An Optimised Reaction Mechanism for Predicting Laminar Flame Speed in NH_3 and NH_3/H_2 Flames

MariNH3
Clean, green ammonia engines for maritime

Cardiff University / Prifysgol Caerdydd

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Introduction

- Ammonia (NH_3) is considered a zero-carbon fuel and hydrogen (H_2) carrier due to its good infrastructure and high hydrogen density.
- Harnessing NH_3 as a fuel presents challenges due to low flammability and high emissions, but blending NH_3 with H_2 improves combustibility while increasing NOx emissions, especially in fuel-rich conditions.
- Addressing these challenges requires a detailed analysis of NH_3 chemistry using a kinetic reaction mechanism.
- The study aims to develop a kinetic reaction mechanism for NH_3/O_2 and $NH_3/H_2/O_2$ flame chemistry, ensuring efficient CFD simulation under complex engine chamber conditions and turbulent flow dynamics.

Methodology

The methodology involves tuning the Arrhenius parameters of the rate constants within predefined uncertainty limits [1] using the Optima++ code [2]. This tuning is applied to the most influential reactions affecting flame speed under various operational conditions. The aim is to align the results with experimental observations from previous studies while considering their associated uncertainties. The process is detailed in the following steps.

1. Experimental data were encoded in **ReSpecTh Kinetics Data** (RKD) **2.3 format** XML files [3].
2. Program **Optima++** [2] reads the XML data file, sets up the simulation environment and calls the **Cantera** [4] simulation code to carry out the simulation.
3. All simulations were carried out with Cantera [4] using a **1D model** (LBV).

Experimental data

Exp. type	XML/Ds./Dp.	T / K	p / atm	φ
LBV	185/3381/1311	295-584.1	0.50–36.6	0.2–2.0

Error function

Quantitative evaluation of mechanism performance using an average error function.

$$E(\mathbf{P}) = \frac{1}{N_s}\sum_{s=1}^{N_s}\frac{1}{N_{sd}}\sum_{d=1}^{N_{sd}}\left(\frac{Y_{sd}^{\mathrm{sim}}(\mathbf{P}) - Y_{sd}^{\mathrm{exp}}}{\sigma_{sd}^{\mathrm{exp,tot}}}\right)^2$$

s,d: data series index, data points index
P: vector of model parameters
N: the total number of the data series
$N_{s/d}$: the number of the data series/points
$Y_{sd}^{\mathrm{exp/sim}}$: experimental data and simulation result
$\sigma_{sd}^{\mathrm{exp}}$: standard deviation of exp. data *d* in data series *s*

$\sqrt{E}$ measures the RMS deviation between the model and the experimental results, with respect to σ^{exp}.
A mechanism is typically considered accurate if $\sqrt{E} < 3$.

