

Experimental and Kinetic Modeling Study of 2-Methylfuran Pyrolysis at Low and Atmospheric Pressures

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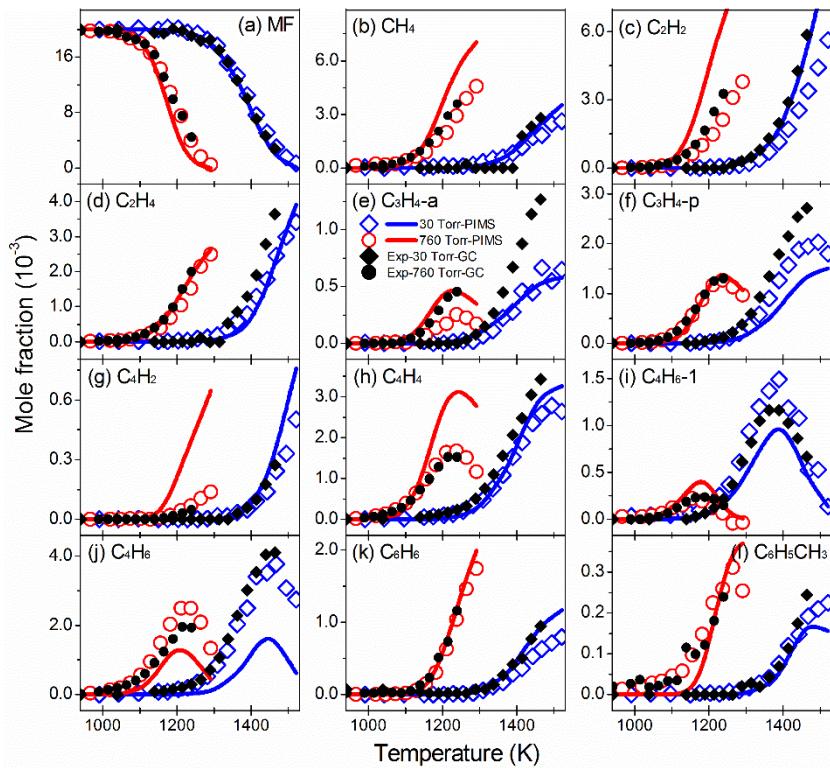


Fig. S1 Comparison of experimental results of SVUV-PIMS (open symbols) and GC (solid symbols) at 30 and 760 Torr in MF pyrolysis. Lines represent the simulated results by the updated model.

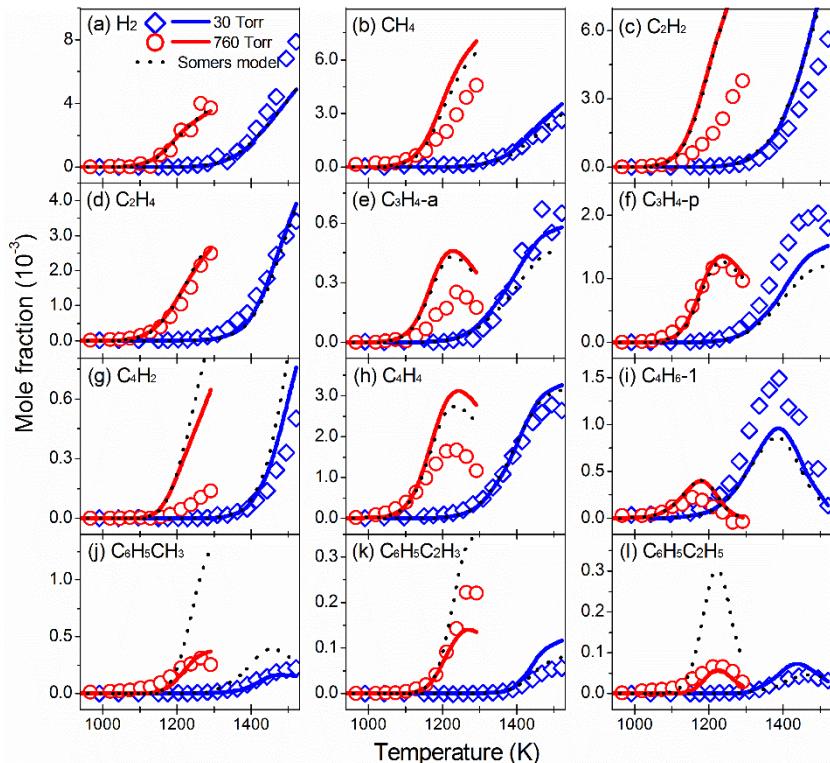


Fig. S2 Experimental and simulated mole fraction profiles of many decomposition products and aromatic specie in MF pyrolysis. Symbols, solid lines, and dashed lines represent the SVUV-PIMS data, the simulated results by the updated model, and the simulated results by the Somers model.¹

