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Open burning of rice, corn and wheat straws: primary emissions, photochemical aging, and secondary organic aerosol formation

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Table S1. Emission factors for the non-methane hydrocarbons (NMHCs) species from the straw burning.

No.	Species	EF ($g\ kg^{-1}$)		
		Rice	Corn	Wheat
1	ethene	1.316±0.492	0.540±0.484	0.777±0.666
2	acetylene	0.958±0.328	0.149±0.108	0.293±0.294
3	propene	0.315±0.323	0.342±0.295	0.332±0.272
4	1-butene	0.045±0.018	0.027±0.029	0.044±0.071
5	1,3-butadiene	0.030±0.038	0.116±0.110	0.104±0.080
6	trans-2-butene	0.016±0.005	0.035±0.031	0.040±0.038
7	cis-2-butene	0.013±0.004	0.025±0.022	0.030±0.028
8	3-methyl-1-butene	0.007±0.003	0.009±0.009	0.008±0.006
9	1-pentene	0.017±0.011	0.029±0.031	0.021±0.025
10	2-methyl-1-butene	0.012±0.008	0.004±0.002	0.013±0.011
11	isoprene	0.096±0.101	0.026±0.035	0.060±0.045
12	trans-2-pentene	0.010±0.011	0.012±0.010	0.016±0.013
13	cis-2-pentene	0.010±0.005	0.007±0.006	0.007±0.006
14	2-methyl-2-butene	0.018±0.021	0.013±0.012	0.015±0.012
15	cyclopentene	0.005±0.007	0.008±0.007	0.008±0.007
16	4-methyl-1-pentene	0.003±0.004	0.002±0.003	0.001±0.001
17	1-hexene	0.007±0.004	0.016±0.025	ND
18	trans-2-hexene	ND	0.003±0.005	ND
19	cis-2-hexene	0.001±0.003	0.001±0.001	0.001±0.001
20	3-hexene	0.002±0.003	0.002±0.002	0.001±0.002
21	a-pinene	0.008±0.022	ND	ND
22	b-pinene	0.011±0.019	ND	ND
23	ethane	0.492±0.603	0.452±0.357	0.586±0.615
24	propane	0.171±0.196	0.127±0.127	0.103±0.155
25	isobutane	0.052±0.043	0.011±0.011	0.004±0.007
26	n-butane	0.062±0.060	0.034±0.030	0.078±0.129
27	isopentane	0.036±0.051	0.015±0.016	0.031±0.035
28	n-pentane	0.016±0.008	0.011±0.014	0.006±0.009
29	2,2-dimethyl-butane	0.004±0.007	ND	ND
30	cyclopentane	ND	0.001±0.001	0.002±0.004
31	2,3-dimethylbutane	ND	ND	0.001±0.001
32	2-methylpentane	0.008±0.011	0.002±0.002	0.001±0.001
33	3-methylpentane	0.006±0.007	0.008±0.014	ND
34	n-hexane	0.120±0.175	0.001±0.002	0.001±0.001
35	methyl-cyclopentane	0.003±0.004	0.001±0.001	0.001±0.001
36	2,4-dimethylpentane	0.001±0.002	ND[a]	ND
37	cyclohexane	0.020±0.042	0.001±0.001	ND
38	2-methyl-hexane	0.002±0.004	ND	0.001±0.001
39	2,3-dimethyl-pentane	0.001±0.004	ND	ND
40	3-methyl-hexane	0.006±0.009	0.001±0.002	ND
41	2,2,4-trimethyl-pentane	0.002±0.003	ND	ND
42	n-heptane	0.037±0.058	0.003±0.004	0.003±0.002
43	methyl-cyclohexane	0.003±0.006	ND	ND
44	2,3,4-trimethyl-pentane	0.000±0.001	ND	ND
45	2-methyl-heptane	0.011±0.025	0.001±0.001	ND
46	3-methyl-heptane	0.001±0.001	ND	ND
47	n-octane	0.005±0.005	0.002±0.003	0.002±0.002
48	n-nonane	0.015±0.024	0.002±0.003	0.002±0.001
49	n-decane	0.005±0.006	0.004±0.005	ND
50	n-undecane	ND	0.007±0.012	ND
51	benzene	0.567±0.172	0.163±0.124	0.249±0.200
52	toluene	0.206±0.148	0.142±0.186	0.134±0.099
53	ethyl-benzene	0.027±0.017	0.016±0.024	0.012±0.009
54	m/p-xylene	0.045±0.043	0.020±0.029	0.030±0.023
55	styrene	0.095±0.033	0.035±0.031	0.029±0.021
56	o-xylene	0.016±0.014	0.008±0.011	0.008±0.006
57	isopropylbenzene	0.003±0.004	0.001±0.001	0.001±0.001
58	n-propylbenzene	0.003±0.003	0.003±0.004	0.002±0.001
59	m-ethyltoluene	0.005±0.003	0.003±0.003	0.005±0.004
60	p-ethyltoluene	0.005±0.004	0.002±0.003	0.003±0.003
61	1,3,5-trimethyl-benzene	0.003±0.004	0.001±0.002	0.002±0.003
62	o-ethyltoluene	0.003±0.002	0.002±0.003	0.002±0.002
63	1,2,4-trimethylbenzene	0.006±0.006	0.004±0.006	0.006±0.006
64	1,2,3-trimethylbenzene	0.039±0.086	0.007±0.010	0.005±0.005
65	m-diethylbenzene	0.003±0.005	0.001±0.001	0.001±0.001
66	p-diethylbenzene	0.004±0.007	0.002±0.002	0.001±0.001
67	o-diethylbenzene	0.002±0.004	0.001±0.001	ND

