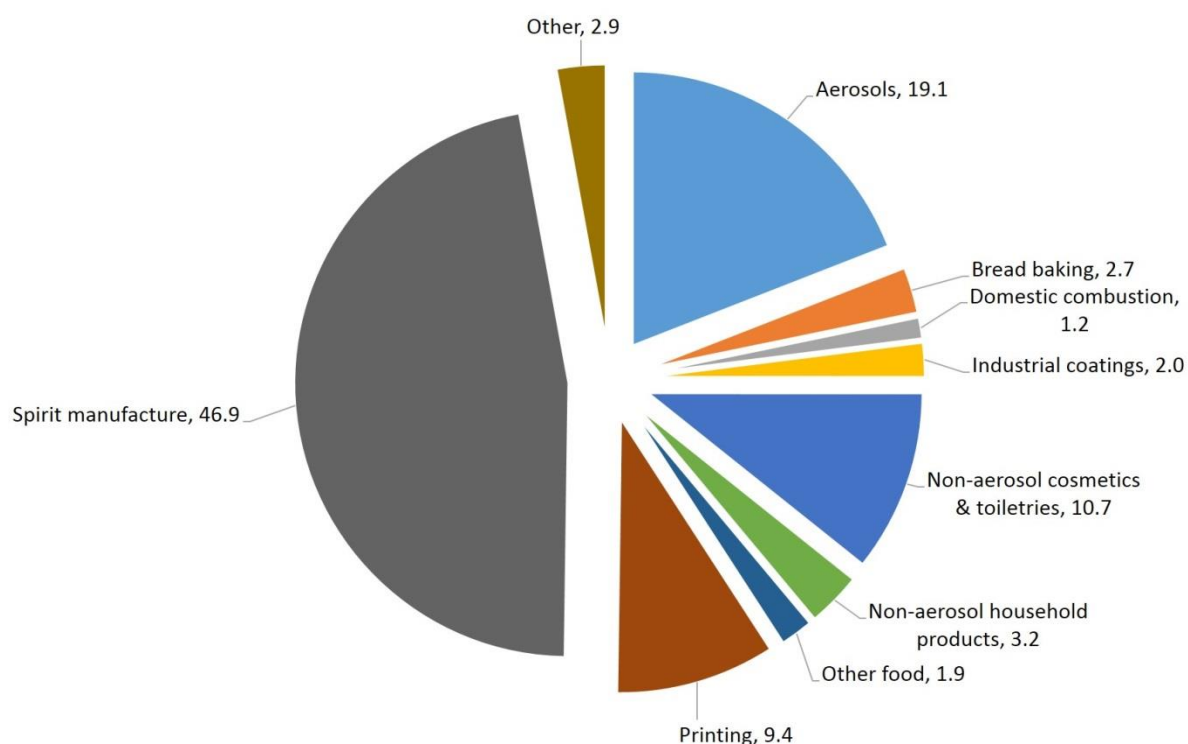


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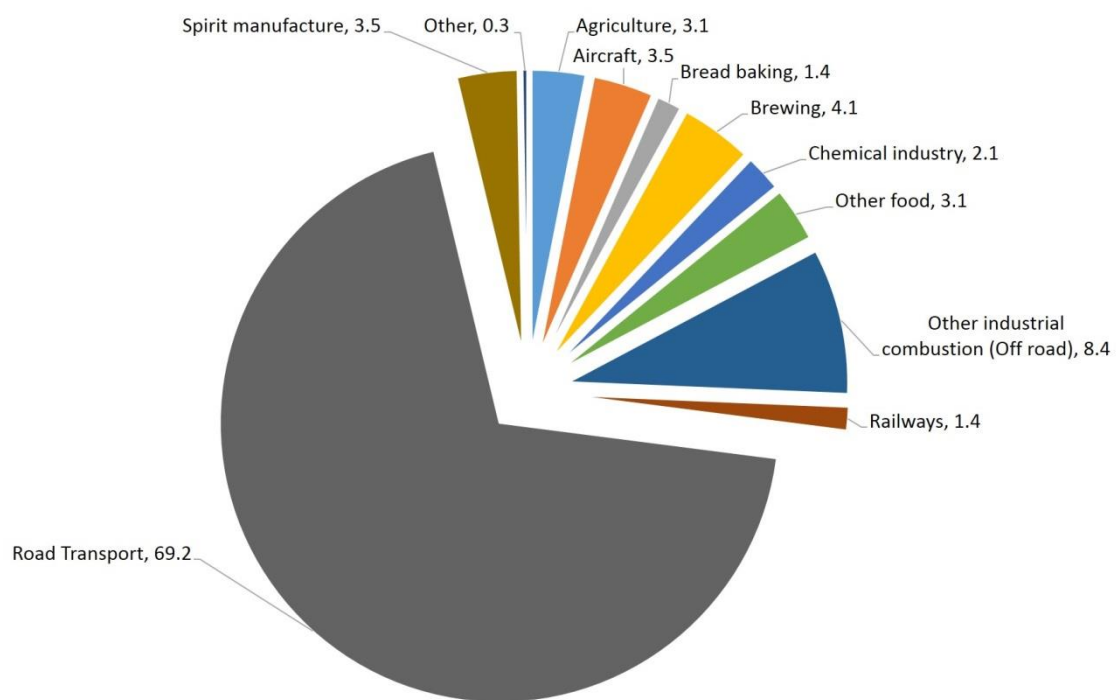
Atmospheric ethanol in London and the potential impacts of future fuel formulations

R.E. Dunmore et al.

Supplementary Figures 1 and 2 show the emission source contributions for ethanol and acetaldehyde respectively from the National Atmospheric Emissions Inventory (NAEI) using the Passant (2002) VOC speciation profiles.



Supplementary Figure 1: Emission source contributions for ethanol from the NAEI. The Other category refers to the sum of categories that have less than 1% each: agrochemicals use, brewing, chemical industry, cider manufacture, coating manufacture, domestic adhesives, film coating, glass, industrial adhesives, landfill, non-aerosol automotive products, other industrial combustion (wood), paper printing, solvent and oil recovery, textile coating and wine manufacture.



Supplementary Figure 2: Emission source contributions for acetaldehyde from the NAEI. The Other category refers to the sum of categories that have less than 1% each: cement (non-de-carbonising), glass, house and garden machinery, miscellaneous-landfill gas, power stations, public services and solvent and oil recovery.

Supplementary Tables 1 and 2 show the linear regression coefficient values for all individual and grouped VOC species with ethanol.

