Limit phenomena and kinetic modeling of ammonia fuels in an unstrained diffusion flame burner

Elie Antar[a,*], Philippe Versailles[a], Etienne Robert[a]

[a]Department of Mechanical Engineering, Polytechnique Montreal, Montreal, Quebec, H3T 1J4, Canada

Supplementary material

Extinction limit measurements:

The uncertainty in the extinction limits reported in the tables below and Figure 5 (error bars) refers to the range of values obtained from repeated experiments, incorporates the specified uncertainty of the flow controllers used to regulate the reactant flow rates, and takes into account the discreetness of the 0.25% X_F step size used in the experiments.

NH_3-H_2 (Figure 5a)

CO_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	H_2	±	CO_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	35.7	1.6	1.43	0.03	0.00	0.00	2.58	0.07	36.38	1.82	34.19	1.71	19.93	1.00	9.51	0.48	800.7	35.9
87.5	32.0	1.4	1.12	0.02	0.16	0.02	2.72	0.05	39.10	1.95	38.44	1.92	14.71	0.74	7.76	0.39	808.9	32.1
75	28.5	1.3	0.86	0.02	0.29	0.02	2.86	0.05	39.90	1.99	39.37	1.97	15.14	0.76	5.59	0.28	677.2	38.3
62.5	26.0	1.3	0.65	0.02	0.39	0.02	2.96	0.05	39.86	1.99	43.42	2.17	12.59	0.63	4.13	0.21	658.8	25.0
50	24.8	1.6	0.50	0.02	0.50	0.02	3.01	0.06	41.94	2.72	41.10	2.71	13.34	1.93	3.61	0.20	669.5	47.1
37.5	22.2	1.4	0.33	0.02	0.55	0.02	3.12	0.06	44.51	2.56	42.12	2.16	10.75	0.93	2.61	0.13	623.6	26.1
25	21.4	1.4	0.21	0.02	0.64	0.02	3.15	0.06	43.36	2.72	44.85	2.65	9.96	0.64	1.84	0.09	601.6	38.2
12.5	19.3	1.5	0.10	0.02	0.67	0.02	3.23	0.06	42.84	2.65	49.53	2.53	6.56	0.75	1.06	0.09	528.5	30.7
0	17.8	1.0	0.00	0.00	0.71	0.03	3.29	0.06	53.15	3.04	36.02	3.64	10.84	1.99	0.00	0.00	462.8	45.6

N_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	H_2	±	N_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	24.4	1.0	0.98	0.02	0.00	0.00	3.03	0.06	0.00	0.00	24.33	1.22	18.59	0.93	57.08	2.85	831.7	35.7
87.5	22.7	1.4	0.79	0.02	0.11	0.02	3.10	0.06	0.00	0.00	23.15	1.36	16.17	1.59	60.68	3.61	796.4	31.9
75	20.7	1.3	0.62	0.02	0.21	0.02	3.18	0.05	0.00	0.00	24.37	1.45	15.62	1.24	60.02	3.23	759.6	25.3
62.5	18.8	1.5	0.47	0.02	0.28	0.02	3.25	0.06	0.00	0.00	19.69	1.22	17.23	1.20	63.08	3.26	728.7	25.5
50	18.3	1.5	0.37	0.02	0.37	0.02	3.27	0.06	0.00	0.00	17.28	1.24	15.93	0.94	66.79	3.57	701.6	25.9
37.5	16.8	1.4	0.25	0.02	0.42	0.02	3.33	0.06	0.00	0.00	23.52	2.22	16.24	2.22	60.24	3.37	646.7	77.2

NH_3-CH_4 (Figure 5b)