([a] ND=not deteced)

Table S2. Secondary organic aerosol yields reported in literature and used in our work for different precursors.

compound	yields reported in literature			yield used in our work		
	yield reference	seed[a]	yield range[b]	applied yield[c]	lower bound	upper bound
acrolein	Chhabra et al., 2011	yes	0.022	0.026	0.022	0.035
	Chan et al., 2010	yes	0.022-0.035			
furan	Gómez Alvarez et al., 2009	no	0.019-0.072	0.019	0.019	0.072
crotonaldehyde or methacrolein[d]	Chhabra et al., 2011	yes	0.02	0.02	0.019	0.194
	Chan et al., 2010	yes	0.019-0.194			
	Chhabra et al., 2011	yes	0.02			
	Chan et al., 2010	yes	0.019-0.044			
benzene	Ng et al., 2007	yes	0.28-0.37	0.33	0.28	0.37
	Nakao et al., 2011	no	0.19-0.28			
	Borras and Tortajada-Genaro, 2012	no	0.016-0.097			
2/3-methylfuran	Gómez Alvarez et al., 2009	no	0.055-0.085	0.085	0.055	0.085
	Chan et al., 2010	yes	0.008-0.391			

Table S2. Secondary organic aerosol yields reported in literature and used in our work for different precursors (continued).

compound	literature data			application of yield data		
	yield reference	seed[a]	yield range[b]	applied yield[c]	lower bound	upper bound
toluene	Chhabra et al., 2011	yes	0.11-0.36	0.26	0.08	0.66
	Ng et al., 2007	yes	0.08-0.31			
	Nakao et al., 2011	no	0.17-0.23			
	Hildebrandt et al., 2009	yes	0.26-0.66			
phenol	Yee et al., 2013	yes	0.24-0.54	0.38	0.13	0.54
	Nakao et al., 2011	no	0.38-0.45			
	Borras and Tortajada-Genaro, 2012	no	0.13-0.18			
	Chhabra et al., 2011	yes	0.34-0.38			
2,4-/2,5-dimethylfuran[e]				0.38	0.13	0.54
styrene[f]				0.22	0.04	0.4
benzaldehyde[g]				0.38	0.27	0.49
m-xylene	Chhabra et al., 2011	yes	0.06-0.4	0.22	0.04	0.4
	Ng et al., 2007	yes	0.04-0.38			
	Nakao et al., 2011	no	0.1-0.32			
o/m-cresol	Nakao et al., 2011	no	0.27-0.49	0.38	0.27	0.49
catechol or benzenediol	Nakao et al., 2011	no	0.39	0.53	0.39	0.53
	Borras and Tortajada-Genaro, 2012	no	0.45-0.53			
dimethylphenol	Nakao et al., 2011	no	0.13-0.9	0.52	0.13	0.9
guaiacol	Yee et al., 2013	yes	0.35-0.5	0.4	0.35	0.5
	Chhabra et al., 2011	yes	0.36-0.39			

Table S2. Secondary organic aerosol yields reported in literature and used in our work for different precursors (continued).