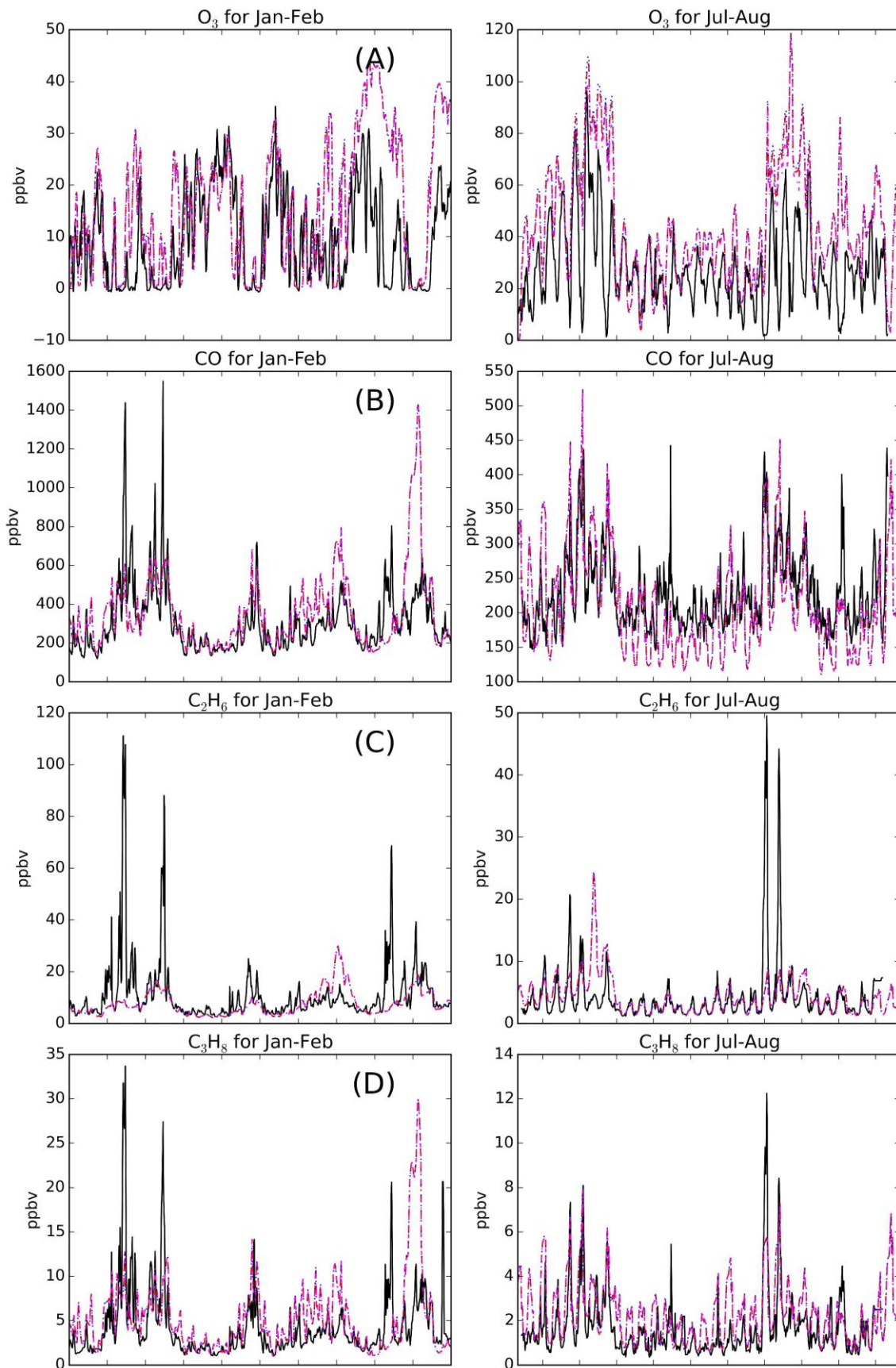
Supplementary Table 1: Correlation of all individually quantified VOCS with ethanol during the ClearLo campaigns. Values in bold indicate R correlations of greater than 0.75.

