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PERFORMANCE OF KINETIC REACTION MECHANISMS IN PREDICTING THE LAMINAR BURNING VELOCITIES OF AMMONIA-HYDROGEN FLAMES

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OBJECTIVES

- To perform a comprehensive comparative study dealing with 36 kinetic reaction mechanisms.
- To study and evaluate the best kinetic model capable of estimating the laminar burning velocity of NH_3-H_2 flames (70-30% in vol.) with a minimum discrepancy with experiments at normal pressure, temperature and with various equivalence ratio.

PRINCIPLES

Kinetic mechanisms depend on experimental measurements to predict flame characteristics (i.e. laminar burning velocity, NOx emissions, extinction limits, ignition delay time, etc.). However, due to the lack of experimental measurement datasets of binary fuels (NH_3-H_2), several kinetic mechanisms tend to over/underestimate flame characteristics of practical combustors. Therefore improving their database by conducting further experiments, comparative analyses and other methods is critical to achieve good correlations.

KINETIC MODELING

- The analysis for 36 kinetic reaction mechanisms of NH_3 oxidation has been performed via CHEMKIN-PRO.
- A premixed laminar flame-speed calculation model (as illustrated in figure 1) was adopted in this work and applied for all kinetic models.
- The numerical calculations for all model tests were performed in a one-dimensional computational domain equal to 10 cm in axial direction.
- The accuracy for all cases was tested and adjusted to give precise results.

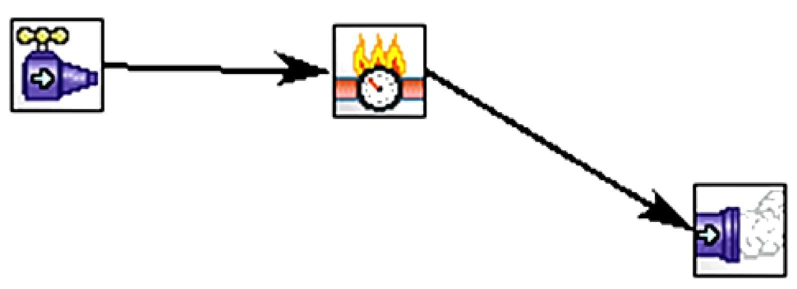


Fig. 1. Layout of a premixed laminar flame-speed calculation model

Chemical kinetic mechanisms used in the present work

Table 1 presents data of kinetic mechanisms that have been developed over the past 22 years.

No.	Kinetic model	No. of Reaction	No. of species	Fuel mixture	Target
1	Bertolino et al. (2021)	264	38	NH_3	LBVs Ignition delay time speciation measurements
2	Mei et al. (2021)	264	38	$NH_3/NO/N_2$	LBVs Markstein length
3	Han et al. (2021)	298	36	NH_3/N_2O	LBVs
4	Mei et al. (2021)	257	40	$NH_3/H_2/N_2$	LBVs NOx formation
5	Gotama et al. (2021)	119	26	NH_3/H_2	LBVs Markstein length
6	Shrestha et al. (2021)	1099	125	NH_3/O_2 NH_3/H_2	LBVs NOx formation
7	Wang et al. (2021)	444	91	NH_3+CH_3OH NH_3+C_2H_5OH	LBVs
8	Zhang et al. (2021)	263	38	NH_3 NH_3/H_2	NOx formation
9	Arunthan. et al. (2021)	203	31	CH_4/NH_3	NOx formation
10	Stagni et al. (2020)	203	31	NH_3	LBVs Ignition delay time speciation measurements
11	Han et al. (2020)	177	35	NH_3+syngas	LBVs Ignition delay time NOx measurements
12	De Persis et al. (2020)	647	103	CH_4	LBVs NOx measurements
13	Mei et al. (2019)	265	38	$NH_3/O_2/N_2$	LBVs
14	Li et al (2019)	957	128	NH_3-H2 NH_3-H_2-CH_4	LBVs Ignition delay time Flame structure
15	Okafor et al. (2019)	356	59	NH_3-CH_4	LBVs NOx measurements Markstein length
16	Glarborg et al. (2018)	231	39	-	NOx measurements
17	Shresth et al. (2018)	1081	124	NH_3 NH_3-H_2	NOx measurements
18	Otomo et al. (2018)	213	32	NH_3 NH_3-H_2	LBVs Ignition delay time