compound	literature data			application of yield data		
	yield reference	seed[a]	yield range[b]	applied yield[c]	lower bound	upper bound
naphthalene	Chhabra et al., 2011	yes	0.36-0.39	0.36	0.11	0.74
	Chhabra et al., 2011	yes	0.33-0.67			
	Chan et al., 2009	yes	0.2-0.74			
	Shakya and Griffin, 2010	no	0.11-0.12			
1/2-methylnaphthalene	Chan et al., 2009	yes	0.19-0.71	0.45	0.19	0.71
	Shakya and Griffin, 2010	no	0.04-0.15			
acenaphthalene	Shakya and Griffin, 2010	no	0.03-0.04	0.03	0.03	0.04
acenaphthene	Shakya and Griffin, 2010	no	0.04-0.05	0.05	0.04	0.05
1,2-dimethylnaphthalene	Chan et al., 2009	yes	0.31	0.31	0.31	0.31

(a Yields obtained without seed aerosol are not taken into account if yields obtained with seed aerosol are available; b the yields at the maximum and minimum NO_x/NMOGs ratios are determined to be the boundary values; c if the NO_x/NMOGs ratio in this study (1.2±0.9) are within the range in the corresponding literature, the average value of boundary values is used, or the yield at NO_x/NMOGs ratio closer to this study is used; besides, yields obtained from different studies were averaged; d averaged SOA yields were applied for isomers since they cannot be resolved by PTR-TOF-MS; e because of lack of available reported value, 2,4-/2,5-dimethylfuran is assumed to have the same SOA yield as phenol; f styrene is assumed to have the same SOA yield as m-xylene; g benzaldehyde is assumed to have the same SOA yield as o/m-cresol)

