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Chemical **inetics**

A compact kinetic reaction mechanism for the oxidation of NH₃/H₂ mixtures

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Marinh engines for maritime

Introduction

Laboratory **ELTE**

- In this poster we present the development and validation of our recently proposed compact NH₃ reaction mechanism [1].
- The potential of ammonia as a zero-carbon fuel and hydrogen carrier has stimulated scientific interest in its application as a fuel in combustion systems.
- However, the use of ammonia as a fuel source for energy applications presents **notable challenges due to** its low flammability and the potential for high emissions [2].

Ħ	Mechanism	$N_{ m spec}$	Nreac ₁	$\overline{E_{\rm LBV}}$	$\sqrt{E_{\rm JSR}}$	$\overline{E_{\rm BSSF}}$	$\sqrt{E_{\text{Overal}}}$	-	•	Th	ne p)e
1	Zhu 2024	39	312	2.97	1.11	2.27	2.25			m	nde	ماد
2	Han 2023	32	171	2.24	1.63	3.70	2.67				Juc	713
3	Present work	21	64	1.97	2.72	3.24	2.70			•••		_
4	Jian 2024	32	233	3 23	1.80	3 79	3.06		•	Si	gni	fi
5	Otomo 2018	32	213	3.67	2.03	3.65	3 21			(n	roc	
5	V 7hong 2021	21	213	2.45	2.03	1 50	2 41			(P	163	
07	A. Zhang 2021	21	224	2.45	2.70	4.59	2.51			pr	edi	C
/	Stagni 2023	22	203	3.40	1.75	4.09	3.51					
8	Gotama 2022	32	165	3.28	2.91	4.59	3.67		-	יח	<u>۸/:</u>	
9	Nakamura 2019	34	229	3.75	2.87	4.71	3.85		•	PV		5 (
10	Stagni 2020	31	203	3.32	3.31	4.90	3.91			th	e s	ha
11	Liu 2024	35	238	3.96	2.39	5.19	4.01					
12	Glarborg 2022	34	227	6.42	2.55	4.45	4.74			Γ.		
13	Glarborg 2023	34	228	6.52	2.54	4.45	4.79		•	FC		53
14	He 2023	34	221	7.37	2.46	4.45	5.17			ac	CU	ra
15	Z. Zhang 2024	34	224	8.46	1.14	4.50	5.57			uu		
16	Mei 2021	35	239	4.02	1.65	9.84	6.21			_		
17	Wang 2022	32	140	2 53	2 64	10.13	6.22		•	EX	(Ce	pt
18	Tamaaki 2022	33	228	3 29	2.01	10.17	6.22					-
10	1 amatri 2024 Mong 2023	30	220	10.14	3 11	10.17 A 62	6.68		•	Th	n n	nc
1) 20 I	Vieng 2023 Zlinnonstoin 2019	22	108	10.14	2.02	4.02	6.76		-			
20 f 21	Clarkarg 2019		211	10.20	2.02	4.75	6.70			Of	H_2)
21	Glarborg 2018	21	211	10.29	5.05	4.75	0.//			ro	ma	, in
22	San Diego 2018	21	04	3.30	2.43	13.94	8.40				ша	
				/ F					/ F .	\		
#	Mechanism	NH		\sqrt{E}	JSR No NO	N-O N		0	$\sqrt{E_{\rm I}}$	BSSF	NO	Na
#	Mechanism Zhu 2024	NH ₃	$H_2 O_2$	\sqrt{E} 2 H ₂ O	$\overline{N_2}$ NO	N ₂ O N	\mathbf{H}_3 \mathbf{H}_2	O_2	$\sqrt{E_{\rm H}}$ H ₂ O	BSSF NO	NO ₂	N ₂
#	Mechanism Zhu 2024 Han 2023	NH ₃ 2.1	H ₂ O ₂ 0.8 0.8	\sqrt{E} $\frac{\sqrt{E}}{2 + H_2O}$ $\frac{1 + 4}{2 + 1 + 3}$	N₂ NO 0.6 0.4	N ₂ O N 0.5	NH ₃ H ₂ 0.9 0.9	O ₂ 1.3 0.7	$\frac{\sqrt{E_{\rm H}}}{\rm H_2O}$	BSSF NO 0.7	NO ₂ 1.5	N ₂ 5.
# 1 2 3	Mechanism Zhu 2024 Han 2023 Present work	NH ₃ 2.1 2.5 4 0	H ₂ O ₂ 0.8 0.8 0.8 0.6 2.3 2.9	\sqrt{E} 2 H ₂ O 3 1.4 5 1.3 9 3 3	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3	N ₂ O N 0.5 2.8 1.5	NH ₃ H ₂ 0.9 0.9 1.1 5.4 0.7 5.6	O ₂ 1.3 0.7 0.8	$\frac{\sqrt{E_{\rm H}}}{1.9}$	BSSF NO 0.7 6.3	NO ₂ 1.5 3.0 3.6	N ₂ 5. 1.
