and related chemistry, Prog Energy Combust Sci. 34 (2008) 1–46. https://doi.org/10.1016/j.pecs.2007.02.004.
[6] B. Mei, S. Ma, X. Zhang, Y. Li, Characterizing ammonia and nitric oxide interaction with outwardly propagating spherical flame method, Proceedings of the Combustion Institute. 38 (2021) 2477–2485. https://doi.org/10.1016/j.proci.2020.07.133.
[7] Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, V.V.L. Jr., Zhiwei Qin, GRI-Mech 3.0, Http://Www.Me.Berkeley.Edu/Gri_mech/. (2000).
[8] X. Han, L. Lavadera, A.A. Konnov, An experimental and kinetic modeling study on the laminar burning velocity of NH3+N2O+air flames, Combust Flame. 228 (2021) 13–28. https://doi.org/10.1016/j.combustflame.2021.01.027.
[9] E. Coda Zabetta, M. Hupa, A detailed kinetic mechanism including methanol and nitrogen pollutants relevant to the gas-phase combustion and pyrolysis of biomass-derived fuels, Combust Flame. 152 (2008) 14–27. https://doi.org/10.1016/j.combustflame.2007.06.022.

[10] B. Mei, J. Zhang, X. Shi, Z. Xi, Y. Li, Enhancement of ammonia combustion with partial fuel cracking strategy: Laminar flame propagation and kinetic modeling investigation of NH3/H2/N2/air mixtures up to 10 atm, Combust Flame. 231 (2021). https://doi.org/10.1016/j.combustflame.2021.111472.
[11] Alzueta MU, Zaragoza-2016 Mechanism , Personal Communication. (2016).
[12] G.J. Gotama, A. Hayakawa, E.C. Okafor, R. Kanoshima, M. Hayashi, T. Kudo, H. Kobayashi, Measurement of the laminar burning velocity and kinetics study of the importance of the hydrogen recovery mechanism of ammonia/hydrogen/air premixed flames, Combust Flame. 236 (2022). https://doi.org/10.1016/j.combustflame.2021.111753.
[13] A.G. Shmakov, O.P. Korobeinichev, I. v. Rybitskaya, A.A. Chernov, D.A. Knyazkov, T.A. Bolshova, A.A. Konnov, Formation and consumption of NO in H2 + O2 + N2 flames doped with NO or NH3 at atmospheric pressure, Combust Flame. 157 (2010) 556–565. https://doi.org/10.1016/j.combustflame.2009.10.008.
[14] K.P. Shrestha, C. Lhuillier, A.A. Barbosa, P. Brequigny, F. Contino, C. Mounaïm-Rousselle, L. Seidel, F. Mauss, An experimental and modeling study of ammonia with enriched oxygen content and ammonia/hydrogen laminar flame speed at elevated pressure and temperature, Proceedings of the Combustion Institute. 38 (2021) 2163–2174. https://doi.org/10.1016/j.proci.2020.06.197.
[15] C. Esarte, M. Peg, M.P. Ruiz, Á. Millera, R. Bilbao, M.U. Alzueta, Pyrolysis of ethanol: Gas and soot products formed, Ind Eng Chem Res. 50 (2011) 4412–4419. https://doi.org/10.1021/ie1022628.
[16] Z. Wang, X. Han, Y. He, R. Zhu, Y. Zhu, Z. Zhou, K. Cen, Experimental and kinetic study on the laminar burning velocities of NH3 mixing with CH3OH and C2H5OH in premixed flames, Combust Flame. 229 (2021). https://doi.org/10.1016/j.combustflame.2021.02.038.
[17] M. Abian, M.U. Alzueta, P. Glarborg, Formation of NO from N2/O2 mixtures in a flow reactor: Toward an accurate prediction of thermal NO, Int J Chem Kinet. 47 (2015) 518–532. https://doi.org/10.1002/kin.20929.
[18] X. Zhang, S.P. Moosakutty, R.P. Rajan, M. Younes, S.M. Sarathy, Combustion chemistry of ammonia/hydrogen mixtures: Jet-stirred reactor measurements and comprehensive kinetic modeling, Combust Flame. 234 (2021). https://doi.org/10.1016/j.combustflame.2021.111653.
[19] T. Wang, X. Zhang, J. Zhang, X. Hou, Automatic generation of a kinetic skeletal mechanism for methane-hydrogen blends with nitrogen chemistry, Int J Hydrogen Energy. 43 (2018) 3330–3341. https://doi.org/10.1016/j.ijhydene.2017.12.116.
[20] S. Arunthanayothin, A. Stagni, Y. Song, O. Herbinet, T. Faravelli, F. Battin-Leclerc, Ammonia-methane interaction in jet-stirred and flow reactors: An experimental and kinetic modeling study, in: Proceedings of the Combustion Institute, Elsevier Ltd, 2021: pp. 345–353. https://doi.org/10.1016/j.proci.2020.07.061.
[21] T. Faravelli, POLIMI-2017, Personal Communication. (2017).
[22] A. Stagni, C. Cavallotti, S. Arunthanayothin, Y. Song, O. Herbinet, F. Battin-Leclerc, T. Faravelli, An experimental, theoretical and kinetic-modeling study of the gas-phase oxidation of ammonia, React Chem Eng. 5 (2020) 696–711. https://doi.org/10.1039/c9re00429g.
[23] POLIMI, The CRECK Modeling Group,C1-C3 mechanism , Http://Creckmodeling.Chem.Polimi.It. (2014).
[24] X. Han, Z. Wang, M. Costa, Z. Sun, Y. He, K. Cen, Experimental and kinetic modeling study of laminar burning velocities of NH3/air, NH3/H2/air, NH3/CO/air and NH3/CH4/air premixed flames, Combust Flame. 206 (2019) 214–226. https://doi.org/10.1016/j.combustflame.2019.05.003.
[25] C.S.T. Marques, L.R. dos Santos, M.E. Sbampato, L.G. Barreta, A.M. dos Santos, TEMPERATURE MEASUREMENTS BY OH LIF AND CHEMILUMINESCENCE KINETIC MODELING FOR ETHANOL FLAMES, 2073.
[26] S. de Persis, L. Pillier, M. Idir, J. Molet, N. Lamoureux, P. Desgroux, NO formation in high pressure premixed flames: Experimental results and validation of a new revised reaction mechanism, Fuel. 260 (2020). https://doi.org/10.1016/j.fuel.2019.116331.
[27] V. Aranda, J.M. Christensen, M.U. Alzueta, P. Glarborg, S. Gersen, Y. Gao, P. Marshall, Experimental and kinetic modeling study of methanol ignition and oxidation at high pressure, Int J Chem Kinet. 45 (2013) 283–294. https://doi.org/10.1002/kin.20764.
[28] B. Mei, X. Zhang, S. Ma, M. Cui, H. Guo, Z. Cao, Y. Li, Experimental and kinetic modeling investigation on the laminar flame propagation of ammonia under oxygen enrichment and elevated pressure conditions, Combust Flame. 210 (2019) 236–246. https://doi.org/10.1016/j.combustflame.2019.08.033.
[29] Y. Jiang, A. Gruber, K. Seshadri, F. Williams, An updated short chemical-kinetic nitrogen mechanism for carbon-free combustion applications, Int J Energy Res. 44 (2020) 795–810. https://doi.org/10.1002/er.4891.
[30] R. Li, A.A. Konnov, G. He, F. Qin, D. Zhang, Chemical mechanism development and reduction for combustion of NH3/H2/CH4 mixtures, Fuel. 257 (2019). https://doi.org/10.1016/j.fuel.2019.116059.
[31] J. Sun, Q. Yang, N. Zhao, M. Chen, H. Zheng, Numerically study of CH4/NH3 combustion characteristics in an industrial gas turbine combustor based on a reduced mechanism, Fuel. 327 (2022) 124897. https://doi.org/10.1016/J.FUEL.2022.124897.

