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Carbonyl compounds from typical combustion sources: emission characteristics, influencing factors, and their contribution to ozone formation

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Text S1 The uncertainty analysis of ozone formation potential

The Monte Carlo method was employed to analyze the uncertainty in estimating the ozone formation potentials(OFPs) of carbonyl compounds(CCs) from different combustion sources in this study, as it has been widely applied for uncertainty assessment in numerous emission inventory studies (Streets et al., 2003; Zhao et al., 2011, 2012; Shen et al., 2022; Yu et al., 2023). Prior to conducting the Monte Carlo simulation, the mathematical distributions and coefficients of variation (CV, standard deviation divided by the mean) of the input variables needed to be determined. In this study, the emission factor of CCs obtained from experimental measurements for different sources (Zhao et al., 2011) and the maximum incremental reactivity(MIR) values(Shen et al., 2022; Yu et al., 2023) were assumed to follow a normal distribution. Generally, parameters derived from the literature, such as the MIR values in this study, are assigned a lower CV (set at 5%), whereas the emission factors typically exhibit higher variability, with a CV of 50% adopted in this study(Zhou et al., 2015). After defining these parameters, 100,000 iterations of Monte Carlo simulations were performed to quantify the uncertainty (95% confidence interval) in the OFPs of CCs emitted from different combustion sources. The uncertainty ranges for OFPs estimates of carbonyl compounds across different emission sources are summarized in Table S1.

Table S1 The uncertainty ranges for OFPs from different combustion sources.

Combustion sources	Max	Min
BB	21.5%	-3.1%
RCC	13.8%	-10.9%
E-GVs	3.66%	-2.68%
GVs	3.84%	-2.31%
DVs	8.38%	-6.63%
AMs	10.27%	-4.52%

Notes: BB: Biomass Burning; RCC: Residential coal combustion; E-GVs: Ethanol gasoline vehicles; GVs: Gasoline vehicles; DVs: Diesel vehicles; AMs: Agricultural machineries.

The Table S1 presents the uncertainty ranges of the OFPs estimates for different combustion sources, expressed as maximum (Max) and minimum (Min) deviation percentages. It can be observed that the deviations are generally positively correlated with the emission factor of CCs, meaning that the higher the emission factor of CCs, the greater the uncertainty in the calculated OFPs for the combustion source. Among these, BB, RCC, and RCC are identified as high-uncertainty combustion sources, indicating that their emission characteristics are complex and may significantly contribute to ozone formation. It is recommended to conduct more precise measurements and modeling of the emission factor of CCs for these combustion sources to reduce uncertainty.

Text S2 Quality assurance/ quality control (QA/QC)

Before sampling, the entire combustion system and combustion setup were inspected, and the flow rate was measured before each sample collection to ensure that the system was airtight. Additionally, 3 to 5 laboratory blanks were prepared for each batch of sample tubes. During sampling, a field blank group was included, which was identical to the sample tubes in all conditions except for not being connected to the sampler, and it was analyzed together with the samples. Each group of samples included 2 to 4 replicate samples to eliminate randomness. To prevent breakthrough, two identical sampling tubes were connected in series to the sampler. After processing and analysis, if the detected substance in the rear tube exceeded 3% of the total amount in both tubes, it was considered a breakthrough, and the results were deemed unusable. Moreover, the linear regression coefficient R^2 of the standard curve for sample analysis was greater than 0.999. To ensure the stability of the instrument, a known concentration standard sample was inserted every 10 samples to ensure that the instrument deviation was within 10%.

Table S2 Volatile content values of six raw coals.

Coal type	**LL**	**GJ**	**DT**	**SH**	**NM**	**PX**
V_{daf} (%)	20	25	26~27	30	32	35

Table S3 Basic information of on-road gasoline vehicles (ethanol gasoline).

Vehicle model	**Emission standard**	**Model year**	**Engine model**	**Engine size (L)**
Gasoline vehicles	V	2016	DAM15R1	1.5
	V	2017	TNN4G115B	1.5
	V	2020	LZW1028SP6	1.5
	V	2014	LQG5029XXYBF	1.2
	VI	2017	LZW1029PY	1.5
	VI	2021	LZW5028CCYPWV	1.5

Table S4 Basic information of on-road diesel vehicles.

Vehicle model	**Emission standard**	**Model year**	**Mileage**	**Engine model**	**Engine size (L)**
Diesel vehicles	V	2019	40068	UK12030066	1.5
	V	2018	69000	LJ4A15Q	1.5
	V	2018	100700	H2116228	1.5
	VI	2021	13634	LJ469Q-AEC	1.3
	VI	2021	39000	DAM16KL	1.6
	VI	2021	98122	LJ4A18Q6	1.8

Table S5 Basic information of agricultural machinery sampling vehicles.

Machinery type	**Emission standard**	**Model year**	**Engine power(kW)**	**Tail gas treatment**
Small Tractor	China II	2015/2	11(＜22.1)	
Medium Tractor	China II	2014/2	73.5（22.1＜73.6）	
Medium Tractor	China III	2022/4	118（＞73.6）	ECU、Intercooler、Supercharger
Small Harvester	China III	2015/8	46	
Medium Harvester	China III	2021/11	92	ECU、EGR、Intercooler、Supercharger

Table S6 The MIR value of carbonyl compounds(Zhang et al., 2021) .

Carbonyl compounds	MIR
Formaldehyde	6.71
Acetaldehyde	4.10
Acetone	0.22
Acrolein	3.01
Propionaldehyde	2.60
Crotonaldehyde	3.97
Butyraldehyde	4.54
Benzaldehyde	-1.02
Cyclohexanone	0.97
Isovaleraldehyde	3.75
Valeraldehyde	6.27
o-Tolualdehyde	-1.19
m-Tolualdehyde	-1.16
p-Tolualdehyde	-0.65
Hexaldehyde	5.72
2,5-Dimethylbenzaldehyde	0
Heptaldehyde	4.63

Table S7 EF_{CCs}（mg/kg）in real stoves from residential solid fuel combustion.

mg/kg	Straw	Wood	Coal
FA	1006.8 ± 608.7	557.9 ± 264.0	160.1 ± 54.1
ALD	714.1 ± 507.3	173.0 ± 99.3	44.8 ± 17.5
ACE	138.8 ± 122.2	51.0 ± 26.3	25.8 ± 9.3
UA	273.5 ± 210.4	64.6 ± 34.1	11.4 ± 5.3
AA	69.6 ± 47.0	50.8 ± 36.0	22.9 ± 13.5
Other CCs	245.7 ± 164.9	63.7 ± 30.7	22.7 ± 9.0
ΣCCs	2384.1 ± 1515.0	968.6 ± 464.0	287.9 ± 79.2

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