# 1 2 3 4	Mechanism Zhu 2024 Han 2023 Present work Jian 2024	NH ₃ 2.1 2.5 4.0 2.2	H ₂ O ₂ 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0	$ \sqrt{E} \frac{\sqrt{E}}{1.20} \frac{1.4}{1.3} \frac{1.3}{1.3} \frac{1.3}{1.3} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5	N ₂ O N 0.5 2.8 1.5 0.5	NH ₃ H ₂ 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1	O ₂ 1.3 0.7 0.8 0.7	$\sqrt{E_{\rm H}}$ H ₂ O 1.9 3.9 3.9 4.0	BSSF NO 0.7 6.3 1.5 2.8	NO ₂ 1.5 3.0 3.6 2.2	N ₂ 5. 1. 3.
# 1 2 3 4 5	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018	NH ₃ 2.1 2.5 4.0 2.2 2.9	H ₂ O ₂ 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.4	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1.4}{1.3} \frac{3.3}{1.3} 1.3 1.3 5 2.3 $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5	N ₂ O N 0.5 2.8 1.5 0.5 1.0	NH ₃ H ₂ 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3	O ₂ 1.3 0.7 0.8 0.7 0.8	$\sqrt{E_{\rm H}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8	BSSF NO 0.7 6.3 1.5 2.8 5.4	NO ₂ 1.5 3.0 3.6 2.2 1.9	N ₂ 5. 1. 3. 6. 4.
# 1 2 3 4 5 6	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5	H ₂ O ₂ 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1.4}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{3.1} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1	N ₂ O N 0.5 2.8 1.5 0.5 1.0 3.0	NH ₃ H ₂ 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6	O ₂ 1.3 0.7 0.8 0.7 0.8 0.7	$\sqrt{E_{\rm H}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 3.8	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8	N ₂ 5. 1. 3. 6. 4. 8.
# 1 2 3 4 5 6 7	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023	NH3 2.1 2.5 4.0 2.2 2.9 3.5 2.0	H2 O2 0.8 0.8 0.8 0.8 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3 1.3 0.8	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1.4}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.1}{3.1} \frac{3.1}{1.8} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 3.0 2.7	H3 H2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4	O ₂ 1.3 0.7 0.8 0.7 0.8 0.7 0.7 0.7	$\sqrt{E_{\rm H}}$ H ₂ O 1.9 3.9 4.0 3.8 3.8 4.0	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3	NO2 1.5 3.0 3.6 2.2 1.9 2.8 2.7	N ₂ 5. 1. 3. 6. 4. 8. 9.
# 1 2 3 4 5 6 7 8	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022	NH3 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9	H2 O2 0.8 0.8 0.8 0.8 2.3 2.9 2.6 1.0 1.4 2.5 1.3 0.8 3.7 2.1	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1.4}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.1}{1.8} \frac{1.8}{2.4} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 5.0	H3 H2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6	O ₂ 1.3 0.7 0.8 0.7 0.8 0.7 0.7 0.7	$ \frac{\sqrt{E_{\rm H}}}{1.9} $ 3.9 3.9 4.0 3.8 3.8 4.0 3.8	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1	N ₂ 5. 1. 3. 6. 4. 8. 9. 8.
# 1 2 3 4 5 6 7 8 9	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019	NH3 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9	H2 O2 0.8 0.8 0.8 0.8 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3 1.3 0.8 3.7 2.1 3.6 0.9	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{14}{5} \frac{1.3}{3.3} \frac{3.3}{5} \frac{3.3}{3.1} \frac{3.1}{1.8} \frac{1.8}{1.2} \frac{1.8}{4.2} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 .	