

SUPPLEMENTAL MATERIAL

to

Combustion chemistry and flame structure of furan group biofuels using molecular-beam mass spectrometry and gas chromatography – Part III: 2,5-dimethylfuran

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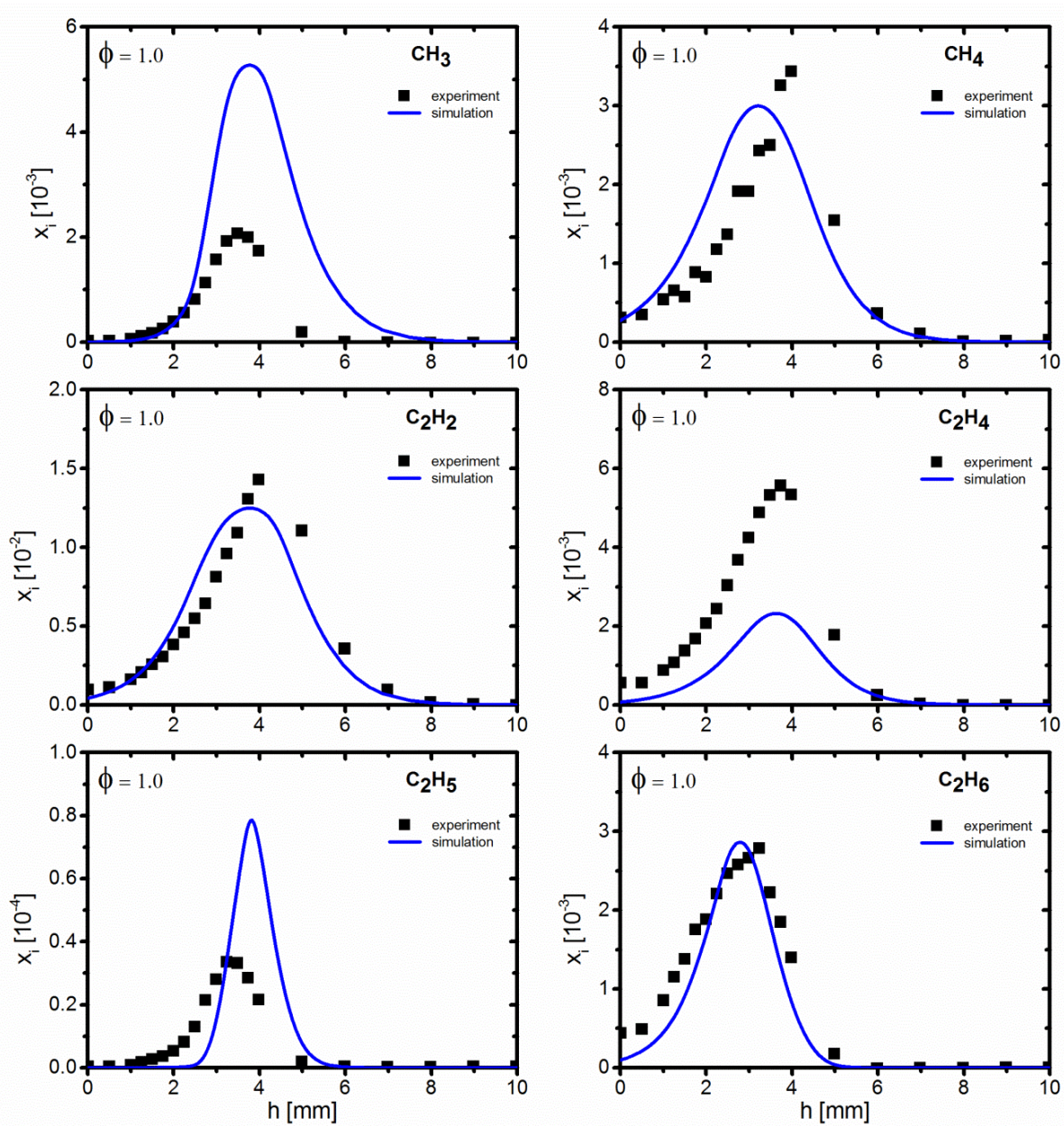


Figure S1. Mole fraction profiles of selected C_1 and C_2 species profiles for $\phi = 1.0$. Symbols: experiment; lines: simulation.