No	Kinetic model	No. of Reaction	No. of species	Fuel mixture	Target
19	UCSD Mechanism (2018)	41	20	-	NOx formation
20	Klippenstein et al. (2018)	211	33	-	NOx formation
21	Nakamura et al. (2017)	232	33	NH_3	LBVs Ignition delay time Species measurements
22	Zhang et al. (2017)	251	44	H_2/NOx Syngas/NOx	NOx formation
23	Lamoureux et al. (2016)	934	123	-	N-species sub-mechanism
24	Xiao et al. (2016)	276	55	NH_3/CH_4	Ignition delay time
25	Song et al. (2016)	204	32	NH_3/O_2	NOx measurements
26	Nozari and Karabeyoğlu (2015)	91	21	NH_3/H_2	LBVs NOx measurements
27	Mathieu and Petersen (2015)	278	54	NH_3	Ignition delay time NOx measurements
28	Duynslaegher et al. (2012)	80	19	NH_3/H_2	NOx formation
29	Klippenstein et al. (2011)	202	31	-	NO formation
30	Zhang et al. (2011)	701	88	CH_3NO_2	Species measurements (hydrocarbons and nitrogen species)
31	Lamoureux et al. (2010)	883	119	CH_4; C_2H_2	NO formation
32	Konnov (2009)	1207	127	-	NO formation
33	Mendiara and Glarborg (2009)	779	79	CH_4/N_2 CH_4/CO_2	NO reduction
34	Tian et al. (2009)	703	84	NH_3/CH_4	Species measurements (hydrocarbons and nitrogen species)
35	Dagaut (2008)	250	41	-	NOx formation
36	GRI mech 3.0 (2000)	325	53	CH_4	NO formation

RESULTS

The absolute percentage error (APE) relation has been adopted in this work to calculate the error percentage between the predicted numerical data of the laminar burning velocity (LBV) and experimental results given by C. Lhuillier et al. (2020) using two ranges of equivalence ratios (lean and rich conditions).

$$APE_{m,h,s} = \left| \frac{F_m - A_{h,s}}{A_{h,s}} \right|$$

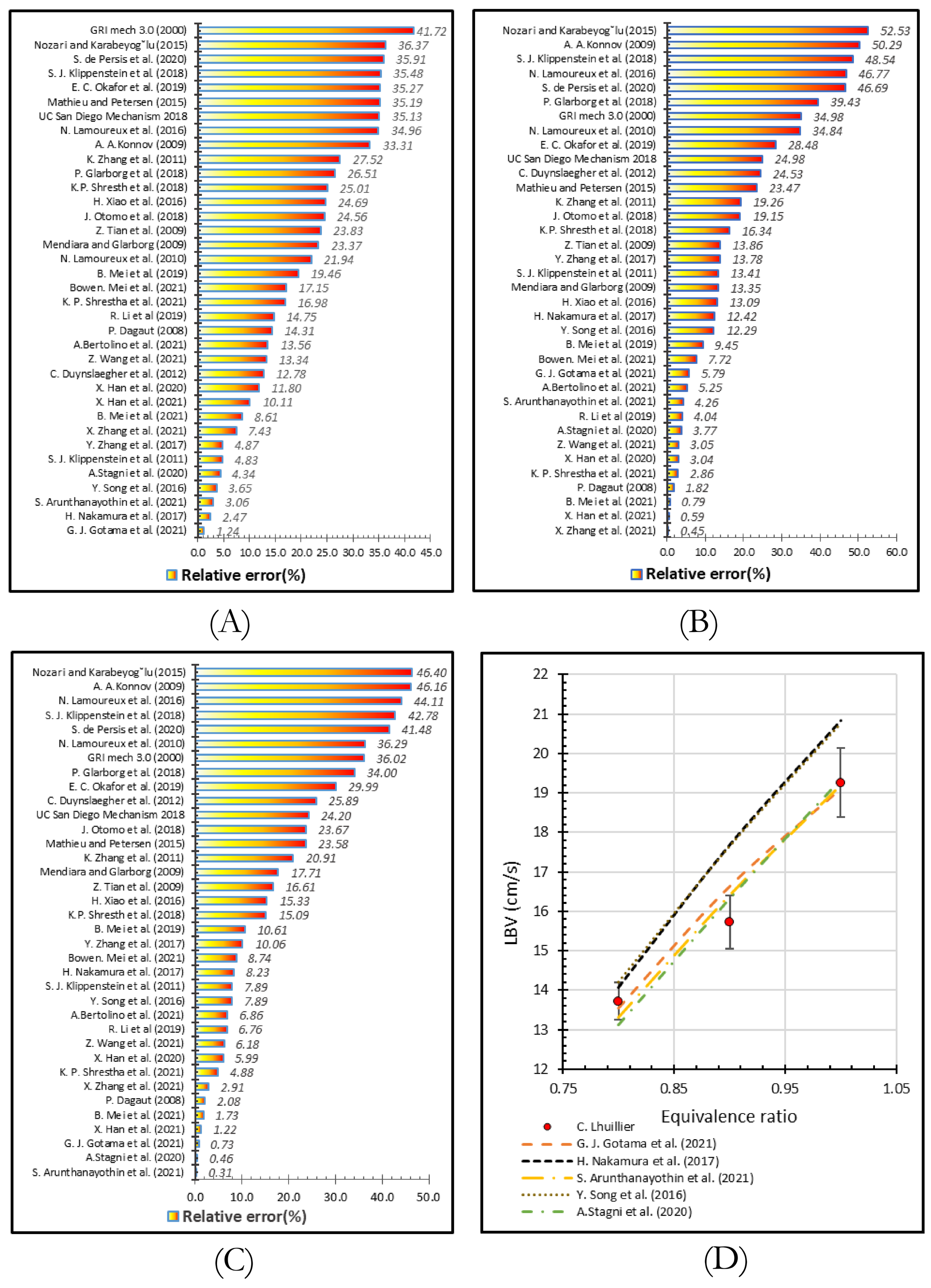
Where :