CO_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	CH_4	±	CO_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	35.7	1.6	1.43	0.03	0.00	0.00	2.58	0.07	36.38	1.82	34.19	1.71	19.93	1.00	9.51	0.48	800.7	35.9
87.5	28.0	1.6	0.98	0.02	0.14	0.03	2.88	0.05	40.10	2.01	32.91	1.65	20.33	1.02	6.66	0.33	797.3	25.0
75	22.0	1.5	0.66	0.02	0.22	0.03	3.12	0.05	43.11	2.16	30.58	1.53	21.67	1.08	4.63	0.23	804.7	25.0
62.5	18.5	1.4	0.46	0.02	0.28	0.03	3.26	0.05	45.50	2.27	30.93	1.55	20.29	1.01	3.28	0.16	793.4	25.0
50	15.8	1.4	0.32	0.02	0.32	0.03	3.37	0.05	46.91	2.35	29.54	1.48	21.31	1.07	2.24	0.11	759.0	48.5
37.5	13.9	1.5	0.21	0.02	0.35	0.03	3.45	0.06	49.50	3.59	31.20	1.87	17.91	2.14	1.38	0.25	783.5	31.1
25	12.3	1.3	0.12	0.02	0.37	0.03	3.51	0.05	49.61	2.48	33.72	1.69	15.49	0.77	1.17	0.06	770.8	25.0
12.5	10.8	1.2	0.05	0.02	0.38	0.03	3.57	0.05	51.35	2.57	33.30	1.67	15.35	0.77	0.00	0.00	779.7	25.0
0	10.0	0.8	0.00	0.00	0.40	0.03	3.60	0.05	57.04	2.85	36.01	1.80	6.95	0.35	0.00	0.00	739.2	48.5

N_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	CH_4	±	N_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	24.4	1.0	0.98	0.02	0.00	0.00	3.03	0.06	0.00	0.00	24.33	1.22	18.59	0.93	57.08	2.85	831.7	35.7
87.5	18.0	1.4	0.63	0.02	0.09	0.03	3.28	0.05	2.48	0.12	22.98	1.15	14.60	0.73	59.94	3.00	804.9	30.1
75	14.2	1.5	0.42	0.02	0.14	0.03	3.44	0.05	3.33	0.21	23.68	1.37	17.58	1.32	55.40	2.99	776.5	35.8
62.5	11.8	1.3	0.29	0.02	0.18	0.03	3.53	0.05	3.79	0.19	23.30	1.16	13.58	0.68	59.33	2.97	768.1	25.0
50	10.0	1.5	0.20	0.02	0.20	0.03	3.60	0.06	4.13	0.21	24.17	1.21	17.15	0.86	54.55	2.73	751.8	25.0
37.5	8.2	1.3	0.12	0.02	0.20	0.03	3.68	0.06	4.25	0.21	24.03	1.20	14.96	0.75	56.76	2.84	724.5	25.0
25	7.2	1.3	0.07	0.02	0.21	0.03	3.72	0.06	4.23	0.21	24.05	1.20	17.04	0.85	54.68	2.73	709.3	25.0
12.5	6.0	1.1	0.03	0.02	0.21	0.03	3.76	0.05	4.70	0.23	25.64	1.28	14.35	0.72	55.31	2.77	713.7	25.0
0	6.4	0.9	0.00	0.00	0.26	0.03	3.75	0.05	5.20	0.26	18.27	0.91	17.02	0.85	59.51	2.98	704.5	25.0

NH_3-CH_3OH (Figure 5c)