[32] E.C. Okafor, Y. Naito, S. Colson, A. Ichikawa, T. Kudo, A. Hayakawa, H. Kobayashi, Measurement and modelling of the laminar burning velocity of methane-ammonia-air flames at high pressures using a reduced reaction mechanism, Combust Flame. 204 (2019) 162–175. https://doi.org/10.1016/j.combustflame.2019.03.008.

[33] Y. Song, L. Marrodán, N. Vin, O. Herbinet, E. Assaf, C. Fittschen, A. Stagni, T. Faravelli, M.U. Alzueta, F. Battin-Leclerc, The sensitizing effects of NO 2 and NO on methane low temperature oxidation in a jet stirred reactor, Proceedings of the Combustion Institute. 37 (2019) 667–675. https://doi.org/10.1016/j.proci.2018.06.115.

[34] P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Modeling nitrogen chemistry in combustion, Prog Energy Combust Sci. 67 (2018) 31–68. https://doi.org/10.1016/j.pecs.2018.01.002.

[35] R. Mével, S. Javoy, F. Lafosse, N. Chaumeix, G. Dupré, C.E. Paillard, Hydrogen–nitrous oxide delay times: Shock tube experimental study and kinetic modelling, Proceedings of the Combustion Institute. 32 (2009) 359–366. https://doi.org/10.1016/J.PROCI.2008.06.171.

