

Supplementary Materials:

Characteristics and Secondary Organic Aerosol Formation of Volatile Organic Compounds from Vehicle and Cooking Emissions

Rui Tan ¹, Song Guo ^{1,2,*}, Sihua Lu ¹, Hui Wang ³, Wenfei Zhu ⁴, Ying Yu ^{1,2}, Rongzhi Tang ¹, Ruizhe Shen ¹, Kai Song ¹, Daqi Lv ¹, Wenbin Zhang ⁵, Zhou Zhang ⁵, Shijin Shuai ⁵, Shuangde Li ⁶, Yunfa Chen ⁶ and Yan Ding ^{7,*}

- ¹ State Key Joint Laboratory of Environmental Simulation and Pollution Control, International Joint Laboratory for Regional Pollution Control, Ministry of Education (IJRC), College of Environmental Sciences and Engineering, Peking University, Beijing 100871, China; 2001111891@pku.edu.cn (R.T.); lshua@pku.edu.cn (S.L.); ying.yu@pku.edu.cn (Y.Y.); rongzhi.tang@cityu.edu.hk (R.T.); ruizhe_shen@pku.edu.cn (R.S.); 1901111786@pku.edu.cn (K.S.); dqlv@pku.edu.cn (D.L.)
 - ² Collaborative Innovation Center of Atmospheric Environment and Equipment Technology, Nanjing University of Information Science & Technology, Nanjing 210044, China
 - ³ Institute of Energy and Climate Research, Troposphere (IEK-8), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany
 - ⁴ School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China
 - ⁵ State Key Laboratory of Automotive Safety and Energy, Tsinghua University, Beijing 100871, China; sjshuai@tsinghua.edu.cn (S.S.)
 - ⁶ State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China; sdli@ipe.ac.cn (S.L.)
 - ⁷ State Environmental Protection Key Laboratory of Vehicle Emission Control and Simulation, Chinese Research Academy of Environmental Sciences, Beijing 100012, China
- * Correspondence: songguo@pku.edu.cn (S.G.); dingyan@craes.org.cn (Y.D.)

Table S1. Parameters of the engine used in this study.

Parameter	Reference Value
Stroke	78.6mm
Cylinder Number	3
Cylinder Diameter	73.4mm
Compression Ratio	9.6:1
Maximum Power	100kW 6000rpm
Peak Torque	205 N m 2000~3000rpm

Table S2. Materials of each dishes.

	Bean	Vegetable	Meat
Materials	500g Tofu	300g cabbage	170g chicken
Corn Oil	200mL	40mL	500mL
Cooking Time	11mins	8mins	10mins
Oil Temperature ^a	106°C	101°C	149°C

^a Temperature here referred to the initial temperature when materials were added.

Table S3. VOCs species measured in this study and their calibration correlation coefficients.