NH3H20.90.91.15.40.75.61.85.10.85.31.35.61.55.41.05.62.75.3	O ₂ 1.3 0.7 0.8 0.7 0.8 0.7 0.7 0.7 0.7 0.7	$ \frac{\sqrt{E_{\rm H}}}{1.9} $ 3.9 3.9 4.0 3.8 3.8 4.0 3.8 4.0 3.8 4.0	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7	N2 5. 1. 3. 6. 4. 8. 9. 8. 9.
# 1 2 3 4 5 6 7 8 9 10	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3 3.7 2.1 3.6 0.9 1.3 0.5	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{14}{5} \frac{1.3}{3.3} \frac{3.3}{5} \frac{3.3}{3.1} \frac{3.1}{3} \frac{3.1}{1.8} \frac{1.8}{1.2} \frac{1.8}{1.6} \frac{4.2}{5} \frac{1.6}{1.6} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 .	NH3H20.90.91.15.40.75.61.85.10.85.31.35.61.55.41.05.62.75.31.15.7	O ₂ 1.3 0.7 0.8 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7	$ \frac{\sqrt{E_{\rm H}}}{1.9} $ 3.9 3.9 4.0 3.8 3.8 4.0 4.0 3.8 4.0 4.0 4.0 4.0 4.0 4.0 4.0 4.0 4.0 4.0	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7.
# 1 2 3 4 5 6 7 8 9 10 11	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.7	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 3.6 0.9 1.3 0.8 1.4 1.4	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{14}{5} \frac{1.3}{2.3} \frac{3.3}{5} \frac{3.3}{2.3} \frac{3.1}{3} \frac{3.1}{1.8} \frac{3.1}{1.8} \frac{1.8}{1.8} \frac{1.2}{5} \frac{4.2}{5} \frac{1.6}{4} \frac{2.7}{2.7} $	N2NO0.60.40.90.72.71.32.80.52.40.53.51.12.10.61.21.23.00.61.50.71.11.2	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 . 8.1 . 4.3 .	NH3H20.90.91.15.40.75.61.85.10.85.31.35.61.55.41.05.62.75.31.15.71.55.5	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$ \sqrt{E_{\rm H}} $ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 3.8 3.8 3.8 3.8 3.9 3.8 3.9 3.9 3.9 3.8 3.9	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2	NO2 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9.
# 1 2 3 4 5 6 7 8 9 10 11 12	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.7 3.1	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 3.7 2.1 3.6 0.9 1.3 0.5 1.4 1.4 2.4 1.2	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{3} \frac{1}{3} \frac{1}{3} \frac{3}{3} \frac{3}{1} \frac{1}{3} \frac{3}{1} \frac{3}{1} \frac{1}{8} \frac{1}{2} \frac{4}{2} \frac{4}{2} \frac{1}{6} \frac{4}{2} \frac{2}{7} \frac{2}{2} \frac{8}{3} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 . 8.1 . 4.3 . 2.9 .	NH3H20.90.91.15.40.75.61.85.10.85.31.35.61.55.41.05.62.75.31.15.71.55.52.15.3	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$ \sqrt{E_{I}} H_2O 1.9 3.9 3.9 4.0 3.8 4.1 4.1 $	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8	NO2 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9.
# 1 2 3 4 5 6 7 8 9 10 11 12 13	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3 1.3 0.8 3.7 2.1 3.6 0.9 1.3 0.5 1.4 1.4 2.4 1.2 2.4 1.2	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{14}{13} \frac{1.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.1}{1.8} \frac{3.1}{1.8} \frac{3.1}{1.8} \frac{1.8}{1.2.4} \frac{4.2}{1.6} \frac{4.2}{2.7} \frac{1.6}{2.7} \frac{2.8}{2.8} \frac{2.8}{2.8} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 . 