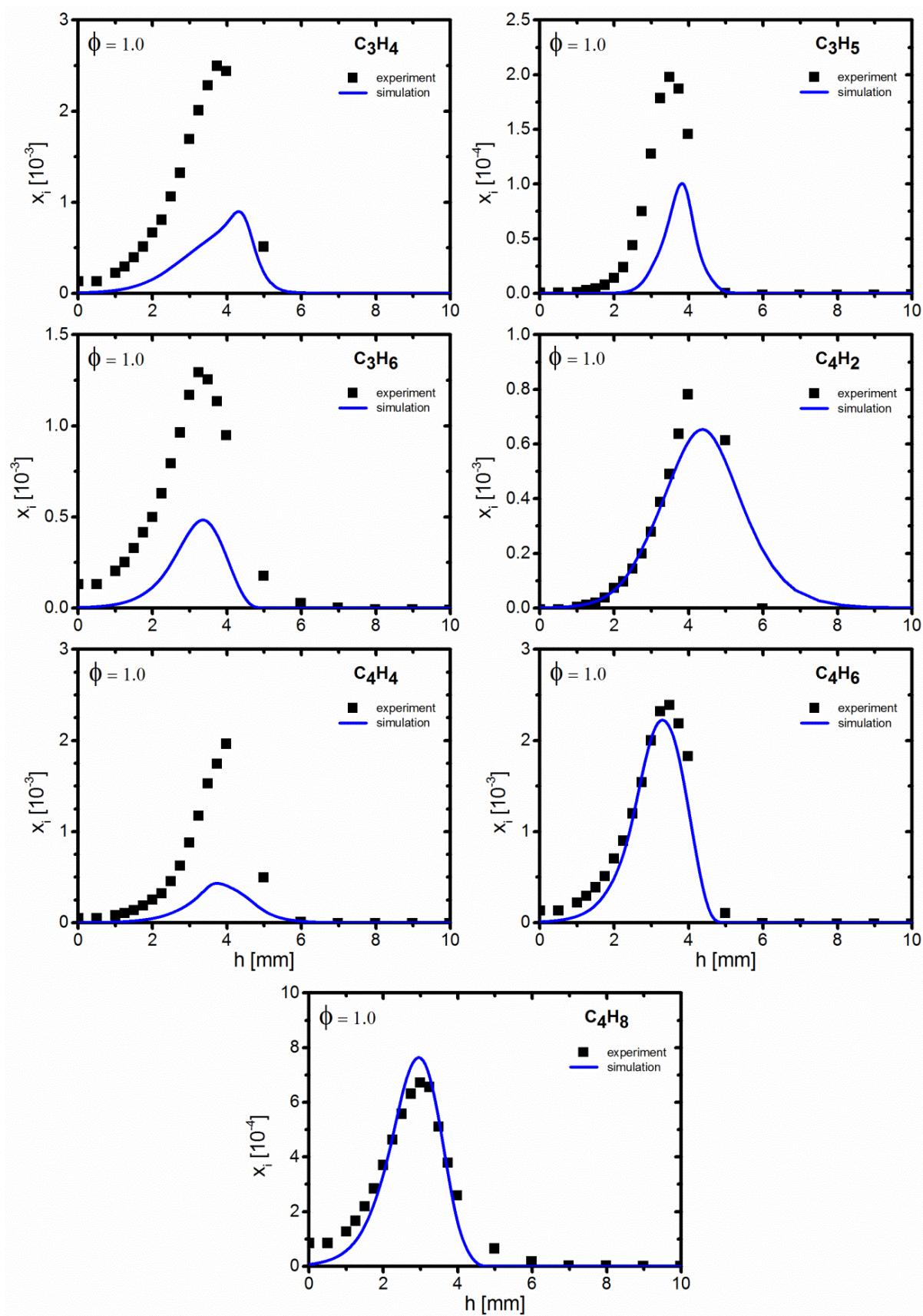


Figure S2. Mole fraction profiles of selected C₃ and C₄ species profiles for $\phi = 1.0$. Symbols: experiment; lines: simulation.