[36] K.P. Shrestha, L. Seidel, T. Zeuch, F. Mauss, Detailed Kinetic Mechanism for the Oxidation of Ammonia Including the Formation and Reduction of Nitrogen Oxides, Energy and Fuels. 32 (2018) 10202–10217. https://doi.org/10.1021/acs.energyfuels.8b01056.

[37] R.C. da Rocha, M. Costa, X.S. Bai, Chemical kinetic modelling of ammonia/hydrogen/air ignition, premixed flame propagation and NO emission, Fuel. 246 (2019) 24–33. https://doi.org/10.1016/J.FUEL.2019.02.102.

[38] U. Mechanism, Chemical-kinetic mechanisms for combustion applications, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego. (2018).

[39] S.J. Klippenstein, M. Pfeifle, A.W. Jasper, P. Glarborg, Theory and modeling of relevance to prompt-NO formation at high pressure, Combust Flame. 195 (2018) 3–17. https://doi.org/10.1016/j.combustflame.2018.04.029.

[40] M. Kovaleva, A. Hayakawa, S. Colson, E.C. Okafor, T. Kudo, A. Valera-Medina, H. Kobayashi, Numerical and experimental study of product gas characteristics in premixed ammonia/methane/air laminar flames stabilised in a stagnation flow, Fuel Communications. 10 (2022) 100054. https://doi.org/10.1016/j.jfueco.2022.100054.

[41] H. Nakamura, S. Hasegawa, T. Tezuka, Kinetic modeling of ammonia/air weak flames in a micro flow reactor with a controlled temperature profile, Combust Flame. 185 (2017) 16–27. https://doi.org/10.1016/j.combustflame.2017.06.021.

[42] E. Houshfar, Ø. Skreiberg, P. Glarborg, T. Løvas, Reduced chemical kinetic mechanisms for NO x emission prediction in biomass combustion, Int J Chem Kinet. 44 (2012) 219–231. https://doi.org/10.1002/kin.20716.

[43] Y. Zhang, O. Mathieu, E.L. Petersen, G. Bourque, H.J. Curran, Assessing the predictions of a NOx kinetic mechanism on recent hydrogen and syngas experimental data, Combust Flame. 182 (2017) 122–141. https://doi.org/10.1016/j.combustflame.2017.03.019.

[44] N. Lamoureux, H. El Merhubi, L. Pillier, S. de Persis, P. Desgroux, Modeling of NO formation in low pressure premixed flames, Combust Flame. 163 (2016) 557–575. https://doi.org/10.1016/j.combustflame.2015.11.007.

[45] H. Xiao, A. Valera-Medina, P.J. Bowen, Modeling Combustion of Ammonia/Hydrogen Fuel Blends under Gas Turbine Conditions, Energy and Fuels. 31 (2017) 8631–8642. https://doi.org/10.1021/acs.energyfuels.7b00709.

[46] G. Capriolo, C. Brackmann, M. Lubrano Lavadera, T. Methling, A.A. Konnov, An experimental and kinetic modeling study on nitric oxide formation in premixed C3alcohols flames, in: Proceedings of the Combustion Institute, Elsevier Ltd, 2021: pp. 805–812. https://doi.org/10.1016/j.proci.2020.07.051.

[47] Y. Song, H. Hashemi, J.M. Christensen, C. Zou, P. Marshall, P. Glarborg, Ammonia oxidation at high pressure and intermediate temperatures, Fuel. 181 (2016) 358–365. https://doi.org/10.1016/j.fuel.2016.04.100.

[48] L. Xu, Y. Chang, M. Treacy, Y. Zhou, M. Jia, X.S. Bai, A skeletal chemical kinetic mechanism for ammonia/n-heptane combustion, Fuel. 331 (2023). https://doi.org/10.1016/j.fuel.2022.125830.

[49] H. Nozari, A. Karabeyoğlu, Numerical study of combustion characteristics of ammonia as a renewable fuel and establishment of reduced reaction mechanisms, Fuel. 159 (2015) 223–233. https://doi.org/10.1016/j.fuel.2015.06.075.

[50] D.E. Thomas, K.P. Shrestha, F. Mauss, W.F. Northrop, ARTICLE IN PRESS Extinction and NO formation of ammonia-hydrogen and air non-premixed counterflow flames, Proceedings of the Combustion Institute. (2022). https://doi.org/10.1016/j.proci.2022.08.067.

[51] O. Mathieu, E.L. Petersen, Experimental and modeling study on the high-temperature oxidation of Ammonia and related NOx chemistry, Combust Flame. 162 (2015) 554–570. https://doi.org/10.1016/j.combustflame.2014.08.022.