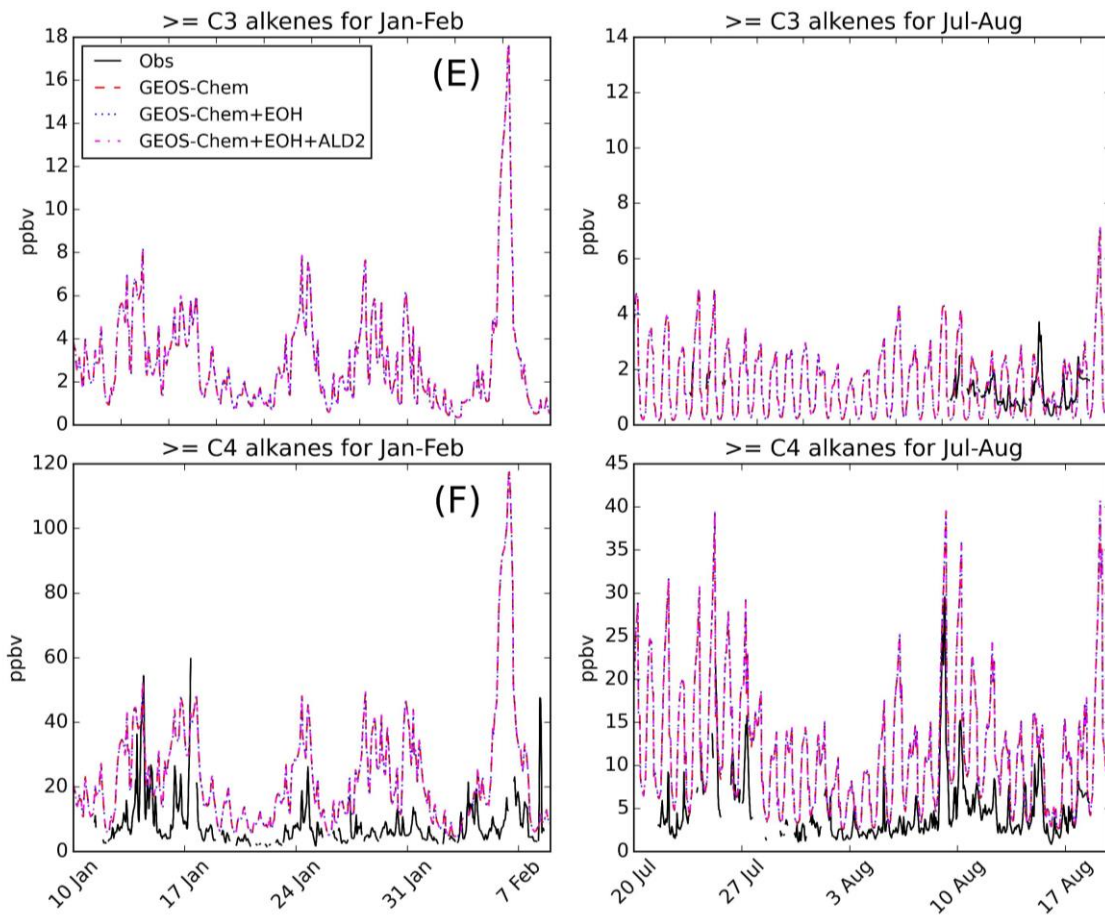
Compound	Correlation with Ethanol		Compound	Correlation with Ethanol	
	Winter	Summer		Winter	Summer
Saturated			Aromatics continued		
Methane	0.88	0.75	m- and p-Xylene	0.88	0.90
Ethane	0.86	0.81	o-Xylene	0.86	0.90
Propane	0.89	0.89	Benzene, iso-propyl-	0.71	-
n-Butane	0.89	0.85	Benzene, propyl-	0.84	0.67
iso-Butane	0.86	0.84	Toluene, 3-ethyl-	0.85	0.68
n-Pentane	0.91	0.88	Toluene, 4-ethyl-	0.77	0.66
iso-Pentane	0.89	0.87	Benzene, 1,3,5-trimethyl-	0.82	0.73
Cyclopentane	0.76	0.82	Toluene, 2-ethyl-	0.78	0.63
n-Hexane	0.91	0.79	Benzene, 1,2,4-trimethyl-	0.79	0.60
Pentane, 2+3-methyl-	0.89	0.88	Toluene, 4-isopropyl-	0.63	0.31
n-Heptane	0.80	0.84	Benzene, 1,2,3-trimethyl-	0.88	0.72
Butane, 2,2,3-trimethyl-	0.83	0.85	Indan	0.84	-
n-Octane	0.90	0.85	Benzene, tert-butyl-	0.28	0.41
Pentane, 2,2,4-trimethyl-	0.80	0.87	Benzene, 1,3-diethyl-	0.86	0.61
n-Nonane	0.88	0.77	Benzene, 1,4-diethyl-	0.86	0.79
n-Decane	0.89	0.65	Naphthalene	0.83	0.66
Nonane, 2-methyl-	0.83	0.66	Oxygenates		