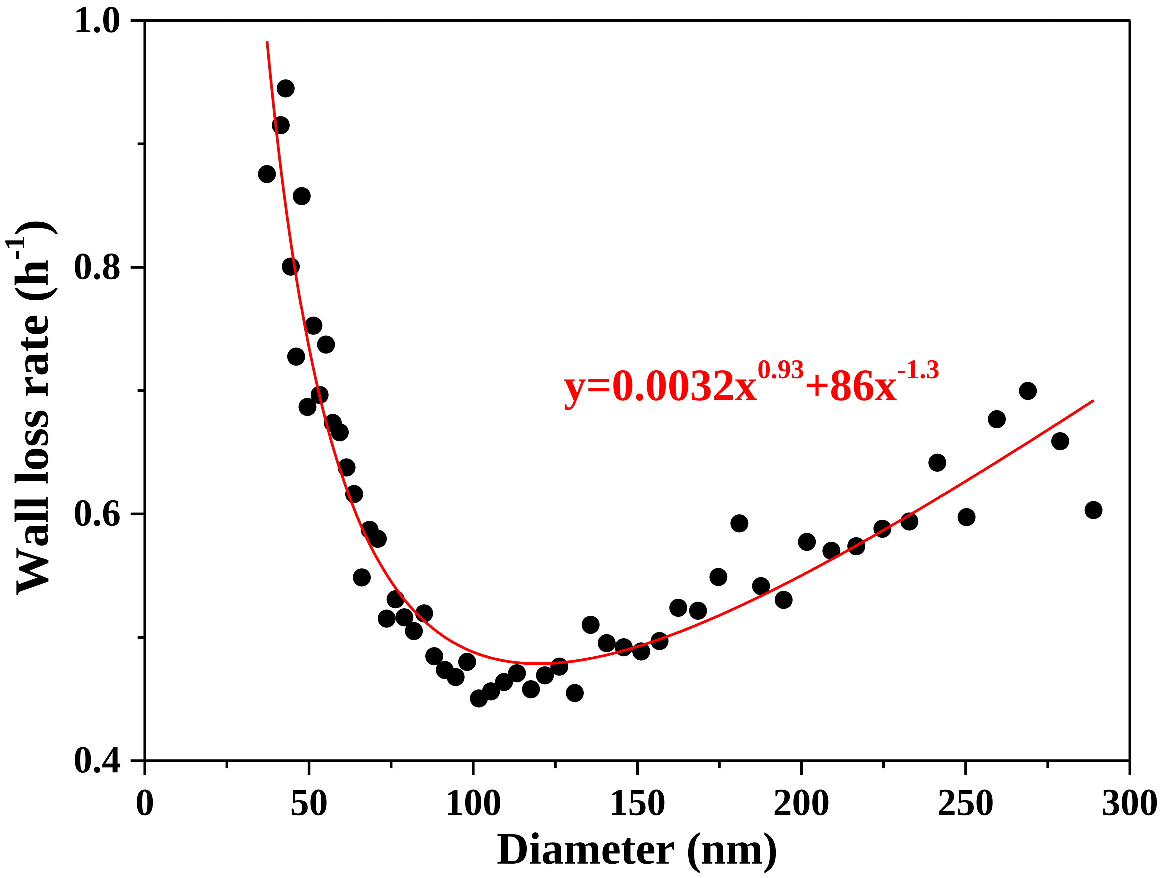

Figure S1 The relationship between the particle wall loss rate and the particle diameter. The data were calculated from burn 6 in which wheat straws were burned. The fitting was based on the equation suggested by Takekawa et al. (2003). From burn 1 to 6, the uncorrected particle size grew from 68 to 92, 71 to 148, 57 to 91, 61 to 98, 82 to 150 and 57 to 105 nm during the photoreaction. Assuming that the wall loss rates during the whole photoreaction should correspond to the averaged size of the primary particles and the aged particles, they were underestimated by 5.4%, -2.0%, 8.8%, 7.3%, -2.8% and 7.8%, respectively when we use the wall loss rates after lights were off for simplification.

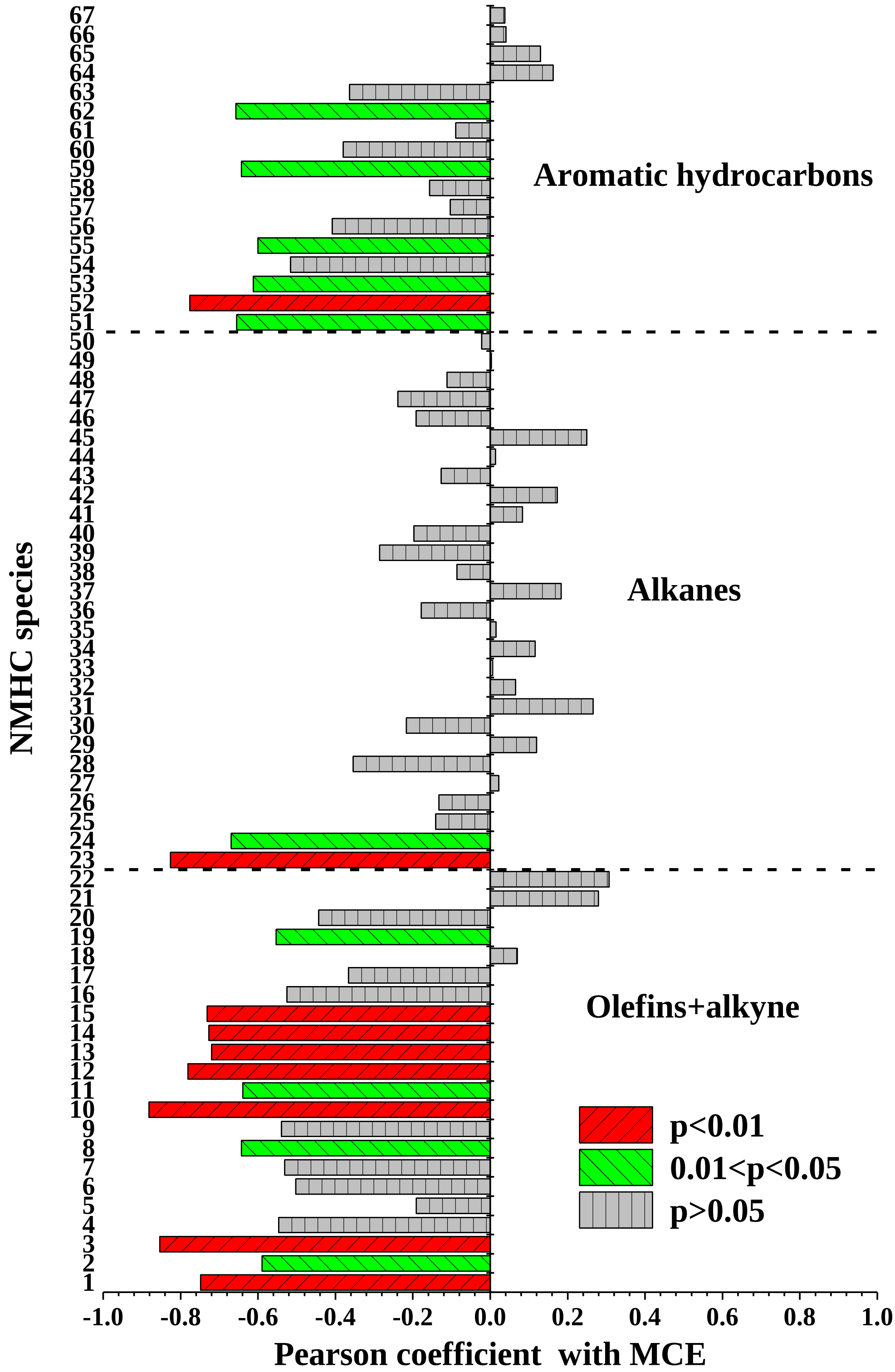

Figure S2 Pearson coefficients of correlations between the modified combustion efficiency (MCE) and individual NMHC concentrations. The number order of NMHC species is the same as Table S1.