8.1 . 4.3 . 2.9 .	NH3H20.90.91.15.40.75.61.85.10.85.31.35.61.55.41.05.62.75.31.15.71.55.52.15.32.25.3	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.8 0.8	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9.
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.2	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 3.6 0.9 1.3 0.5 1.4 1.4 2.4 1.2 2.4 1.2 2.7 1.1	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{120}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.1}{1.8} \frac{3.1}{1.8} \frac{2.4}{2.4} \frac{4.2}{1.6} \frac{4.2}{1.6} \frac{4.2}{2.8} \frac{2.8}{2.8} \frac{2.7}{2.8} \frac{2.7}{2.8} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 1.6 1.5 0.7 1.1 1.2 3.2 1.4 3.1 1.0	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 . 8.1 . 4.3 . 2.9 . 2.4 .	NH ₃ H ₂ 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 3.9	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.5	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.3	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9. 9.
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023 Z. Zhang 2024	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.1 3.2 2.1	 H₂ O₂ 0.8 0.8 0.8 0.8 0.8 2.3 2.9 2.6 1.4 2.4 1.2 2.4 1.2 2.4 1.2 2.7 1.1 0.6 1.1 	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{120}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.1}{1.3} \frac{3.1}{1.8} \frac{2.4}{1.6} \frac{4.2}{1.6} \frac{4.2}{2.8} \frac{2.8}{2.8} \frac{2.7}{1.5} \frac{1.5}{1.6} \frac{1.5}{1.5} \frac{1.5}{1.5} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4 3.1 1.0 0.6 0.5	N2O N 0.5 . 2.8 . 1.5 . 0.5 . 1.0 . 3.0 . 2.7 . 5.0 . 1.4 . 8.1 . 4.3 . 2.9 . 2.9 . 2.4 . 0.4 .	H_3 H_2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1 3.1 4.1	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{\rm H}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 3.9	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.5 2.9	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.2 2.2 2.3 2.4	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9. 9. 9.
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023 Z. Zhang 2024 Mei 2021	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.1 3.1 3.2 2.1 2.3	 H₂ O₂ 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.4 2.4 1.2 2.4 1.2 2.4 1.2 2.7 1.1 0.6 1.7 2.0 	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{120}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.3}{1.3} \frac{3.1}{1.3} \frac{3.1}{1.8} \frac{3.1}{1.8} \frac{2.4}{2.4} \frac{4.2}{1.6} \frac{4.2}{2.8} \frac{2.8}{2.8} \frac{2.7}{1.5} \frac{1.5}{1.6} \frac{1.6}{1.6} \frac{2.7}{1.5} \frac{1.6}{1.6} \frac{1.6}{1.6} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4 3.1 1.0 0.6 0.5 1.8 0.6	N2O N 0.5 1 2.8 1 1.5 1 0.5 1 1.0 1 3.0 2 2.7 1 5.0 1 1.4 2 8.1 4 4.3 2 2.9 2 2.9 2 2.9 2 0.4 0 0.8 1	NH ₃ H ₂ 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1 3.1 4.1 7.1 6.1	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 3.9 4.1 4.0 3.9	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.5 2.9 1.8 2.5 2.9 1.8	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.3 2.4 3.6	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9. 9. 9. 11