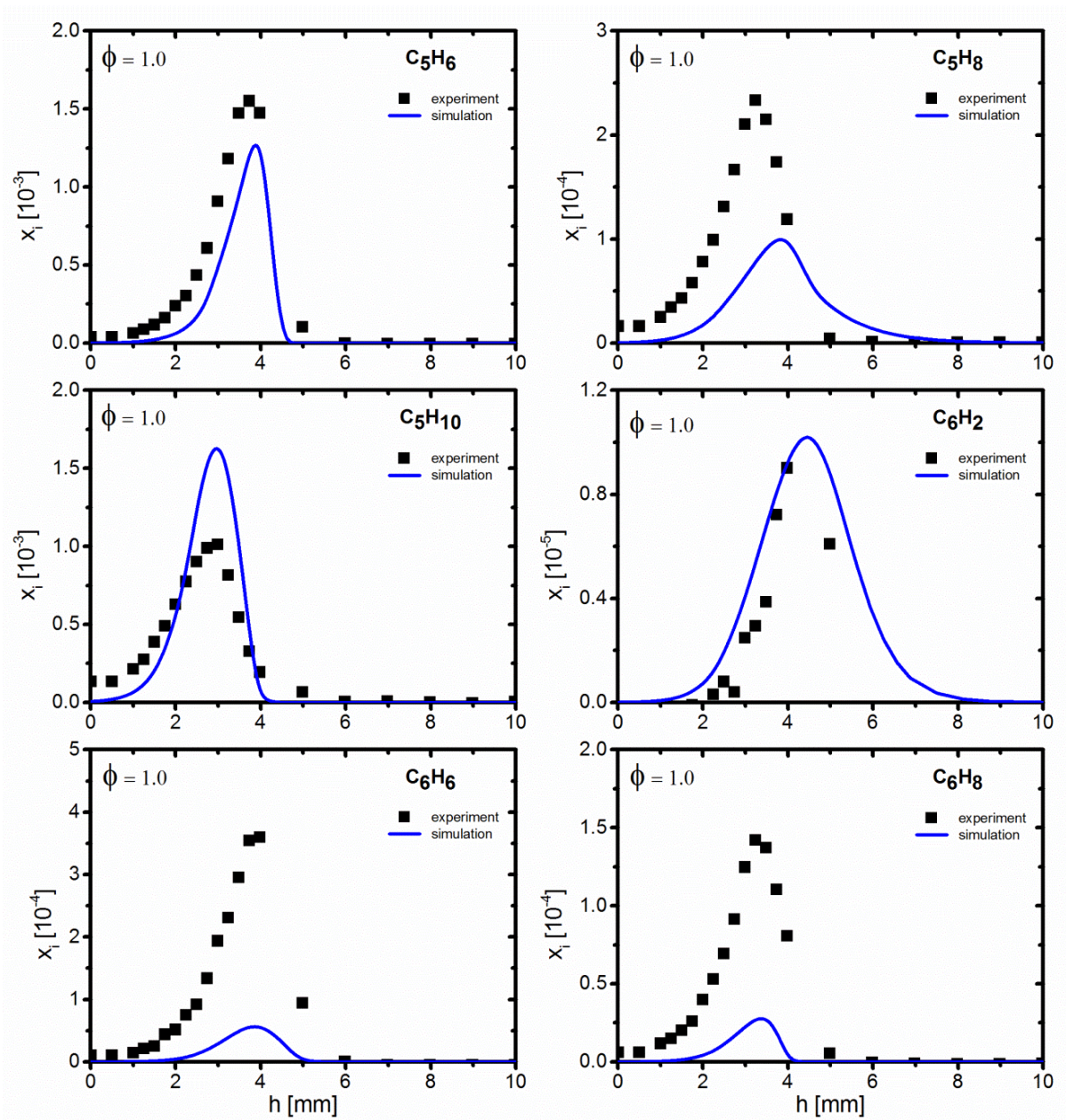


Figure S3. Mole fraction profiles of selected C₅ and C₆ species profiles for $\phi = 1.0$. Symbols: experiment; lines: simulation.