Alkanes	R ²	Alkenes	R ²	Aromatics	R ²	Halocarbons	R ²	OVOCs	R ²
Ethane	0.9998	Ethylene	0.9996	Benzene	0.9999	Chloro-methane	0.9973	Acetaldehyde	0.9634
Propane	0.9987	Propylene	0.9997	Toluene	0.9999	Bromo-methane	0.9984	Acrolein	0.9999
iso-Butane	0.9997	trans-2-Butene	0.9989	Ethylbenzene	0.9992	Freon-11	0.9990	Propanal	0.9992
n-Butane	0.9999	1-Butene	0.9995	m/p-Xylene	0.9984	CarbonTetra-chloride	0.9933	Acetone	0.9995
Cyclopentane	0.9999	cis-2-Butene	0.9995	o-Xylene	0.9995	Bromodi-chloro-methane	0.9998	Methacrolein	0.9992
iso-Pentane	0.9998	1,3-Butadiene	0.9983	Styrene	0.9991	Freon-114	0.9999	n-Butanal	1.0000
n-Pentane	0.9997	1-Pentene	0.9989	Iso-propylbenzene	0.9997	Vinylchloride	1.0000	MethylVinyl-Ketone	0.9980
2,2-Dimethylbutane	0.9999	trans-2-Pentene	0.9992	n-Propylbenzene	0.9987	Chloro-ethane	0.9988	MethylEthyl-Ketone	0.9983
2,3-Dimethylbutane	0.9999	cis-2-Pentene	0.9998	m-Ethyltoluene	0.9984	1,1-Dichloro-ethene	0.9981	2-Pentanone	0.9714
2-Methylpentane	0.9995	Isoprene	0.9992	p-Ethyltoluene	0.9978	Freon-113	0.9979	Pentanal	0.9972
3-Methylpentane	0.9999	1-Hexene	0.9999	1,3,5-Trime-thylbenzene	0.9985	1,1-Dichloro-ethane	0.9977	3-Pentanone	0.9857
n-Hexane	0.9998			o-Ethyltoluene	0.9989	cis-1,2-Di-chloroethene	0.9998	Hexanal	0.9708
Methylcyclopentane	0.9998			1,2,4-Trime-thylbenzene	0.9977	1,1,1-Trichlo-roethane	0.9998		
Cyclohexane	1.0000			1,2,3-Trime-thylbenzene	0.9964	Trichloroeth-ylene	0.9999		
2,4-Dimethylpentane	0.9997			m-Dieth-ylbenzene	0.9892	1,1,2-Trichlo-roethane	0.9999		
2-Methylhexane	0.9999			p-Dieth-ylbenzene	0.9849	1,2-Dibromo-ethane	0.9999		
2,3-Dimethylpentane	0.9998					1,2-Dichloro-propane	0.9999		
3-Methylhexane	0.9998					trans-1,3-Di-chloropro-pene	1.0000		
n-Heptane	0.9999					cis-1,3-Di-chloropro-pene	1.0000		
Methylcyclohexane	0.9999					Chloroben-zene	0.9997		
2,2,4-Trime-thylpentane	0.9998					1,3-Dichloro-benzene	1.0000		

2,3,4-Trime- thylpentane	0.9998	1,4-Dichloro- benzene	0.9999
2- Methylhep- tane	0.9997	1,2-Dichloro- benzene	0.9998
3- Methylhep- tane	0.9996	BenzylChlo- ride	0.9997
n-Octane	0.9995		
Nonane	0.9992		
n-Decane	0.9980		
n-Undecane	0.9001		
n-Dodecane	1.0000		

Table S4. MIR values of the VOCs used in this study.

