

A Comparative Study of Benzene Oxidation in Lean-to-Rich Laminar Premixed Flames

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Laminar premixed benzene flames are important tools for understanding the combustion chemistry of practical fuels with a significant aromatic content. Despite numerous experimental and numerical investigations [1, 2], uncertainties still exist regarding even major benzene combustion features. A handful of very recent premixed benzene flame data sets [3] offer a unique possibility for the judicious evaluation both of experimental and simulated data under similar or even virtually identical operating conditions. In the present work, a single, comprehensive detailed chemical kinetic mechanism [4] is utilized in order to model and analyze twelve low-pressure laminar premixed benzene flames, see Table 1

Flame	Φ	C/O	P(Torr)	X _{fuel}	X _{O₂}	X _{Ar}	V(cm/s)	m(mg/cm2s)
A	0.7	0.31	33.75	3	29	68		2.931
B	0.75	0.3	30	5.91	59.09	35	36.1	
C	1	0.45	33.75	3	20	77		2.984
D	1	0.4	30	7.64	57.36	35	36.1	
E	1.25	0.5	30	9.27	55.73	35	36.1	
F	1.5	0.6	30	10.84	54.16	35	36.1	
G	1.75	0.7	30	12.32	52.68	35	36.1	
H	1.78	0.7	30	9.5	40.5	50		2.1
I	1.8	0.72	20.03	13.5	56.5	30	50	
J	2	0.82	33.75	12	44	44		3.102
K	2	0.8	37.5	11.8	44.2	44	35	
L	2	0.8	30	13.68	51.32	35	36.1	

Table 1. Investigated flames

Although the level of agreement between experimental results and simulations is generally good, several uncertainties remain relating to important features of benzene combustion. The first relates to the phenyl, phenoxy, and phenol chemistry, and in particular the rate and product distribution of the $C_6H_5+O_2$ reaction. The original mechanism postulates phenoxy as the major product of this reaction, which leads to an over-prediction of phenol levels, particularly for lean stoichiometric flames. In this work a channeling of the above reaction directly to C_5 species, as suggested by the recent literature, is proposed, yielding satisfying results, and greatly improved predictions of phenol and cyclopentadiene profiles. This is depicted in Figure 1. A further issue relates to the over-prediction of carbonaceous species in the post flame zone of rich flames (see Figure 2). This is a persistent feature of rich hydrocarbon flames regardless the kinetic scheme used. The wealth of flame datasets examined in this study makes it possible to quantify experimental uncertainties and assess their influence on modelling. Figure-2a and b compare temperature and species data from the virtually identical Flames J and K – only differing slightly in the temperature profiles. This however is insufficient to explain the (more than a factor of 2) differences in key intermediate species profiles (such as C_3H_4). It may lay

on measurement uncertainty, but complicates modelling efforts. Another aspect investigated in the context of the current work is the effect of varying dilution levels. This can be quantified by examining Flames C and D which are characterized by the same C/O ratio but vary in the levels of argon dilution. This results in significant temperature differences and the rates of fuel (and oxygen) decay. Major species are also affected (at a ratio close to the dilution ratio) since their levels are mainly controlled by pressure dependent reactions with rates largely determined by diluent levels. On the other hand stable intermediates are not seriously affected.

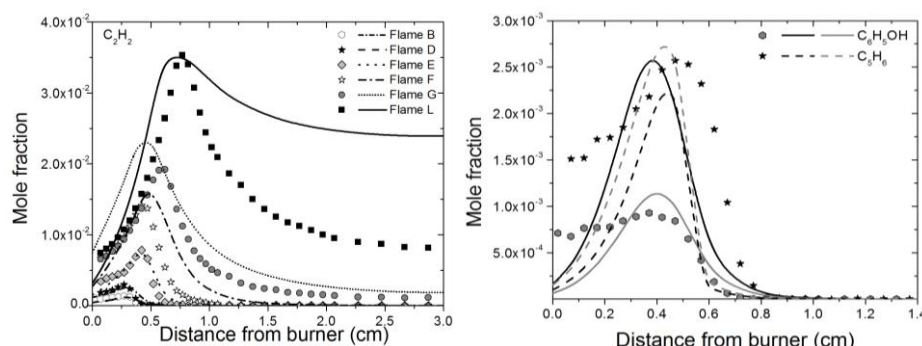


Figure 1. Comparison of experimental (points) and simulated (lines) a: C_2H_2 and b: C_6H_5OH and C_5H_6 Grey lines correspond to the revised mechanism ()

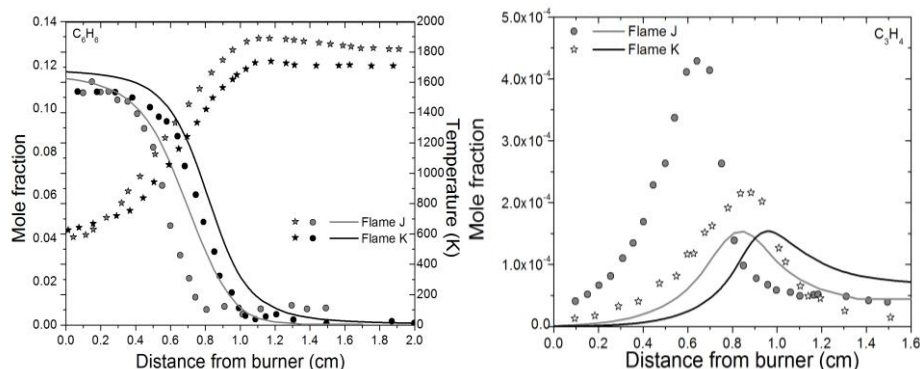


Figure 2.a: Measured temperature profiles (stars) and comparison of experimental (dots) and simulated (lines) C_6H_6 species data, b: Comparison of experimental (points) and simulated (lines) C_3H_4 species data

References

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