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023 Z. Zhang 2024 Mei 2021 Wang 2022	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.1 3.2 2.1 2.3 3.6	 H₂ O₂ 0.8 0.8 0.8 0.8 2.3 2.9 2.6 1.4 2.4 1.2 2.4 1.2 2.4 1.2 2.4 1.2 2.7 1.1 0.6 1.1 1.7 2.0 3.5 2.7 	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{120}{13} \frac{1.4}{5} \frac{1.3}{2.3} \frac{3.3}{5} \frac{3.3}{5} \frac{3.1}{2.3} \frac{3.1}{2.4} \frac{4.2}{4.2} \frac{4.2}{5} \frac{1.6}{1.6} \frac{2.7}{2.8} \frac{2.8}{2.8} \frac{2.7}{1.5} \frac{1.5}{1.6} \frac{1.5}$	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4 3.1 1.0 0.6 0.5 1.8 0.6 2.0 1.5	N2O N 0.5 1 2.8 1 1.5 1 0.5 1 1.0 1 3.0 1 2.7 1 5.0 1 1.4 1 8.1 1 4.3 1 2.9 1 2.9 1 2.9 1 0.4 1 0.4 1 0.4 1 0.9 1	H_3 H_2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1 3.1 4.1 7.1 6.1 7.2 8.2	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 3.9 4.1 4.0 3.9 4.1 4.0 3.9	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.5 2.9 1.8 5.1	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9. 9. 9. 9. 11
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 10	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023 Z. Zhang 2024 Mei 2021 Wang 2022 Tamaoki 2024	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.1 3.1 3.1 3.2 2.1 2.3 3.6 2.9 4.1	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 3.6 0.9 1.3 0.8 3.6 0.9 1.3 0.5 1.4 1.4 2.4 1.2 2.7 1.1 0.6 1.1 1.7 2.0 3.5 2.7 1.2 2.3 2.4 1.2	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{3} \frac{1}{3} \frac{1}{3} \frac{3}{3} \frac{3}{3} \frac{1}{3} \frac{3}{3} \frac{3}{3} \frac{1}{3} \frac{3}{3} \frac{3}{1} \frac{1}{3} \frac{3}{3} \frac{3}{1} \frac{1}{3} \frac{1}{3} \frac{2}{4} \frac{4}{2} \frac{2}{5} \frac{1}{6} \frac{4}{2} \frac{2}{7} \frac{2}{2} \frac{8}{2} \frac{2}{8} \frac{2}{2} \frac{8}{2} \frac{2}{8} \frac{2}{5} \frac{1}{5} \frac{1}{5} \frac{5}{1} \frac{1}{5} \frac{1}{5} \frac{1}{5} \frac{1}{5} \frac{1}{5} \frac{3}{1} \frac{1}{8} \frac{1}{8} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4 3.1 1.0 0.6 0.5 1.8 0.6 2.0 1.5 2.3 1.8 2.4 1.2	N2O N 0.5 1 2.8 1 1.5 1 0.5 1 1.0 1 3.0 1 2.7 1 5.0 1 1.4 1 8.1 1 4.3 2.9 2.9 1 2.9 1 2.9 1 0.4 1 0.4 1 0.7 1 2.9 1 2.9 1 2.9 1 2.4 1 0.4 1 0.7 1 1.2 1	H_3 H_2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1 3.1 4.1 7.1 6.1 7.2 8.2 2.9 5.1	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 3.9 4.1 4.0 3.9 4.1 4.0 3.9 4.1 4.0 3.9 4.0 3.9 4.0 3.9 4.0 3.8 4.0 3.9 4.1 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.1 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 3.9 4.0 4.0 3.9 4.0 4.0 3.9 4.0 3.9 4.0 3.9 4.0 3.9 4.0 1.0 5.9 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.9 1.8 5.1 2.5 2.9 1.8 5.1 2.5 2.9 1.8 5.1 5.7	NO ₂ 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9. 9. 9. 9. 11 10 10
# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023 Z. Zhang 2024 Mei 2021 Wang 2022 Tamaoki 2024 Meng 2023	NH ₃ 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.1 3.1 3.2 2.1 2.3 3.6 2.9 4.1 4.1	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3 1.3 0.8 3.7 2.1 3.6 0.9 1.3 0.5 1.4 1.4 2.4 1.2 2.4 1.2 2.7 1.1 0.6 1.1 1.7 2.0 3.5 2.7 1.2 2.3 2.4 1.6 2.4 1.6	$ \sqrt{E} \frac{\sqrt{E}}{120} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{3} \frac{1}{3} \frac{1}{3} \frac{3}{3} \frac{3}{3} \frac{1}{3} \frac{3}{3} \frac{1}{3} \frac{3}{3} \frac{1}{3} \frac{1}{3} \frac{2}{4} \frac{4}{2} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{2}{3} \frac{3}{3} \frac{1}{3} \frac{1}{3} \frac{5}{3} \frac{1}{3} \frac{3}{3} \frac{1}{3} \frac{1}{3} $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4 3.1 1.0 0.6 0.5 1.8 0.6 2.0 1.5 2.3 1.8 3.6 1.3 3.6 1.3	N2O N 0.5 1 2.8 1 1.5 1 0.5 1 1.0 1 3.0 1 2.7 1 5.0 1 1.4 1 8.1 1 4.3 1 2.9 1 2.9 1 2.9 1 2.9 1 0.4 1 0.4 1 0.5 1 1.4 1	NH3H2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1 3.1 4.1 7.2 8.2 7.2 8.2 2.9 5.1	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 10.4 10.9 10.8 4.1 4.2	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.5 2.9 1.8 5.1 2.5 2.9 1.8 5.1 2.5 2.9 1.8 5.1 5.7 2.5 2.5 2.9 1.8 5.1 5.7 2.5	NO2 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2	N2 5. 1. 3. 6. 4. 8. 9. 8. 9. 7. 9. 9. 9. 9. 9. 9. 11 10 10 9. 0.
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# 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 1 21 22	Mechanism Zhu 2024 Han 2023 Present work Jian 2024 Otomo 2018 X. Zhang 2021 Stagni 2023 Gotama 2022 Nakamura 2019 Stagni 2020 Liu 2024 Glarborg 2022 Glarborg 2023 He 2023 Z. Zhang 2024 Mei 2021 Wang 2022 Tamaoki 2024 Meng 2023 Klippenstein 2018	NH3 2.1 2.5 4.0 2.2 2.9 3.5 2.0 2.9 3.9 2.0 2.7 3.1 3.1 3.1 3.1 3.1 3.2 2.1 2.3 3.6 2.9 4.1 4.1 4.1 4.1 4.1	H2 O2 0.8 0.8 0.8 0.6 2.3 2.9 2.6 1.0 1.4 2.5 2.8 1.3 1.3 0.8 3.7 2.1 3.6 0.9 1.3 0.5 1.4 1.2 2.4 1.2 2.4 1.2 2.7 1.1 0.6 1.1 1.7 2.0 3.5 2.7 1.2 2.3 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 2.4 1.6 3.1 1.4	$ \sqrt{E} \sqrt{E} - H_2O - H_2O - H_2O - H_2O - H_2O - H_2O $	N2 NO 0.6 0.4 0.9 0.7 2.7 1.3 2.8 0.5 2.4 0.5 3.5 1.1 2.1 0.6 1.2 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.0 0.6 1.5 0.7 1.1 1.2 3.2 1.4 3.2 1.4 3.1 1.0 0.6 0.5 1.8 0.6 2.0 1.5 2.3 1.8 3.6 1.3 3.6 1.3 3.6 1.3 3.6 1.3 3.6 1.3	N2O N 0.5 1 2.8 1 1.5 1 0.5 1 1.0 1 3.0 1 2.7 1 5.0 1 1.4 1 8.1 1 4.3 1 2.9 1 2.9 1 2.9 1 2.9 1 2.9 1 0.4 1 0.4 1 0.4 1 0.5 1 2.9 1 2.9 1 2.9 1 3.4 1 0.4 1 0.5 1 3.4 1	NH3H2 0.9 0.9 1.1 5.4 0.7 5.6 1.8 5.1 0.8 5.3 1.3 5.6 1.5 5.4 1.0 5.6 2.7 5.3 1.1 5.7 1.5 5.5 2.1 5.3 2.2 5.3 2.9 4.1 3.1 4.1 7.2 8.2 7.2 8.2 2.9 5.1 2.9 5.1 2.9 5.1 2.9 5.1	O ₂ 1.3 0.7 0.8 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	$\sqrt{E_{II}}$ H ₂ O 1.9 3.9 3.9 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.8 4.0 3.9 4.1 4.0 10.4 10.9 10.8 4.1 4.2 4.1 4.2 4.1	BSSF NO 0.7 6.3 1.5 2.8 5.4 3.9 3.3 5.1 2.7 7.2 6.2 1.8 1.8 2.9 1.8 5.1 2.5 2.9 1.8 5.1 2.5 2.9 1.8 5.1 2.5 2.9 2.5 2.9 3.9 3.9	NO2 1.5 3.0 3.6 2.2 1.9 2.8 2.7 3.1 2.7 2.8 3.2 2.2 2.2 2.2 2.2 2.3 2.4 3.6 3.8 3.8 3.8 2.4 2.2 2.2 2.3 2.4 3.6 3.8 3.8 2.4 2.5 5.5	N ₂ 5. 1. 3. 6. 4. 8. 9. 7. 9. 9. 9. 9. 9. 9. 9. 9. 9. 9. 10