CO_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	CH_3OH (mLPM)	±	CO_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	35.7	1.6	1.43	0.03	0.00	0.00	2.58	0.07	36.38	1.82	34.19	1.71	19.93	1.00	9.51	0.48	800.7	35.9
87.5	28.8	1.7	1.02	0.03	0.24	0.00	2.90	0.10	39.86	1.99	30.02	1.50	22.99	1.15	7.13	0.36	842.9	40.0
75	23.0	1.5	0.74	0.03	0.41	0.00	3.31	0.10	41.38	2.07	32.64	1.63	21.13	1.06	4.85	0.24	832.1	25.0
62.5	20.3	1.5	0.50	0.03	0.50	0.00	3.16	0.10	46.35	2.32	31.27	1.56	18.42	0.92	3.96	0.20	802.9	25.0
50	16.8	1.4	0.34	0.03	0.56	0.01	3.35	0.10	47.55	2.38	33.98	1.70	15.41	0.77	3.06	0.15	736.1	51.1
37.5	14.0	1.1	0.25	0.03	0.69	0.01	4.08	0.10	49.10	3.95	34.11	1.96	14.62	2.39	2.17	0.20	724.6	46.6
25	12.8	1.3	0.13	0.03	0.64	0.01	3.53	0.10	51.05	2.55	33.60	1.68	13.70	0.68	1.65	0.08	730.3	25.0
12.5	11.8	1.2	0.06	0.03	0.74	0.01	3.84	0.10	54.85	4.78	28.53	3.95	15.21	1.14	1.41	0.17	738.0	27.5
0	11.3	0.5	0.00	0.00	0.74	0.01	3.53	0.10	57.63	2.88	24.63	1.23	16.82	0.84	0.92	0.05	737.4	25.0

N_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	CH_3OH (mLPM)	±	N_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	24.4	1.0	0.98	0.02	0.00	0.00	3.03	0.06	0.00	0.00	24.33	1.22	18.59	0.93	57.08	2.85	831.7	35.7
87.5	20.6	1.5	0.68	0.03	0.16	0.00	3.00	0.10	2.20	0.11	20.69	1.03	21.62	1.08	55.49	2.77	821.1	25.0
75	17.3	1.5	0.48	0.03	0.26	0.00	3.04	0.10	3.74	0.19	20.48	1.02	17.12	0.86	58.65	2.93	793.0	25.0
62.5	14.0	1.4	0.32	0.03	0.32	0.00	3.16	0.10	4.32	0.22	23.11	1.16	14.20	0.71	58.37	2.92	753.2	25.0
50	11.3	1.2	0.21	0.03	0.35	0.00	3.36	0.10	4.41	0.22	22.29	1.11	14.78	0.74	58.52	2.93	722.6	25.0
37.5	10.0	1.3	0.13	0.03	0.37	0.00	3.21	0.10	5.18	0.26	19.00	0.95	10.23	0.51	65.58	3.28	706.2	25.0
25	8.8	1.2	0.08	0.03	0.39	0.00	3.31	0.10	4.97	0.25	22.38	1.12	13.17	0.66	59.48	2.97	688.2	25.0
12.5	8.0	1.1	0.04	0.03	0.44	0.00	3.53	0.10	5.40	0.27	17.87	0.89	12.04	0.60	64.69	3.23	693.2	25.0
0	7.5	0.5	0.00	0.00	0.49	0.00	3.66	0.10	6.44	0.32	13.70	0.68	12.54	0.63	67.32	3.37	702.2	25.0

NH_3-C_2H_5OH (Figure 5d)

CO_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	C_2H_5OH (mLPM)	±	CO_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	35.7	1.6	1.43	0.03	0.00	0.00	2.58	0.07	36.38	1.82	34.19	1.71	19.93	1.00	9.51	0.48	800.7	35.9
87.5	21.5	1.2	0.80	0.13	0.31	0.00	3.30	0.55	40.25	3.90	50.84	4.66	4.68	0.36	4.23	0.31	796.2	47.4
75	15.8	1.4	0.44	0.03	0.35	0.00	3.17	0.10	40.36	2.02	45.39	2.27	12.24	0.61	2.01	0.10	736.7	25.0
62.5	12.0	1.2	0.30	0.03	0.42	0.00	3.48	0.10	44.54	2.23	43.06	2.15	10.16	0.51	2.24	0.11	737.0	35.1
50	9.0	1.1	0.18	0.03	0.42	0.00	3.60	0.10	45.68	2.28	43.22	2.16	9.54	0.48	1.56	0.08	706.2	25.0
37.5	8.0	1.2	0.10	0.03	0.41	0.00	3.18	0.10	48.36	2.42	39.50	1.98	10.69	0.53	1.45	0.07	706.1	25.0
25	7.3	1.1	0.07	0.03	0.50	0.00	3.54	0.10	43.91	2.20	44.00	2.20	11.23	0.56	0.87	0.04	696.7	25.0
0	6.0	0.5	0.00	0.00	0.57	0.01	3.72	0.10	47.81	2.39	46.43	2.32	5.01	0.25	0.75	0.04	706.7	25.0