Species	MIR(g/gVOCs)	Species	MIR(g/gVOCs)
Alkanes		Aromatics	
Ethane	0.28	Isopropylbenzene	2.52
Propane	0.49	n-Propylbenzene	2.03
iso-Butane	1.23	m-Ethyltoluene	7.39
n-Butane	1.15	p-Ethyltoluene	4.44
Cyclopentane	2.39	1,3,5-Trimethylbenzene	0.00
iso-Pentane	1.45	o-Ethyltoluene	5.59
n-Pentane	1.31	1,2,4-Trimethylbenzene	8.87
2,2-Dimethylbutane	1.17	1,2,3-Trimethylbenzene	11.97
2,3-Dimethylbutane	0.97	m-Diethylbenzene	7.10
2-Methylpentane	1.50	p-Diethylbenzene	4.43
3-Methylpentane	1.80	Halocarbons	
n-Hexane	1.24	Chloromethane	0.04
Methylcyclopentane	2.19	Bromomethane	0.02
Cyclohexane	1.25	Freon-11	0.00
2,4-Dimethylpentane	1.55	CarbonTetrachloride	0.00
2-Methylhexane	1.19	Bromodichloromethane	9.65
2,3-Dimethylpentane	1.34	Freon-114	0.00
3-Methylhexane	1.61	Vinylchloride	2.83
n-Heptane	1.07	Chloroethane	0.29
Methylcyclohexane	1.70	1,1-Dichloroethene	1.79
2,2,4-Trimethylpentane	1.26	Freon-113	0.00
2,3,4-Trimethylpentane	1.03	1,1-Dichloroethane	0.07
2-Methylheptane	1.07	cis-1,2-Dichloroethene	1.70
3-Methylheptane	5.08	1,1,1-Trichloroethane	0.00
n-Octane	0.00	Trichloroethylene	0.64
Nonane	0.78	1,1,2-Trichloroethane	0.09
n-Decane	0.68	1,2-Dibromoethane	0.00
n-Undecane	0.61	1,2-Dichloropropane	0.29
n-Dodecane	0.00	trans-1,3-Dichloropropene	5.03
Alkenes		cis-1,3-Dichloropropene	3.70
Ethylene	9.00	Chlorobenzene	1.79
Propylene	11.66	1,3-Dichlorobenzene	0.18
trans-2-Butene	15.16	1,4-Dichlorobenzene	0.18
1-Butene	9.73	1,2-Dichlorobenzene	0.18
cis-2-Butene	14.24	BenzylChloride	0.00
1,3-Butadiene	12.61	OVOCs	
1-Pentene	7.21	Acetaldehyde	6.54
trans-2-Pentene	10.56	Acrolein	7.45
cis-2-Pentene	10.38	Propanal	7.08
Isoprene	10.61	Acetone	0.36
1-Hexene	5.49	Methacrolein	6.01
Aromatics		n-Butanal	5.97
Benzene	0.72	MethylVinylKetone	9.65
Toluene	4.00	MethylEthylKetone	1.48
Ethylbenzene	0.00	2-Pentanone	2.81
m/p-Xylene	7.80	Pentanal	6.01
o-Xylene	7.64	3-Pentanone	1.24

Styrene	0.02	Hexanal	4.35
---------	------	---------	------

Table S5. SOA yield used in this study.

Species	Yield (g/g VOC)	Species	Yield (g SOA/g VOC)
Alkanes		Aromatics	
Methylcyclopentane	0.046	Benzene	0.196
Cyclohexane	0.046	Toluene	0.944
Methylcyclohexane	0.14	Ethylbenzene	0.063
2,4-Dimethylpentane	0.01	m/p-Xylene	0.063
2-Methylhexane	0.01	o-Xylene	0.063
2,3-Dimethylpentane	0.01	Styrene	0.063
3-Methylhexane	0.01	Isopropylbenzene	0.063
n-Heptane	0.01	n-Propylbenzene	0.063
2,2,4-Trimethylpentane	0.048	m-Ethyltoluene	0.063
2,3,4-Trimethylpentane	0.048	p-Ethyltoluene	0.063
2-Methylheptane	0.048	1,3,5-Trimethylbenzene	0.063
3-Methylheptane	0.048	o-Ethyltoluene	0.063
n-Octane	0.048	1,2,4-Trimethylbenzene	0.063
Nonane	0.093	1,2,3-Trimethylbenzene	0.063
n-Decane	0.169	m-Diethylbenzene	0.063
n-Undecane	0.313	p-Diethylbenzene	0.063
OVOCs			
MethylEthylKetone	0.008		
n-Pentanal	0.093		
n-Hexanal	0.093		

Table S6. Top ten species in cooking emission and vehicle emission.