Results

- erformance of the initial and optimized San Diego 2018 s were compared with 19 recent models (refs \rightarrow ECM paper).
- cantly improved accuracy of the optimised mechanism nt work, PW) vs. the San Diego 2018 (SD) model in ting the LBVs (\sqrt{E} : 3.36 \rightarrow 1.97)
- currently the most accurate model for LBV simulations with ortest computational time.
- SF simulations of 70/30 vol% NH₃/H₂ mixtures, the cy of the model improved greatly (\sqrt{E} : 13.91 \rightarrow 3.24).

- Blending NH_3 with H_2 offers the prospect of improving combustibility, albeit with a notable increase in NOx emissions, especially under fuel-rich conditions [3].
- The design of burners, turbines, and engines is aided by computational fluid dynamics (CFD) simulations, which require small-sized mechanisms.
- According to a recent review of the performance of ammonia combustion mechanisms [4], the San Diego **2018 mechanism** [5], which has an **exceptionally small** size (21 species, 64 reactions), shows fair performance in predicting laminar burning velocities (LBV) and concentration data measured in jet-stirred reactors (JSR) under a wide range of conditions.
- The current study aims to develop a small and robust kinetic mechanism for CFD simulations of NH_3/H_2 flames by optimising the rate parameters of the San **Diego 2018 NH₃ mechanism against experimental** data using the Optima++ code [6-8].

Experimental Data Collection

A large collection of LBV and concentration data measured in JSRs, previously compiled from the



- for Zhu 2024, all models perform poorly for BSSF data.
- odel performance for JSR concentrations (with at least 10%) slightly deteriorated upon optimisation (2.43 \rightarrow 2.72) but \sqrt{E} ed below 3.
 - The **Zhu 2024** model shows **outstanding performance** for all species in JSR and BSSF simulations, except for NO₂ in BSSF.
 - The prediction for all species concentrations **improved greatly** upon optimization of the San Diego 2018 model in BSSF.
 - The PW model can accurately predict NO and N₂O **JSR data**, but improvement is needed for other species, especially for NH_3 and H_2O .
 - The PW model accurately predicts NO emissions and NH₃ slip in BSSF, while improvement is needed for H_2 , H_2O and NO_2 .
 - Validation in Reynolds Averaged Navier Stokes (RANS) **CFD simulations of a swirl burner** against experimental data of **Mashruk et al.** [14]
 - All models predict N₂O emission qualitatively well.

- literature [4] was downloaded in ReSpecTh Kinetic Data (RKD) format XML files [9] from the Reaction Kinetic branch **ReSpecTh database** [10-11].
- addition. concentration data from burner-In stabilised stagnation flames (BSSF) [12], and recently published LBV data were collected.
- All newly collected data were coded in RKD files [9] and will be available in the **ReSpecTh database** [10-11].
- See ECM manuscript for corresponding publications.

