An Optimised Reaction Mechanism for Predicting

Laminar Flame Speed in NH₃ and NH₃/H₂ Flames

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Introduction

Ammonia (NH₃) is considered a zero-carbon fuel and hydrogen (H₂) carrier due to its good infrastructure and high hydrogen density.

MoriNH₃ Clean, green ammonia

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engines for maritime

Error function

Quantitative evaluation of mechanism performance using an average error function.

- Harnessing ammonia 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 NH₃ 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.

<u>Methodology</u>

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

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were encoded in XML da				L data f	file, sets u	ip the s	imulatior	n 💦 We	ere car	rried o	ut	Jian2(024	32	233	11.1	3.36	[8]		
ReSpecTh Kinetics environment and c						alls the	e Cantera	a E P wi	th Car	ntera [4]	SD20	18	21	64	16.5	3.77	[9]		
Data (RKD) 2.3 [4] simulation code						to car	ry out the	e us	sing a	a 1	D	Zhang2	2021	34	224	13.4	3.75	[10]		
format XML files [3]. simulation.							model (LBV).					2023	31	203	13.4	3.75	[11]			
				-	•							Liu20)24	35	238	18.3	3.98	[12]		
<u>Experimental data</u>												Moi2(021	35	230	3/1 2	/ 39	[12]		
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- I P				105/2201/1211			205_58/1			0 2-2 0			2024	24		24.9	7.72			
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N failed	0	0	0	0	0	1	0	0	0	0	0	0				Root mean squa	are error			



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 $Y_{sd}^{exp/sim}$: experimental data and simulation result σ_{sd}^{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

speed under various operational conditions. The aim is to align the results														$N_{spec}(C_0)$	N _{Reac}	Max sqrt E _{sd}	VE	Ref.
with experimental observations from previous studies while considering their													nt	21	64	9.0	2.17	-
associated uncertainties. The process is detailed in the following steps.													23	32	171	9.9	2.39	[5]
1 3														32	140	8.7	2.75	[6]
Experimental data Program Optima++ [2] reads the All simulations														39	312	10.3	3.15	[7]
were encoded in XML data file, sets up the simulation were carried out														32	233	11.1	3.36	[8]
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Data (RKD) 2.3 [4] simulation code to carry out the sing a a 1D													021	34	224	13.4	3.75	[10]
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Quantitative mechanism comparison															<u>Distr</u>	ibution functio	<u>n</u>	
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