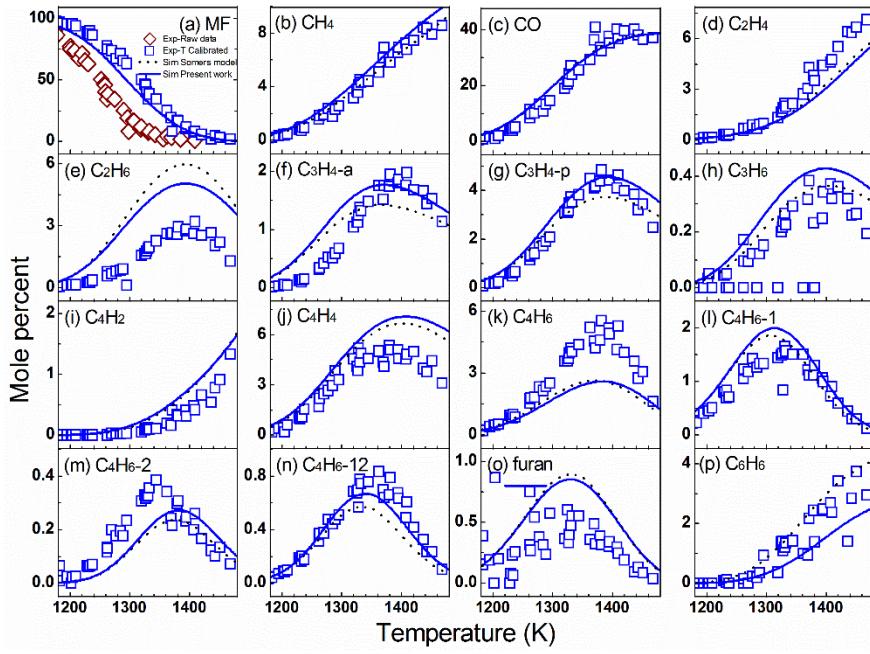


Fig. S3 Simulation of the shock tube pyrolysis of 0.5% MF in argon. The experimental data of Lifshitz et al.² (open squares) were calibrated by Somers et al.¹ Solid lines and dot lines represent the simulated results by the updated model and the Somers model.¹

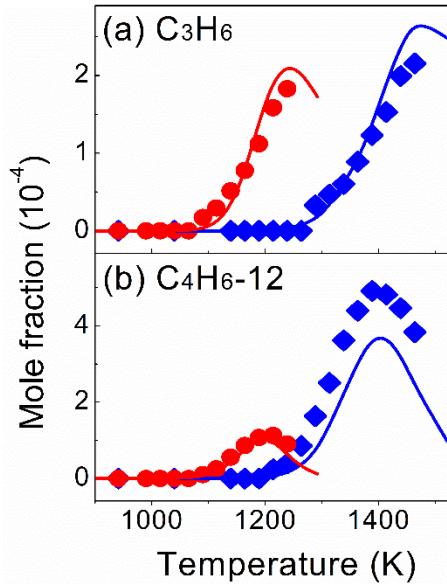


Fig. S4 Experimental and simulated mole fraction profiles of propene (C_3H_6) and 1,2-butadiene (C_4H_6-12) in MF pyrolysis. Symbols and solid lines represent the GC data and the simulated results by the updated mode.

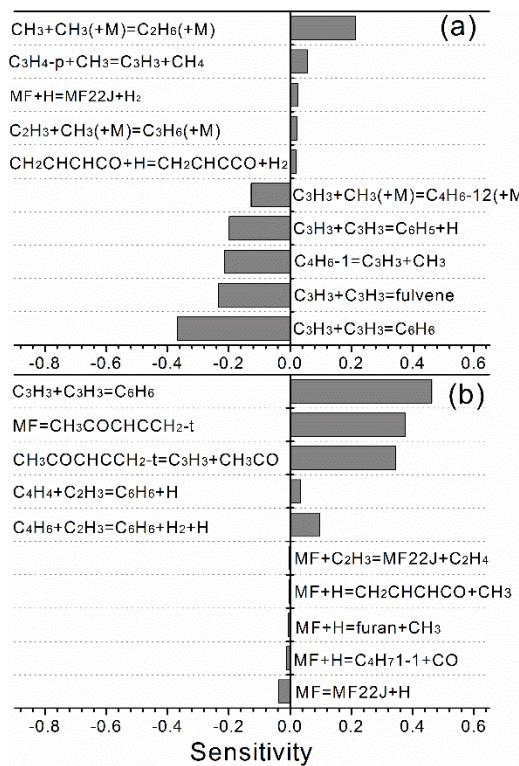


Fig. S5 Sensitivity analysis of (a) C₃H₃ and (b) C₆H₆ at 1442 K and 30 Torr in MF pyrolysis.