n-Undecane	0.88	0.86	Acetaldehyde	0.89	0.91
n-Dodecane	0.88	0.79	Propanal, 2-methyl-	-	0.14
Unsaturated			Butanal	0.49	0.19
Ethene	0.88	0.85	Butanal, 3-methyl-	-	0.18
Acetylene	0.90	0.86	Butanal, 2-methyl-	-	0.17
Propene	0.86	0.81	Methacrolein (MACR)	-	0.16
Propadiene	0.88	0.81	Pentanal	-	0.19
Propyne	-	0.79	Hexanal	0.87	0.24
Butene, trans-2-	0.88	0.82	Benzaldehyde	0.69	0.72
1-Butene	0.91	0.82	Methanol	0.66	0.81
iso-Butene	0.90	0.89	Ethanol	-	-
Butene, cis-2-	0.88	0.82	Propanol	0.54	0.85
1,2-Butadiene	-	-0.17	Butanol	0.49	0.62
1,3-Butadiene	0.88	0.75	Acetone	0.80	0.75
Pentene, trans-2-	0.43	0.83	Butanone	0.81	0.31
1-Pentene	0.49	0.88	Ketone, methyl-vinyl- (MVK)	-	0.19
Isoprene	0.90	0.11	Pentanone, 2-	-	0.15
Styrene	0.80	0.41	Pentanone, 4-methyl-2-	0.70	0.22
α -Pinene	-0.37	0.36	Hexanone, 2-	-	0.17
Limonene	0.90	0.27	Cyclohexanone	-	0.18
Aromatics			Acetate, ethyl-	-0.48	0.23
Benzene	0.87	0.91	Halogenated		
Toluene	0.89	0.91	Methane, dichloro	0.85	0.78
Benzene, ethyl-	0.85	0.90	Trichloroethylene	-	0.85