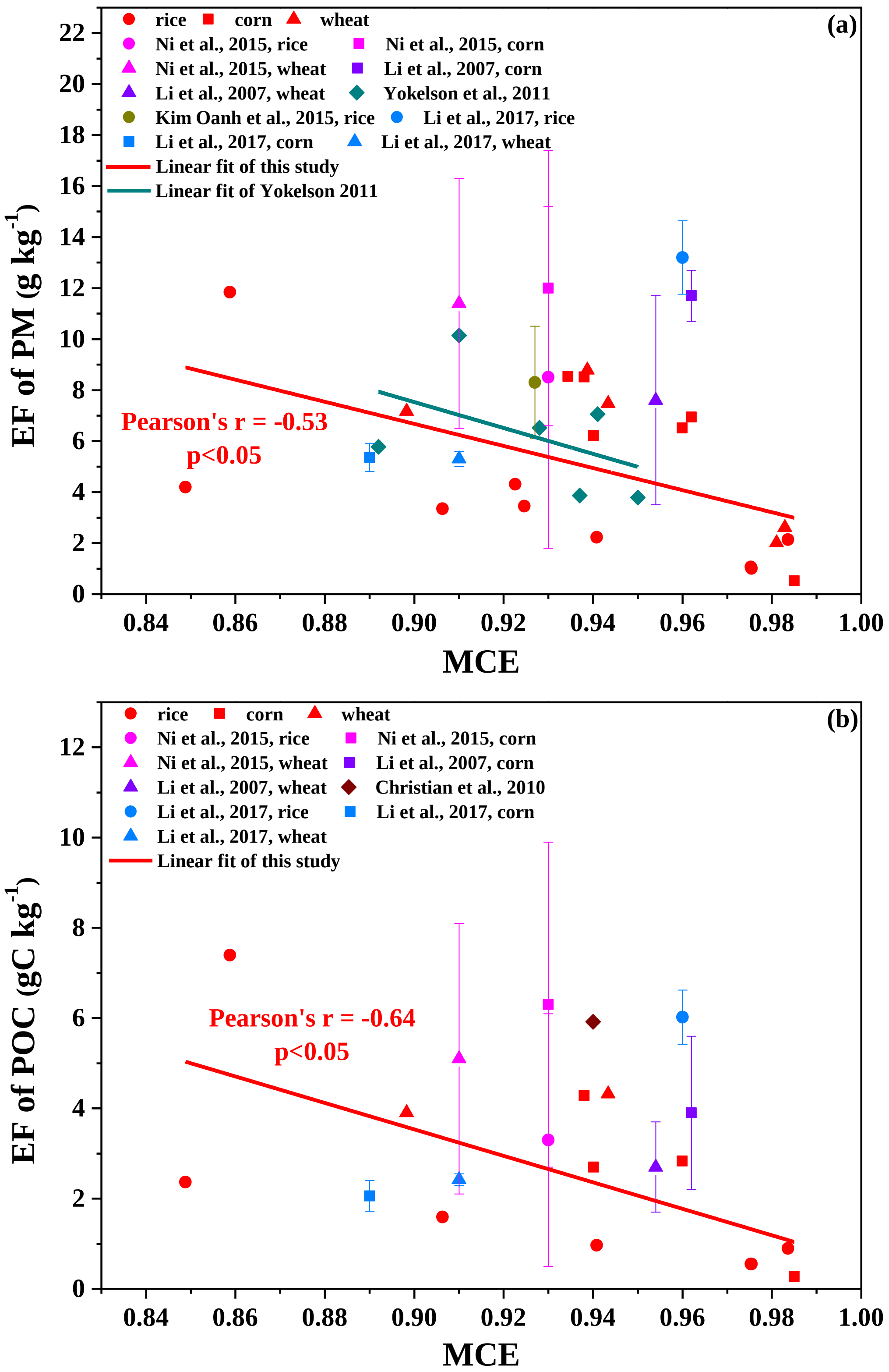

Figure S3 Correlations of modified combustion efficacy (MCE) with emission factors (EFs) for (a) particulate matter and (b) primary organic carbon.

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