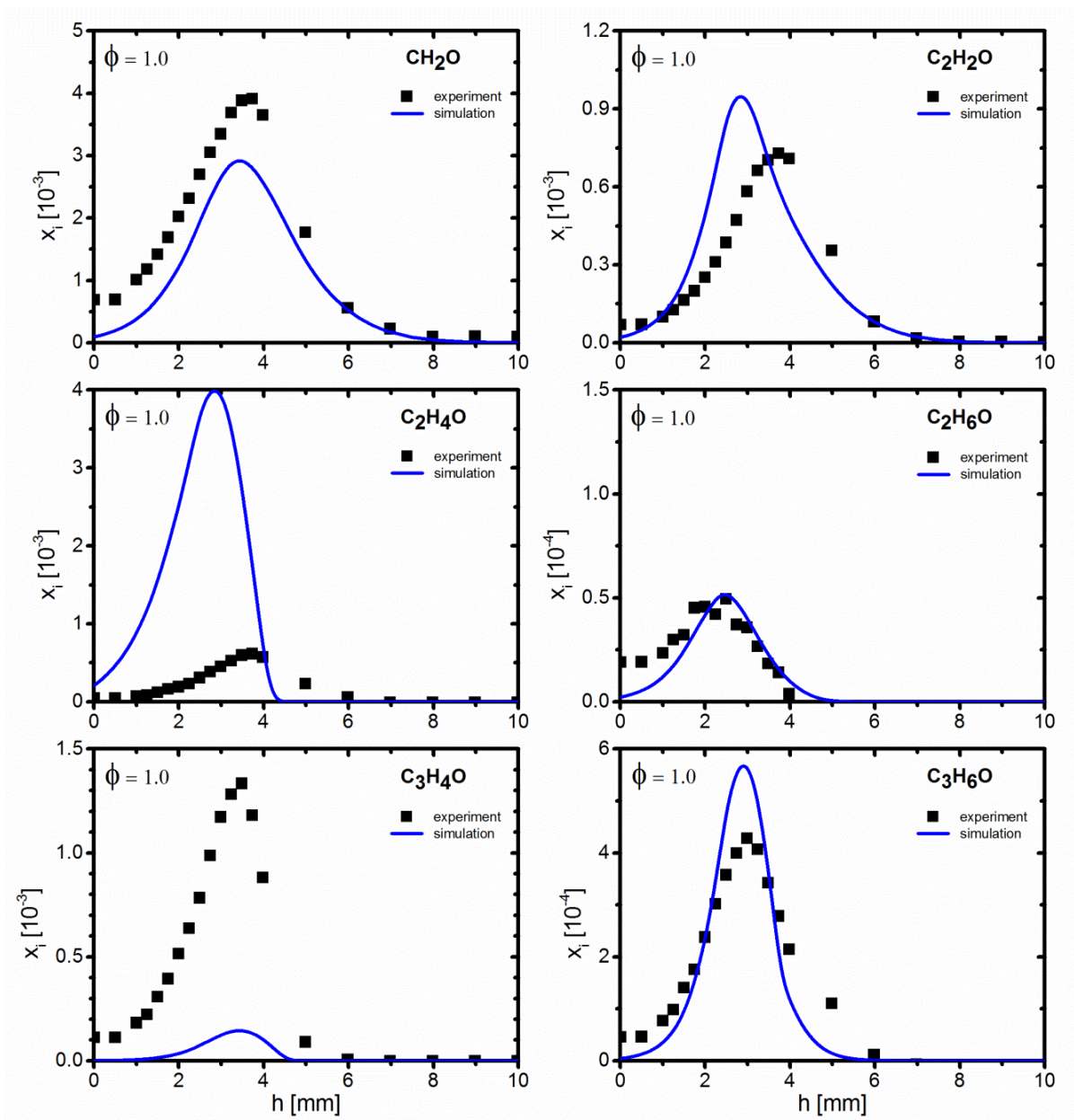


Figure S4. Mole fraction profiles of selected C₁-C₃ oxygenated species profiles for $\phi = 1.0$. Symbols: experiment; lines: simulation.