Supplementary Table 2: Correlation of the grouped species with ethanol during the ClearLo campaigns. Values in bold indicate R correlations of greater than 0.75.

Grouped species	Correlation with Ethanol	
	Winter	Summer
C ₆ Aliphatics	0.79	0.74
C ₇ Aliphatics	0.85	0.77
C ₈ Aliphatics	0.87	0.78
C ₉ Aliphatics	0.85	0.73
C ₁₀ Aliphatics	0.71	0.70
C ₁₁ Aliphatics	0.87	0.65
C ₁₂ Aliphatics	0.85	0.65
C ₁₃ Aliphatics	0.88	0.70
C ₄ substituted monoaromatics	0.86	0.72
C ₁₀ Monoterpenes	0.87	0.17

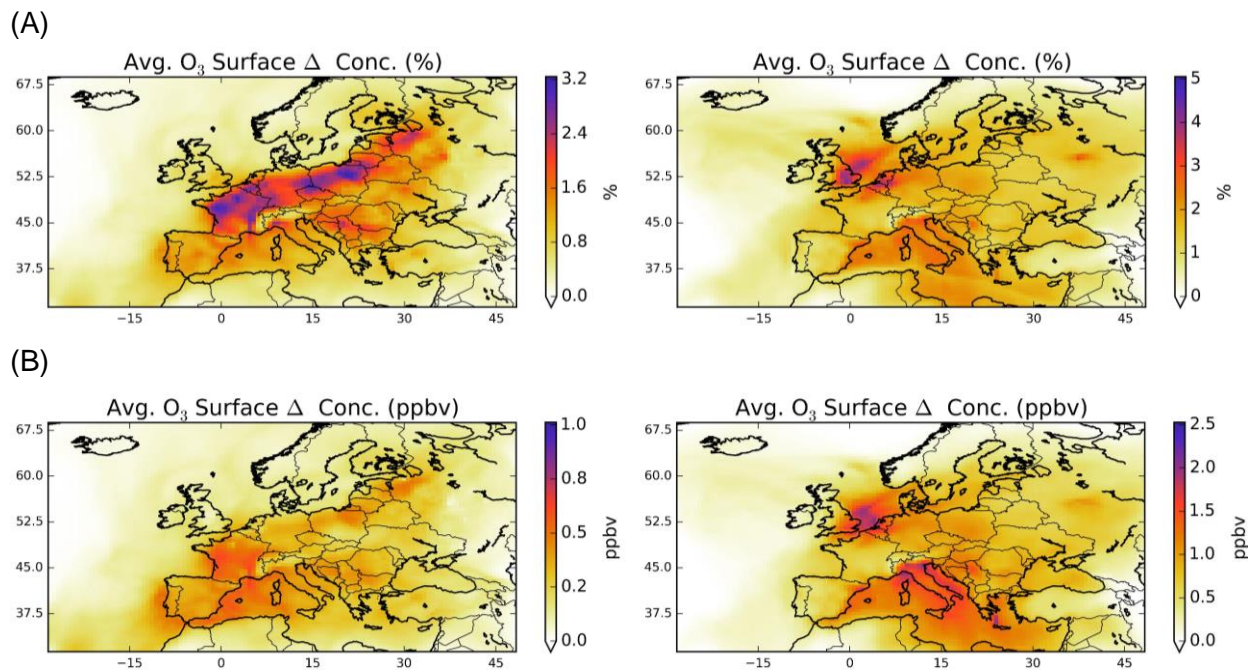
Supplementary Figure 3 shows the time series comparisons between measured and modelled values for multiple species.