Method / Measured Quantity	No. of data series	No. Of data points	H ₂ content in fuel mixture (%)	Pressure range (atm)	Tempera- ture range (K)	Equiva- lence ratio (<i>q</i>)
LBV	179	1283	0-100	1.0–36.6	295-584	0.2–2.0
JSR conc	47	538	10-70	1	800–1300	0.15-1.5
BSSF conc	7	119	30	1	298	0.57–1.4
Overall	239	1968	0-100	0.5-10	295-1300	0.15-2.0

- Stagni 2020 is the most accurate for NO peak conc.
- Both the Stagni 2020 and Nakamura 2019 models give qualitatively incorrect predictions at lean conditions: they fail to predict the very small NO emission, the nonzero NH₃ emission and the low NO₂ emission at φ =0.6.
- The PW model predicts all four emissions qualitatively well over the whole φ range.
- The PW model is the most computationally efficient , as it runs ~2 faster than the other two models.

Concluding remarks

• The accuracy of the San Diego 2018 mechanism could be greatly improved for laminar burning velocities and for concentrations in burner stabilized stagnation flames, and it is on par with best-performing mechanisms.

• However, its performance for concentrations in JSR, and for NO₂ concentration in BSSF need to be improved, which implies that the deficiencies in its chemistry cannot be compensated by the rates of other reaction routes.

• In CFD swirl burner simulations, it ran faster than other models and qualitatively captures all major emissions.

Optimization method	References
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$E(\mathbf{P}) = \frac{1}{N} \sum_{f=1}^{J} \sum_{s=1}^{J} \frac{w_{fsd}}{N_{fsd}} \sum_{d=1}^{J} \begin{pmatrix} Y_{fsd}^{sim}(\mathbf{P}) - Y_{fsd}^{exp} \\ \sigma_{fsd}^{exp,tot} \end{pmatrix}$ <i>f,s,d:</i> data file index, data series index, data $Y_{fsd}^{exp/sim}$: experimental data and simulation result points index	 A review. Applications in Energy and Combustion Science, 15, 100175. [4] A.G. Szanthoffer, I.G. Zsély, L. Kawka, M. Papp, T. Turányi, Testing of NH3/H2 and NH3/syngas combustion mechanisms using a large amount of experimental data, Appl. Energy Combust. Sci. (2023) 100127. [5] Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego, Chemical-Kinetic Mechanisms for Combustion Applications https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html
P: vector of model parameters data series <i>s</i> in data file <i>f</i>	[6] T. Turányi, T. Nagy, I.G. Zsély, M. Cserháti, T. Varga, B.T. Szabó, I. Sedyó, P.T. Kiss, A. Zempléni, H.J. Curran, Int. J. Chem. Kinet. 44 (2012) 284-302.
<i>N:</i> the total number of the data series w_{fsd} : weights to equalize an data collection	optimization. (2024). respecth.hu.
N _{f/s/d} : the number of the data which may contain different number of files /series /points data series of each experiment type	[8] S. Goitom, M. Papp, M. Kovács, T. Nagy, I.Gy. Zsély, T. Turányi, P. László: Combust. Theory. Modell. 26, (2022), 1071-1097.
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• \sqrt{E} measures the RMS deviation between the model and the experimental results, with respect to σ^{exp} . A	[10] <u>https://respectn.eite.nu</u> [11] T. Turányi, IG. Zsély, M. Papp, T. Nagy ,T. Furtenbacher, R. Tóbiás, P. Árendás, A. G. Császár: ReSpecTh: Reaction kinetics, spectroscopy, and thermochemical datasets, Scientific Data (2025), in press
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 The initial model missing important chemistry, which can be compensated by unphysical rate coefficients. 	Acknowledgements Acknowledgements Acknowledgements Acknowledgements
 Thus, one order of magnitude prior uncertainty range was employed for parameter tuning. 	 A. Alnasif: Funded by Al-Furat Al-Awsat Technical University (ATU) for PhD studies in the UK. T. Nagy and T. Turányi: National Research, Development, and Innovation Fund (NKFIH) grants FK134332 and K147024. A.G. Szanthoffer: Funded by DKOP 23 Doctoral Excellence Program of the Ministry for Culture and Innovation of Hundary from NKEIH (Hundary).
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