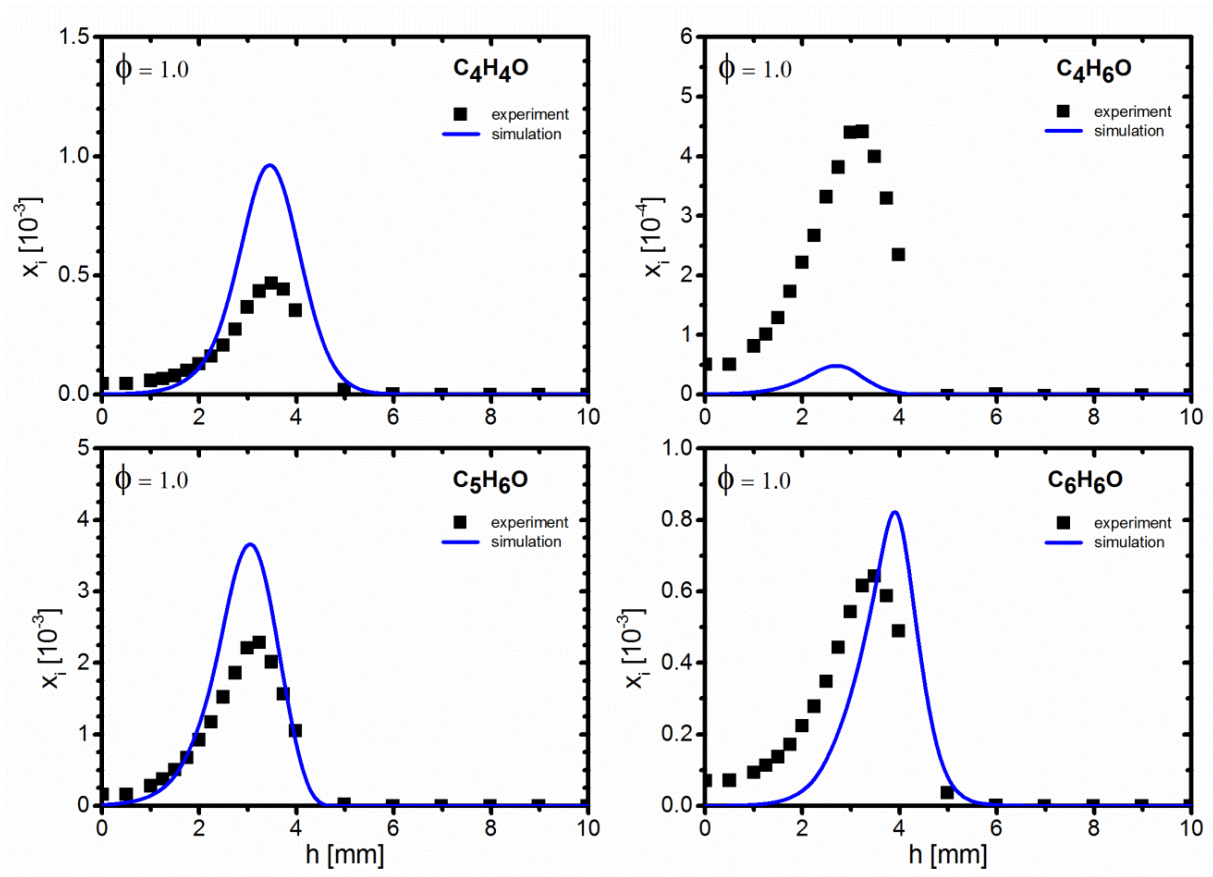


Figure S5. Mole fraction profiles of selected C₄-C₆ oxygenated species profiles for $\phi = 1.0$. Symbols: experiment; lines: simulation.