N_2 dilution

X_{NH3} (%)	Extinction X_F(%)		Fuel preheat temperature = 140 ± 5°C Fuel supply flow rates (SLPM)						Oxidizer boundary mole fractions (%)								Oxidizer temperature	
	Mean	±	NH_3	±	C_2H_5OH (mLPM	±	N_2	±	CO_2	±	O_2	±	H_2O	±	N_2	±	°C	±
100	24.4	1.0	0.98	0.02	0.00	0.00	3.03	0.06	0.00	0.00	24.33	1.22	18.59	0.93	57.08	2.85	831.7	35.7
87.5	17.1	2.0	0.47	0.03	0.16	0.00	2.80	0.28	3.72	1.95	20.66	1.67	13.87	2.19	61.74	5.71	733.5	86.0
75	10.8	1.2	0.30	0.03	0.24	0.00	3.28	0.10	4.06	0.20	22.14	1.11	11.51	0.58	62.29	3.11	712.8	25.0
62.5	8.6	1.3	0.17	0.03	0.25	0.00	2.98	0.10	5.43	0.27	16.02	0.80	9.21	0.46	69.34	3.47	694.4	42.0
50	7.1	1.4	0.10	0.03	0.24	0.00	2.63	0.10	6.87	0.34	12.13	0.61	9.27	0.46	71.73	3.59	683.8	25.0
37.5	5.8	0.9	0.09	0.03	0.35	0.00	3.89	0.10	5.50	0.28	22.83	1.14	6.67	0.33	65.00	3.25	712.0	25.0
25	4.5	0.9	0.05	0.03	0.35	0.00	4.20	0.10	5.57	0.28	20.86	1.04	5.51	0.28	68.05	3.40	691.5	25.0
0	3.5	0.5	0.00	0.00	0.47	0.00	5.45	0.10	6.17	0.31	20.55	1.03	4.55	0.23	68.73	3.44	717.6	25.0

Performance of the kinetic models:

The absolute value of the relative error (E) between the predicted ($X_{F,model}$) and measured ($X_{F,exp}$) extinction limits is computed as:

$$E = \left| \frac{X_{F,model} - X_{F,exp}}{X_{F,exp}} \right|$$

For a given kinetic model, the error is averaged over all the flame conditions (E_{avg}) tests and reported in the table below.

Model	E_{avg} (%)	Applicable NH_3 fuel blends
Wang2021	8.4%	CH_4, H_2, CH_3OH, C_2H_5OH (CO_2 & N_2 dilution)
Okafor2018	9.1%	CH_4, H_2, CH_3OH (CO_2 & N_2 dilution)
GRI3.0	9.9%	CH_4, H_2, CH_3OH (CO_2 & N_2 dilution)
Han2020	11.2%	H_2 (N_2 dilution)
Kovaleva2022	11.8%	CH_4, H_2, CH_3OH (CO_2 & N_2 dilution)
Mie2021	11.2%	H_2 (N_2 dilution)
UCSD	14.0%	CH_4, H_2, CH_3OH, C_2H_5OH (CO_2 & N_2 dilution)
Thomas2023	15.6%	CH_4, H_2, CH_3OH, C_2H_5OH (CO_2 & N_2 dilution)
POLIMI	19.4%	H_2 (N_2 dilution)
Zhang2021	14.9%	H_2 (N_2 dilution)
Shrestha2025	20.3%	H_2 (N_2 dilution)