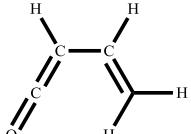
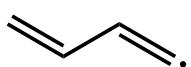
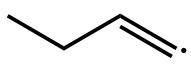
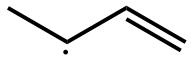
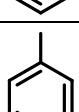
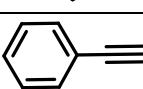
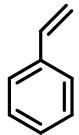
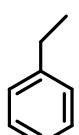
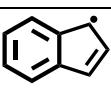
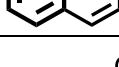
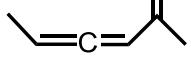
Table S1. A list of reactions in the updated model discussed in the manuscript, units are s⁻¹, cm³ and cal/mol.^a

Selected reactions	A	n	E	Pressure (Torr)	References
<i>Reactions of some important aromatics</i>					
1 C ₃ H ₃ + C ₃ H ₃ = C ₆ H ₆	1.64E+66	-15.9	2.75E+04	30	³
Duplicate	1.20E+35	-7.40	5.06E+03	30	
	1.07E+45	-9.57	1.70E+04	760	⁴
	7.17E+40	-8.24	1.59E+04	7600	
2 C ₃ H ₃ + C ₃ H ₃ = C ₆ H ₅ + H	2.02E+33	-6.00	1.59E+04	30	³
	5.77E+37	-7.00	3.15E+04	760	⁴
	3.87E+33	-5.67	3.04E+04	7600	
3 C ₃ H ₃ + C ₃ H ₃ = fulvene	7.25E+65	-16.00	2.50E+04	30	³
Duplicate	4.19E+03	-9.00	6.10E+03	30	
	8.25E+46	-10.10	1.69E+04	760	⁴
	5.53E+42	-8.77	1.58E+04	7600	
4 fulvene = C ₆ H ₆	5.62E+81	-19.36	1.22E+05	30	⁵
	1.45E+45	-8.90	9.70E+04	760	
	2.95E+31	-4.97	8.85E+04	7600	
5 fulvene+H= C ₆ H ₆ +H	4.94E+18	-1.28	5.41E+03	1	⁶
	2.15E+22	-2.28	8.43E+03	10	
	5.60E+26	-3.47	1.28E+04	100	
	1.66E+25	-2.99	1.37E+04	760	
	5.06E+25	-3.12	1.42E+04	1000	
	2.20E+27	-3.48	1.92E+04	10000	
6 fulvene= C ₆ H ₅ +H	2.57E+97	-23.20	1.53E+05	30	⁵
	2.24E+68	-14.70	1.43E+05	760	
	8.51E+24	-2.50	1.13E+05	7600	
7 C ₃ H ₃ + C ₄ H ₄ = C ₆ H ₅ CH ₂	1.76E-30	3.52	-1.64E+04	7.6	⁷
	9.80E+68	-23.55	6.78E+04	76	
	1.88E+100	-31.77	1.02E+05	760	
	2.43E+67	-22.14	8.76E+04	22800	
8 C ₃ H ₃ + C ₃ H ₅ -a = fulvene + 2H	3.26E+29	-5.40	3.39E+03		⁸
9 C ₆ H ₅ CH ₂ + CH ₃ = C ₆ H ₅ C ₂ H ₅	2.12E+16	-0.97	6.20E+02		⁹
	LOW/ 1.77E+50	-9.67	6.22E+03		
	TROE/ 5.33E-01 1.51E+02	1.04E+03	4.97E+03/		
10 C ₄ H ₄ + C ₂ H ₃ = C ₆ H ₆ + H	1.90E+12	0.00	2.51E+03		¹⁰
11 C ₆ H ₅ CH ₂ + H = C ₆ H ₅ + CH ₃	4.50E+58	-11.90	5.19E+04	30	¹¹
	2.03E+64	-13.37	5.95E+04	150	
	5.83E+67	-14.15	6.83E+04	760	
	8.85E+68	-14.23	7.84E+04	7600	
12 C ₅ H ₅ + C ₃ H ₃ = C ₆ H ₅ C ₂ H ₃	1.64E+66	-15.9	2.75E+04	30	¹²
Duplicate	1.20E+35	-7.40	5.06E+03	30	

1.07E+45	-9.57	1.70E+04	760
7.17E+40	-8.24	1.59E+04	7600

Table S2. The chemical structures of important species discussed in this work.

formula	nomenclature	structure
C ₅ H ₆ O	MF	
C ₅ H ₅ O	MF22J	
CH ₃ CHCCHCHO-t	p23de1o-t	
CH ₃ CHCCHCHO-c	p23de1o-c	
CH ₃ COCHCCH ₂ -t	p34de2o-t	
CH ₃ COCHCCH ₂ -c	p34de2o-c	
C ₅ H ₅ O	p34de1o2j-c2	
C ₅ H ₅ O	p24de1o1j-c1	
C ₅ H ₅ O	p34de1o2j-c1	
C ₅ H ₅ O	p14de1o3j-c1	

C ₄ H ₄ O	CH ₂ CHCHCO	
C ₄ H ₅	C4H5-n	
C ₄ H ₇	C4H71-1	
C ₄ H ₇	C4H71-3	
C ₆ H ₆	C6H6	
C ₇ H ₇	C6H5CH ₂	
C ₇ H ₈	C6H5CH ₃	
C ₈ H ₆	C6H5C2H	
C ₈ H ₈	C6H5C2H3	
C ₈ H ₈	C6H5C2H5	
C ₉ H ₇	C9H7	
C ₉ H ₈	C9H8	
C ₁₀ H ₈	C10H8	
C ₆ H ₈ O	M4C6H8O	

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