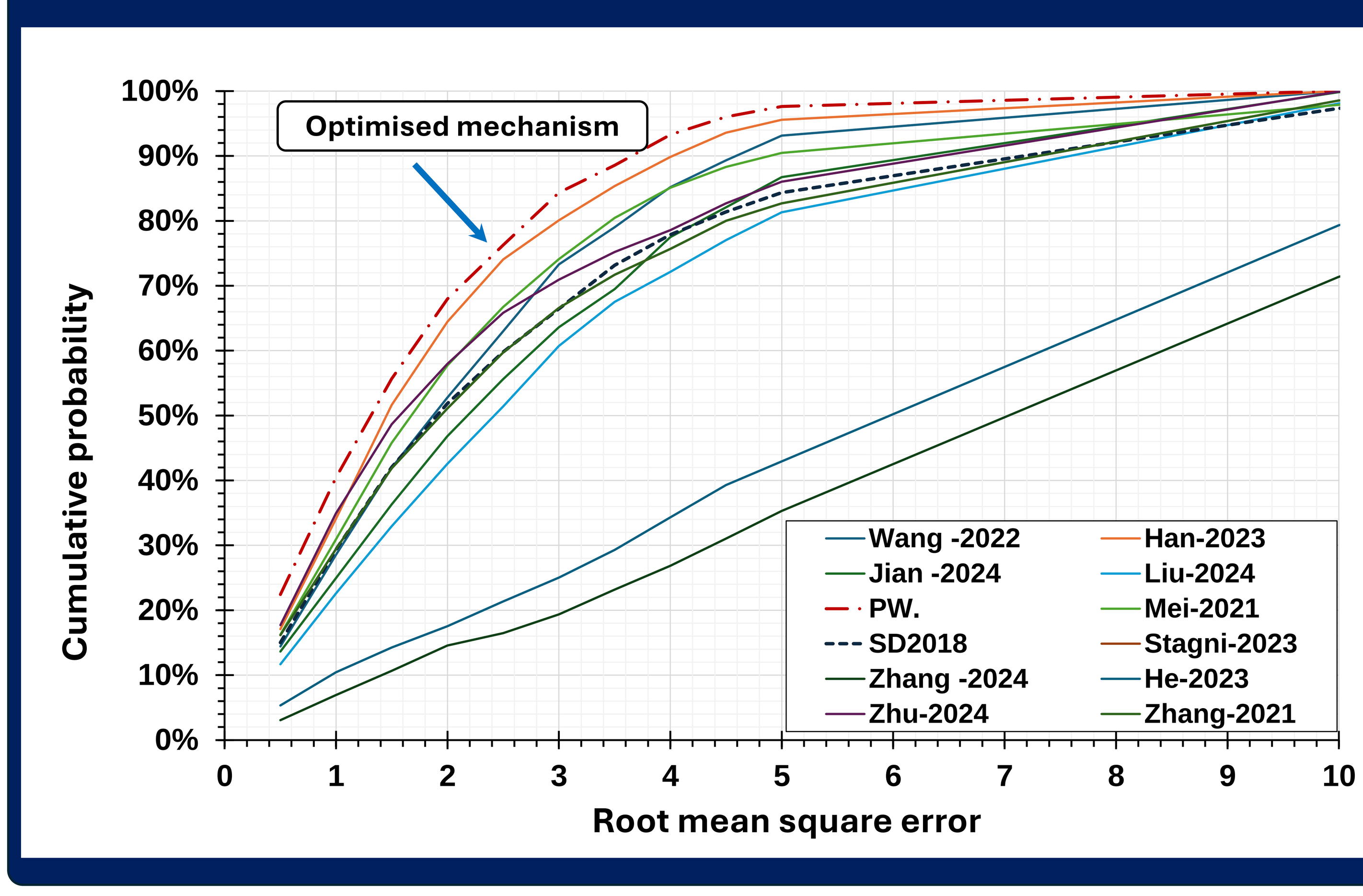
Reaction mechanisms investigated

	$N_{spec}(C_0)$	N_{Reac}	Max sqrt E_{sd}	$\sqrt{E}$	Ref.
Present work	21	64	9.0	2.17	-
Han-2023	32	171	9.9	2.39	[5]
Wang-2022	32	140	8.7	2.75	[6]
Zhu-2024	39	312	10.3	3.15	[7]
Jian-2024	32	233	11.1	3.36	[8]
SD-2018	21	64	16.5	3.77	[9]
Zhang-2021	34	224	13.4	3.75	[10]
Stagni-2023	31	203	13.4	3.75	[11]
Liu-2024	35	238	18.3	3.98	[12]
Mei-2021	35	239	34.2	4.39	[13]
He-2023	34	221	24.9	7.72	[14]
Zhang-2024	34	224	28.2	8.92	[15]

Quantitative mechanism comparison

$\sqrt{E}$	Wang 2022	Han 2023	Jian 2024	Liu 2024	Present work	Mei 2021	SD 2018	Stagni 2023	Zhang 2024	He 2023	Zhu 2024	Zhang 2021
0.5	14%	17%	14%	12%	22%	16%	15%	16%	3%	5%	18%	16%
1.0	29%	34%	25%	23%	40%	31%	29%	29%	7%	10%	35%	29%
1.5	42%	52%	36%	33%	56%	46%	42%	42%	11%	14%	49%	42%
2.0	53%	64%	47%	43%	68%	58%	52%	51%	15%	18%	58%	51%
2.5	63%	74%	56%	51%	76%	67%	60%	60%	16%	21%	66%	60%
3.0	73%	80%	64%	61%	84%	74%	66%	67%	19%	25%	71%	67%
3.5	79%	85%	69%	68%	89%	80%	73%	72%	23%	29%	75%	72%
4.0	85%	90%	77%	72%	93%	85%	78%	76%	27%	34%	79%	76%
4.5	89%	94%	82%	77%	96%	88%	81%	80%	31%	39%	83%	80%
5.0	93%	96%	87%	81%	98%	90%	84%	83%	35%	43%	86%	83%
10.0	100%	100%	100%	98%	100%	98%	97%	99%	71%	79%	100%	99%
15.0	100%	100%	100%	100%	100%	99%	100%	100%	93%	97%	100%	100%
20.0	100%	100%	100%	100%	100%	99%	100%	100%	98%	100%	100%	100%
25.0	100%	100%	100%	100%	100%	99%	100%	100%	100%	100%	100%	100%
30.0	100%	100%	100%	100%	100%	99%	100%	100%	100%	100%	100%	100%
35.0	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
N_{failed}	0	0	0	0	0	1	0	0	0	0	0	0

Distribution function



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