$APE_{m,h,s}$: The absolute percentage error

F_m: the forecast from method (m)

$A_{h,s}$: the actual value at the horizon (h) of series (s)

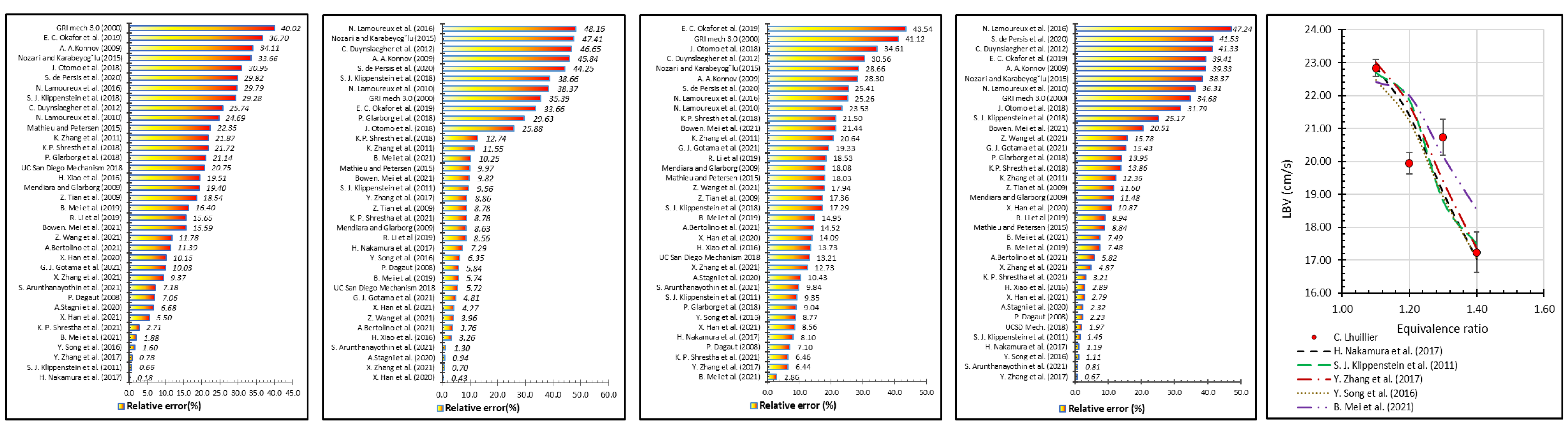
EFFECT OF EQUIVALENCE RATIO (LEAN CONDITIONS)



(A) (B) (C) (D)

Figures A, B and C illustrate the relative error for 36 kinetic reaction mechanisms at 0.8, 0.9 and 1.0, respectively, equivalence ratios, while figure D shows the laminar burning velocity at lean conditions of NH_3/H_2 flames. Symbols refer to experiments, and lines refer to kinetic models.

EFFECT OF EQUIVALENCE RATIO (RICH CONDITIONS)



(E) (F) (G) (H) (I)

Figures E-H show the relative error for 36 kinetic reaction mechanisms at 1.1, 1.2, 1.3 and 1.4, respectively, equivalence ratios, while figure I shows the laminar burning velocity at rich NH_3/H_2 flames conditions. Symbols refer to experiments, and lines refer to kinetic models.

CONCLUSIONS

The study showed Gotama et al. (2021), Arunthanayothin et al. (2021), and Stagni et al. (2020) giving a good prediction and acceptable agreement estimation for the laminar burning velocity of NH_3-H_2 flames at lean conditions. Meanwhile, Nakamura et al. (2017), Zhang et al. (2017), and Song et al. (2016) are the best in estimating the laminar burning velocity in fuel-rich conditions and show better agreement with the experimental results than the other 32 kinetic mechanisms.

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