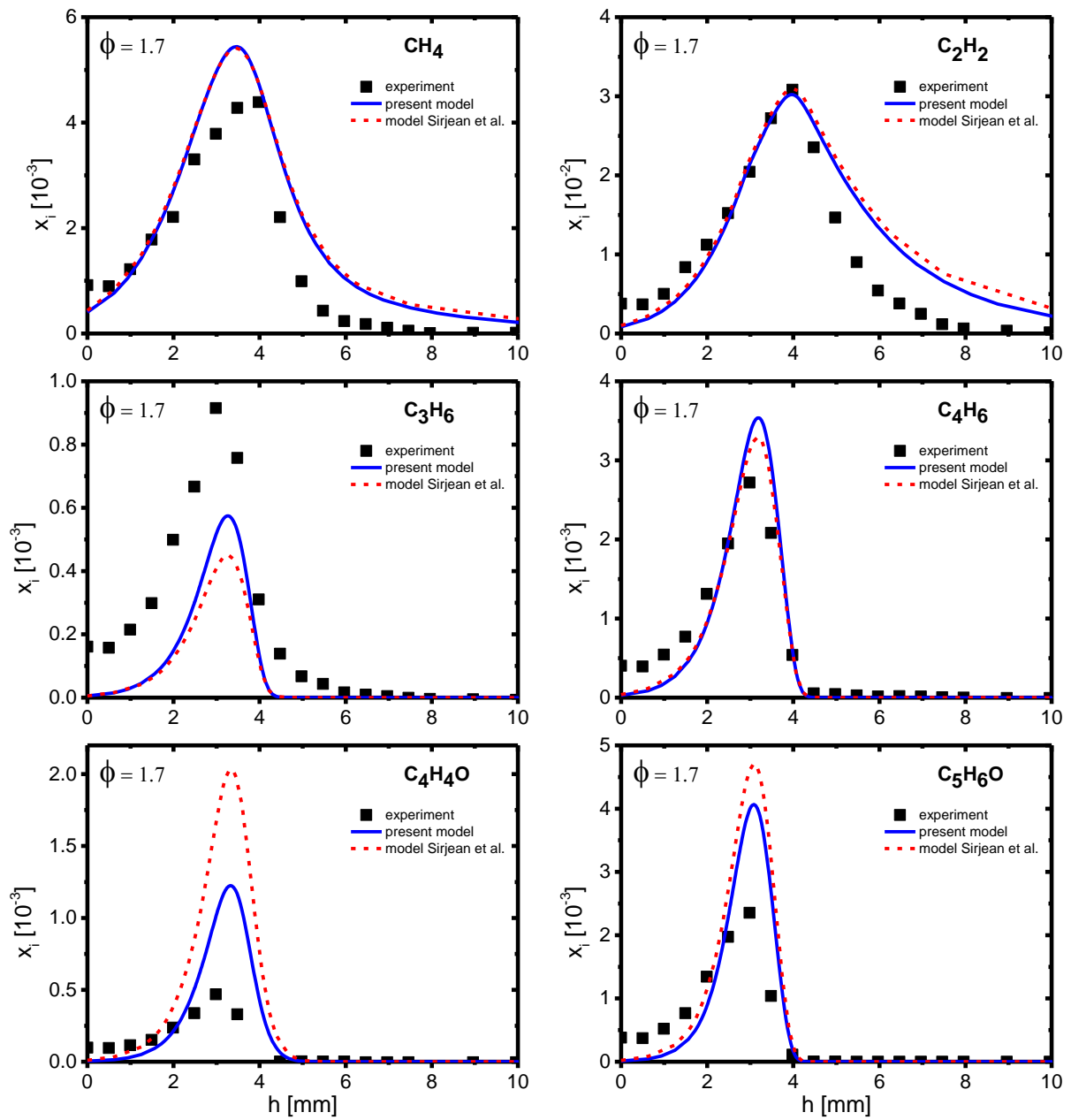


Figure S6. Examples for the comparison between the present model and that of Sirjean et al. [28].