Cooking Emission					
Bean		Vegetable		Meat	
Species	Mass Fraction	Species	Mass Fraction	Species	Mass Fraction
Hexanal	16% ± 2%	Hexanal	14% ± 6%	Hexanal	30% ± 3%
iso-Butane	13% ± 2%	Acetone	10% ± 3%	Acetone	15% ± 10%
Ethane	10% ± 4%	iso-Butane	9% ± 8%	Pentanal	7% ± 1%
Ethylene	7% ± 8%	Ethane	8% ± 3%	iso-Butane	7% ± 6%
Propylene	6% ± 2%	Acetaldehyde	7% ± 5%	Acrolein	6% ± 2%
iso-Pentane	6% ± 10%	Styrene	5% ± 2%	Propylene	5% ± 4%
Acetaldehyde	3% ± 2%	Pentanal	5% ± 0%	n-Butanal	5% ± 1%
m/p-Xylene	3% ± 1%	n-Butanal	4% ± 2%	Propanal	3% ± 1%
Acetone	3% ± 3%	m/p-Xylene	4% ± 1%	n-Butane	2% ± 2%
Pentanal	2% ± 1%	Acrolein	3% ± 1%	1,2,4-Trimethylbenzene	2% ± 1%
Vehicle Emission					
Gasoline			E10		
Species	Mass Fraction		Species	Mass Fraction	
iso-Pentane	20% ± 3%		iso-Pentane	24% ± 6%	
Ethane	8% ± 1%		n-Butane	11% ± 3%	
Ethylene	6% ± 1%		Ethane	8% ± 4%	
Toluene	5% ± 1%		iso-Butane	7% ± 2%	
n-Pentane	5% ± 1%		n-Pentane	6% ± 1%	
2-Methylpentane	4% ± 1%		Propane	5% ± 4%	
Benzene	4% ± 1%		2-Methylpentane	3% ± 1%	

3-Methylhexane	3% \pm 1%	3-Methylpentane	2% \pm 1%
2-Methylhexane	3% \pm 1%	n-Hexane	1% \pm 0%
n-Butane	3% \pm 1%	Methylcyclopentane	1% \pm 1%

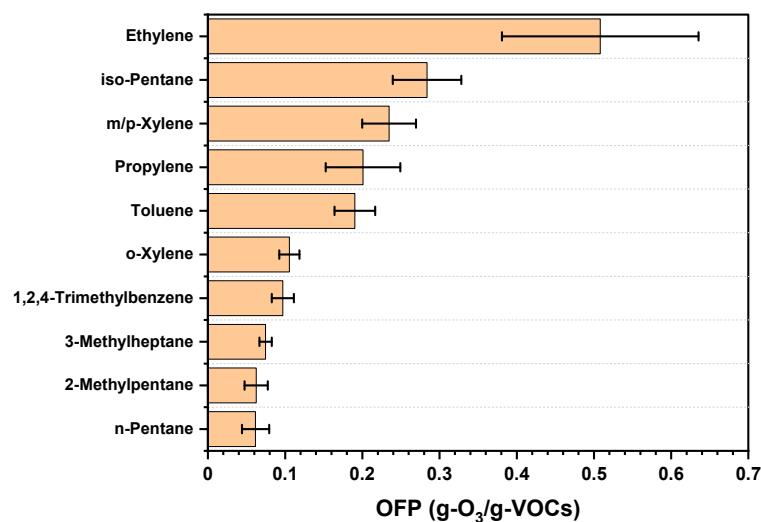


Figure S1. Top ten species contributing to OFP from Gasoline emissions.

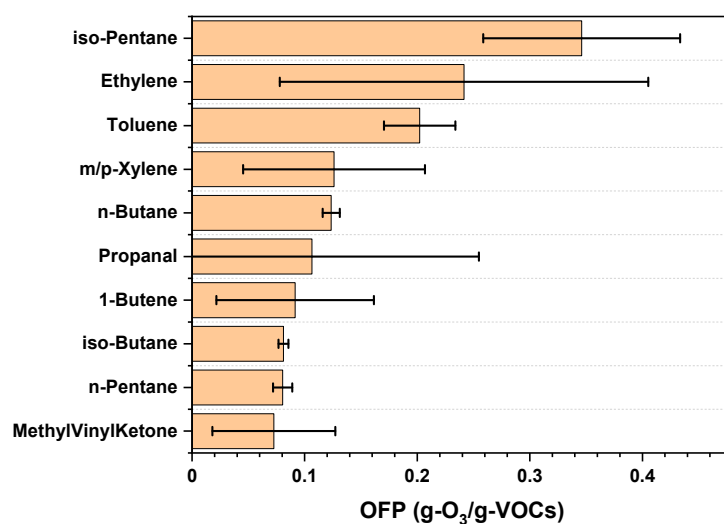


Figure S2. Top ten species contributing to OFP from E10 emissions.