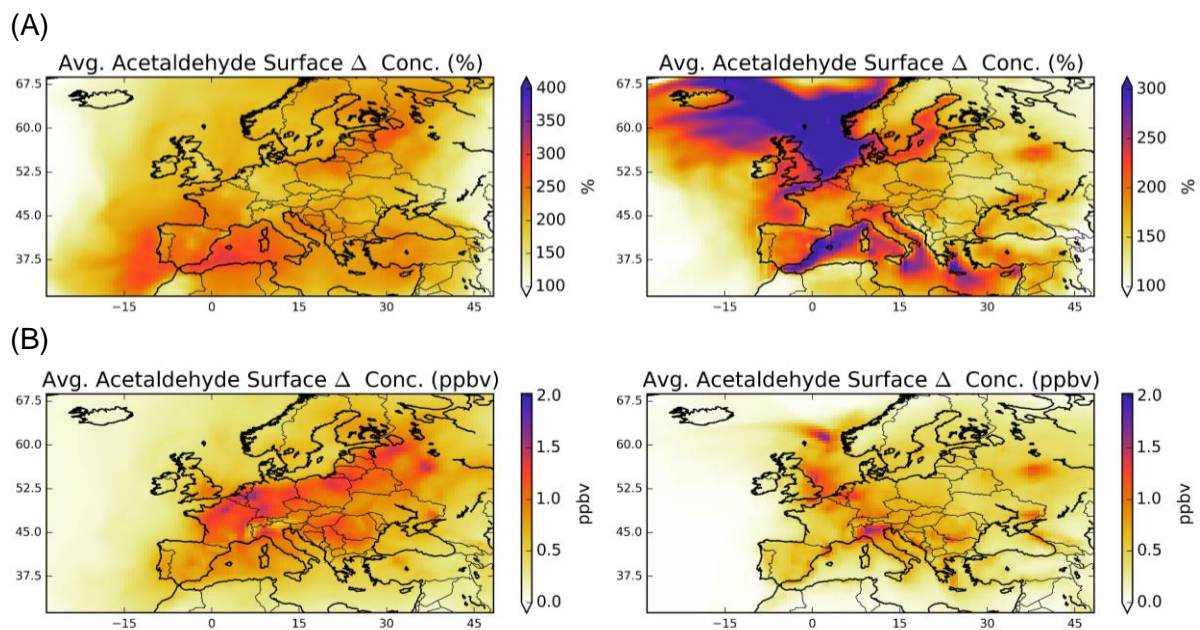


Supplementary Figure 3: Comparison between modelled values and observed for ozone (A), carbon monoxide (B), ethane (C), propane (D), \geq C3 alkenes (E), and \geq C4 alkanes (F), for winter (left) and summer (right) observation periods. Plots show the simulation without increase ethanol or aldehyde emissions ('GEOS-Chem') in magenta, with added EOH emissions ('GEOS-Chem+EOH') in red, and with both additional ethanol and acetaldehyde emissions ('GEOS-Chem+EOH+ALD2') in blue.

Supplementary Figures 4 and 5 show spatial changes in ozone and acetaldehyde concentrations between the 'GEOS-Chem' and 'GEOS-Chem+EOH' models.



Supplementary Figure 4: Spatial change in ozone concentration between ('GEOS-Chem') and additional ethanol emissions ('GEOS-Chem+EOH') for winter (left) and summer (right) observation periods. Actual changes in ppbv are shown below (B), and percentage changes are shown above (A).



Supplementary Figure 5: Spatial change in acetaldehyde concentration between ('GEOS-Chem') and additional ethanol emissions ('GEOS-Chem+EOH') for winter (left) and summer (right) observation periods. Actual changes in ppbv are shown below (B), and percentage changes are shown above (A).