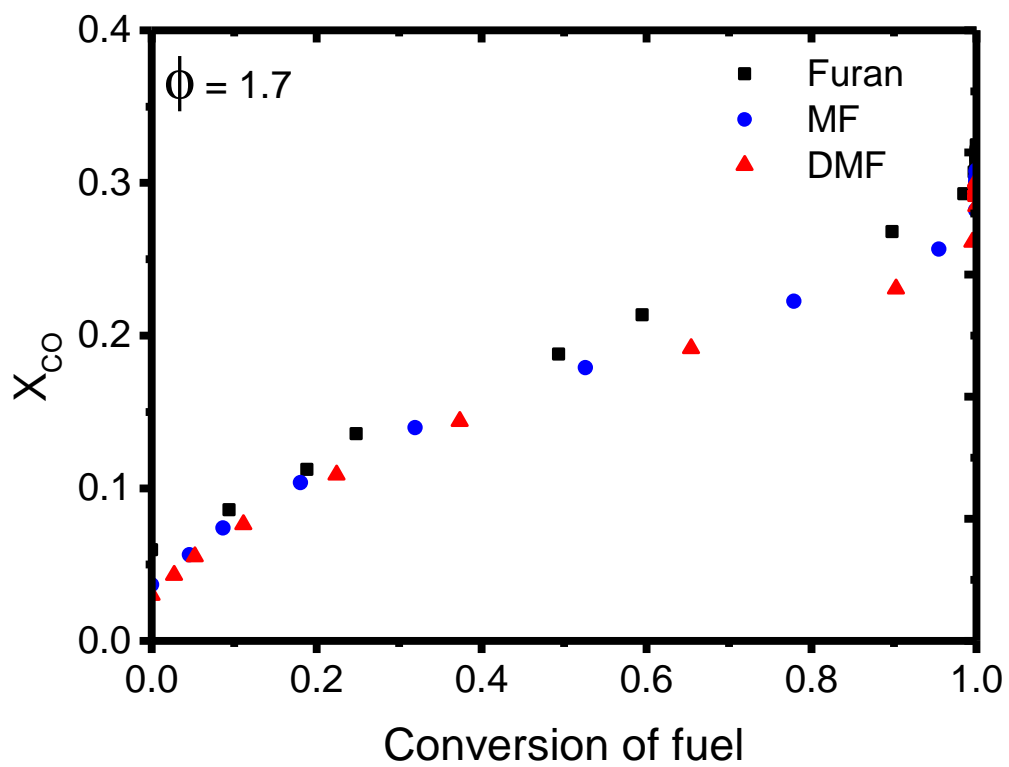


Figure S7. Mole fraction profiles of CO profiles as a function of fuel conversion.

Table S1

Comparison between the maximum mole fractions (x) of the main intermediate species measured in the three fuel flames. The largest mole fractions for each species obtained in the three fuels are written in bold.