[52] M. Kovács, M. Papp, I.G. Zsély, T. Turányi, Determination of rate parameters of key N/H/O elementary reactions based on H2/O2/NOx combustion experiments, Fuel. 264 (2020) 116720. https://doi.org/10.1016/J.FUEL.2019.116720.

[53] C. Duynslaegher, F. Contino, J. Vandooren, H. Jeanmart, Modeling of ammonia combustion at low pressure, Combust Flame. 159 (2012) 2799–2805. https://doi.org/10.1016/j.combustflame.2012.06.003.

[54] M. Kovács Máté Papp István Gy Zsély Tamás Turányi, Main sources of uncertainty in recent methanol/NOx combustion models, Int J Chem Kinet. 53 (2021) 884–900. https://doi.org/10.1002/kin.21490.

[55] S.J. Klippenstein, L.B. Harding, P. Glarborg, J.A. Miller, The role of NNH in NO formation and control, Combust Flame. 158 (2011) 774–789. https://doi.org/10.1016/j.combustflame.2010.12.013.

[56] P. Saxena, F.A. Williams, Numerical and experimental studies of ethanol flames, Proceedings of the Combustion Institute. 31 I (2007) 1149–1156. https://doi.org/10.1016/j.proci.2006.08.097.

[57] K. Zhang, Y. Li, T. Yuan, J. Cai, P. Glarborg, F. Qi, An experimental and kinetic modeling study of premixed nitromethane flames at low pressure, Proceedings of the Combustion Institute. 33 (2011) 407–414. https://doi.org/10.1016/j.proci.2010.06.002.

[58] É. Valkó, M. Papp, M. Kovács, T. Varga, I. Gy Zsély, T. Nagy, T. Turányi, Combustion Theory and Modelling ISSN: (Print) (Design of combustion experiments using differential entropy Design of combustion experiments using differential entropy, Combustion Theory and Modelling. 26 (2022) 67–90. https://doi.org/10.1080/13647830.2021.1992506.

[59] N. Lamoureux, P. Desgroux, A. El Bakali, J.F. Pauwels, Experimental and numerical study of the role of NCN in prompt-NO formation in low-pressure CH4-O2-N2 and C2H2-O2-N2 flames, Combust Flame. 157 (2010) 1929–1941. https://doi.org/10.1016/j.combustflame.2010.03.013.

[60] M.U. Alzueta, R. Bilbao, M. Finestra, Methanol oxidation and its interaction with nitric oxide, Energy and Fuels. 15 (2001) 724–729. https://doi.org/10.1021/ef0002602.

[61] A.A. Konnov, Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism, Combust Flame. 156 (2009) 2093–2105. https://doi.org/10.1016/j.combustflame.2009.03.016.

[62] H. Nakamura, M. Shindo, Effects of radiation heat loss on laminar premixed ammonia/air flames, Proceedings of the Combustion Institute. 37 (2019) 1741–1748. https://doi.org/10.1016/j.proci.2018.06.138.

[63] T. Mendiara, P. Glarborg, Ammonia chemistry in oxy-fuel combustion of methane, Combust Flame. 156 (2009) 1937–1949. https://doi.org/10.1016/j.combustflame.2009.07.006.

[64] P. Glarborg, The NH3/NO2/O2 system: Constraining key steps in ammonia ignition and N2O formation, Combust Flame. (2022). https://doi.org/10.1016/j.combustflame.2022.112311.

[65] Z. Tian, Y. Li, L. Zhang, P. Glarborg, F. Qi, An experimental and kinetic modeling study of premixed NH3/CH4/O2/Ar flames at low pressure, Combust Flame. 156 (2009) 1413–1426. https://doi.org/10.1016/j.combustflame.2009.03.005.

[66] R. Tang, Q. Xu, J. Pan, J. Gao, Z. Wang, H. Wei, G. Shu, An experimental and modeling study of ammonia oxidation in a jet stirred reactor, Combust Flame. 240 (2022). https://doi.org/10.1016/j.combustflame.2022.112007.

[67] A.S. Singh, S.K. Dash, V.M. Reddy, Chemical kinetic analysis on influence of hydrogen enrichment on the combustion characteristics of ammonia air using newly proposed reaction model, Int J Energy Res. 46 (2022) 6144–6163. https://doi.org/10.1002/er.7554.

[68] P. Marshall, P. Glarborg, Probing High-Temperature Amine Chemistry: Is the Reaction NH 3 + NH 2 ⇄ N 2 H 3 + H 2 Important? , J Phys Chem A. (2023). https://doi.org/10.1021/acs.jpca.2c08921.