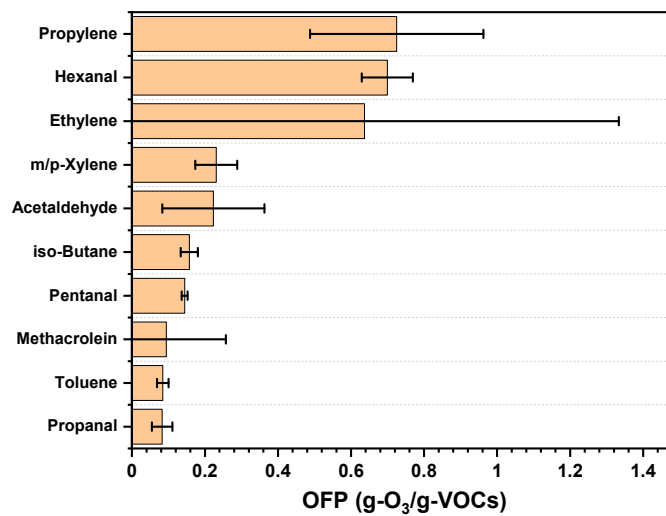


Figure S3. Top ten species contributing to OFP from Bean emissions.

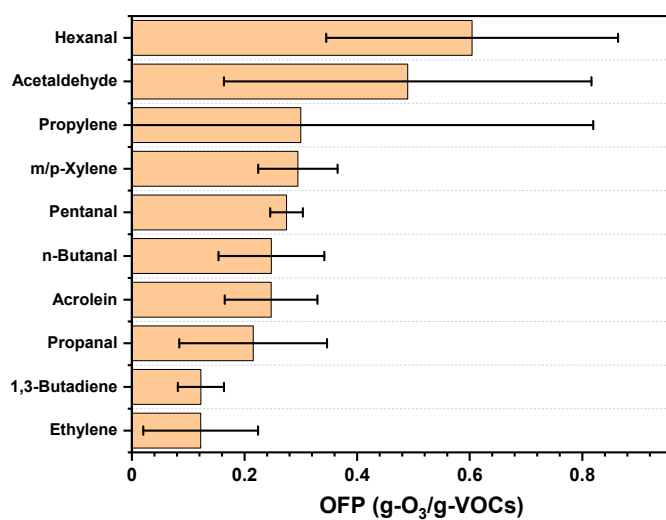


Figure S4. Top ten species contributing to OFP from Vegetable emissions.

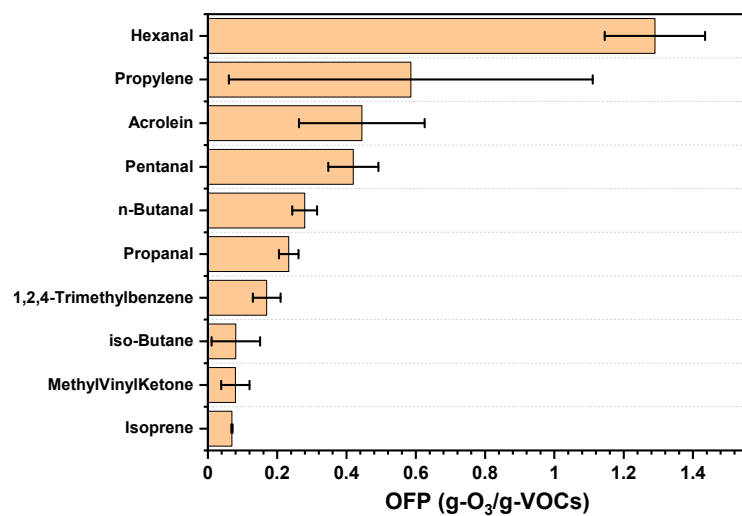


Figure S5. Top ten species contributing to OFP from Meat emissions.