Species quantified		$\phi = 1.0$			$\phi = 1.7$		
Formula	Name	x_{Furan} (ppm)	x_{MF} (ppm)	x_{DMF} (ppm)	x_{Furan} (ppm)	x_{MF} (ppm)	x_{DMF} (ppm)
CH ₃	Methyl	1140	1920	2070	1490	1530	1960
CH ₄	Methane	2360	3050	3440	3300	4260	4390
C ₂ H ₂	Acetylene	18200	15900	14300	34900	33400	30800
C ₂ H ₃	Vinyl	6.32	-	5.30	5.77	5.95	5.65
C ₂ H ₄	Ethylene	5690	6210	5570	6720	8040	7050
C ₂ H ₅	Ethyl	26.9	41.0	33.7	23.6	25.2	24.5
HCO	Formyl	71.1	44.6	34.7	55.0	29.7	25.2
C ₂ H ₆	Ethane	1450	2370	2790	1980	2550	3000
CH ₂ O	Formaldehyde	3950	3980	3920	3840	3300	2910
CH ₄ O	Methanol	492	227	350	436	143	306
C ₃ H ₃	Propargyl	37.2	182	160	104	248	355
C ₃ H ₄	Propyne	1820	2950	2500	2960	4760	3790
C ₃ H ₅	Allyl	152	305	198	151	190	165
C ₂ H ₂ O	Ketene	361	637	2470	358	551	752
C ₃ H ₆	Propene	1430	1830	1290	1110	1130	915
C ₂ H ₄ O	Acetaldehyde	3740	1040	618	3180	608	674
C ₂ H ₆ O	Dimethylether	23.9	34.0	49.6	39.0	25.6	42.0
C ₄ H ₂	1,3-Butadiyne	134	509	782	1080	2150	4200
C ₄ H ₄	1-Buten-3-yne	163	1500	3250	482	2160	3585
C ₄ H ₅	But-2-yn-1-yl	2.38	30.7	42.2	5.33	38.3	122
C ₄ H ₆	1,3-Butadiene	248	2230	2390	456	2020	2720
C ₄ H ₇	But-3-en-1-yl	7.75	171	81.0	14.0	146	42.7
C ₄ H ₈	1-Butene	510	1120	672	643	862	409
C ₃ H ₄ O	Propenal	2750	1960	1330	2450	1370	847
C ₃ H ₆ O	Propanal	859	354	428	417	175	138
C ₅ H ₄	1,3-Pentadiyne	5.93	22.5	39.9	28.2	57.9	126
C ₅ H ₆	1,3-Cyclopentadiene	49.2	158	1550	101	202	2500
C ₅ H ₇	3-Cyclopentenyl	0.9	2.16	7.24	1.3	2.23	17.0
C ₄ H ₄ O	Furan	Fuel	3080	468	Fuel	3100	469
C ₅ H ₈	1,3-Pentadiene	n/a	58	233	n/a	68.9	230
C ₄ H ₆ O	2-Butenal	396	n/a	n/a	291	n/a	n/a
C ₄ H ₆ O	2-Butenone	n/a	395	441.8	n/a	241	243
C ₅ H ₁₀	2-Pentene	13.0	110	101	24.7	124	69.2
C ₄ H ₈ O	Isobutanal	105	114	n/a	102	421	n/a
C ₄ H ₈ O	2-Butenone	n/a	n/a	32.1	n/a	n/a	12.4
C ₆ H ₂	Triacetylene	3.22	12.2	9.02	36.6	60.9	130
C ₆ H ₄	Benzynes	1.74	9.19	11.5	11.9	29.5	54.6
C ₆ H ₆	Benzene	42.3	141	360	131	275	1000
C ₆ H ₈	1,4-Cyclohexadiene	21.4	29.7	142	41	42.8	308
C ₅ H ₄ O	Allenylketene	n/a	5.54	0	n/a	5.49	46.8
C ₅ H ₅ O	2-Furanylmethyl	n/a	82.2	179	n/a	97.4	272
C ₅ H ₆ O	2-Methylfuran	68.8	Fuel	2290	88.9	Fuel	2350
C ₅ H ₈ O	2,5-Dihydro-2MF	20.5	n/a	n/a	10.7	n/a	n/a
C ₅ H ₈ O	3-Pentene-2-one	n/a	516	79.5	n/a	240	40.9
C ₇ H ₈	Toluene	2.98	24.6	43.1	9.63	42.4	45.9
C ₆ H ₆ O	Phenol	6.15	29.0	445	9.70	25.5	626
C ₆ H ₇ O	2-(5-Methyl)furanylmethyl	n/a	n/a	253	n/a	n/a	467
C ₆ H ₈ O	2,5DMF	5.8	259	Fuel	5	284	Fuel

n/a: not applicable

Table S2.

Name and structure of some species involved in the detailed mechanism of the DMF oxidation.

Species	Name	Species	Name	Species	Name
	DMF		R8C ₆ H ₇ O		Furyl-2
	MF		R9C ₆ H ₇ O		Furyl-3
	Furan		M2C ₆ H ₆ O		C ₄ H ₅ O-3
	R1C ₆ H ₇ O		M3C ₆ H ₆ O		C ₄ H ₅ O-2
	R2C ₆ H ₇ O		B1C ₆ H ₆ O		C ₅ H ₅ #
	R3C ₆ H ₇ O		C ₆ H ₅ O#		1,3-C ₅ H ₆
	R4C ₆ H ₇ O		C ₆ H ₅ OH		C ₅ H ₇ Y
	R5C ₆ H ₇ O		Bicycle		C ₅ H ₇ #Y
	R6C ₆ H ₇ O		furylCH ₂		C ₅ H ₇ -1s
	R7C ₆ H ₇ O		M5F-2yl		C ₅ H ₇ #