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Supplement of

Investigating diesel engines as an atmospheric source of isocyanic acid in urban areas

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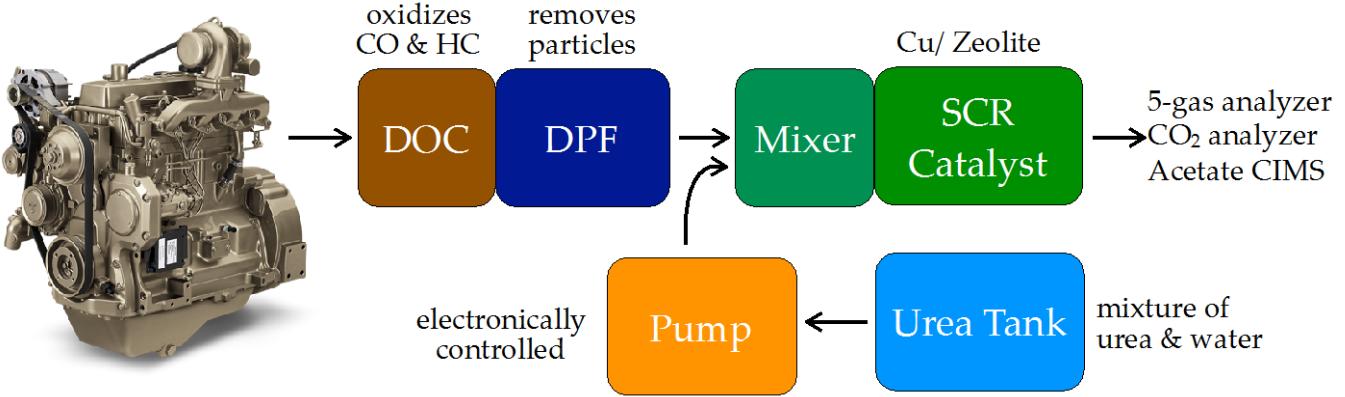


Figure S-1: Schematic showing the diesel engine, selective catalytic reduction (SCR) system, and instrumentation used during the study.

5 Table S-1: HNCO and CO emission factors and HNCO:CO ratios used to determine lower and upper bound for the ratios

<i>Reference/Engine</i>	<i>Engine Mode/Drive Cycle</i>	<i>HNCO (mg kg-fuel⁻¹)</i>	<i>CO (g kg-fuel⁻¹)</i>	<i>HNCO/CO</i>
This work: John Deere 4.5L Tier-3/Tier-4	1500 rpm @ 45 kW	38.80	4.61	8.41E-03
	2400 rpm @ 11 kW	56.20	48.91	1.15E-03
	2400 rpm @ 57 kW	30.90	3.74	8.26E-03
	1500 rpm @ 45 kW	9.40	2.19	4.29E-03
	2400 rpm @ 57 kW	7.60	3.40	2.24E-03
Link et al. (2016): John Deere 4.5L Tier-3	900 rpm @ 0 kW	54.00	49.00	1.10E-03
	2400 rpm @ 60 kW	17.00	3.95	4.30E-03
	900 rpm @ 0 kW	51.00	54.00	9.44E-04
	2400 rpm @ 60 kW	17.00	3.65	4.66E-03
Wentzell et al. (2013): VW Jetta 2001 + DOC	US06	3.98	0.92	4.33E-03
	HWFET	3.54	1.01	3.50E-03
	FTP75	0.21	11.60	1.77E-05
	Idle	0.61	7.09	8.62E-05
Heeb et al. (2011, 2012): IVECO 3L Euro-3 engine	ISO8178 – Mode 7	4.58	5.19	8.82E-04
	ISO8178 – Mode 4	7.50	15.86	4.73E-04
	ISO8178 – Mode 3	2.38	2.01	1.18E-03
Heeb et al. (2011, 2012): IVECO 3L Euro-3 engine (SCR)	ISO8178 – Mode 7	12.50	4.10	3.05E-03
	ISO8178 – Mode 4	32.41	19.03	1.70E-03
	ISO8178 – Mode 3	41.26	2.60	1.59E-02
Heeb et al. (2011, 2012): IVECO 3L Euro-3 engine (DPF+SCR)	ISO8178 – Mode 7	1.64	BDL	NA
	ISO8178 – Mode 4	45.17	3.40	1.33E-02
	ISO8178 – Mode 3	74.88	BDL	NA
Suarez-Bertoa and Astorga (2016): Euro 5 vehicles	WLTC	37.2	7.7	4.8E-03
Suarez-Bertoa and Astorga (2016): Euro 6 vehicles	WLTC	1.3	2.9	4.5E-04
	WLTC	9.7	1.3	7.2E-03

BDL = below detection limit, NA = not applicable

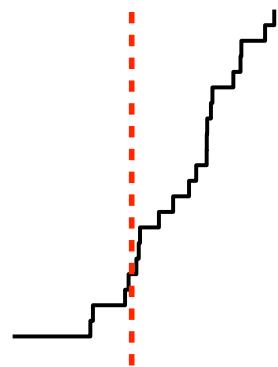


Figure S-2: Cumulative distribution function of the HNCO:CO ratios listed in Table S-1. The low and high bounds represent the low and high estimates of the HNCO:CO ratios used to build the HNCO emissions inventory for diesel sources.



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Figure S-3: (a) Low and (b) high estimates of the 14-day averaged ground-level concentrations of HNCO precursors from the 24 km simulations.

**AGP**SERGEANT BLUFF, IOWA
METHYL ESTER PLANT**Certificate of Analysis**

Load Order 890-57732
Shipping date 1/18/2016
Rail/ Truck # OFC 6210/5237
Lot number M21601-13
Product ID 99000
Product name Methyl Ester

Registration# 4552
Facility# 81733

Customer
Rex Oil Company, Inc.
804 Denver Ave.
Fort Lupton CO 80621

Customer PO: 0053MWB
Schedule PO: 0053MWB

Property	Test Methods	Test Limits	Units	Results
Total glycerin	ASTM D6584	0.240 max	% mass	0.059
Free glycerin	ASTM D6584	0.020 max	% mass	0.001
Monoglycerides	ASTM D6584	0.8 max	% mass	0.185
Diglycerides	ASTM D6584	report	% mass	0.061
Triglycerides	ASTM D6584	report	% mass	0.001
Acid Number	ASTM D974	0.50 max	mg KOH/g	0.19
Moisture	ASTM D6304	Report	% mass	0.0139
Methanol Content	EN 14110	0.2 max	% mass	0.034
Flash Point (closed cup)	ASTM D93	93 min	° C	151.0 *
Water / Sediment	ASTM D2709	0.05	% volume	n.d.
Sulfur	ASTM D5453	15 max	ppm	<1
Cloud Point	ASTM D2500	report	° C	-1.0
Cold Soak Filterability	ASTM D7501	200 max	seconds	91.44
Cold Filter Plugging Point	ASTM D6371	Report***	° C	-4 *
Cold Soak Filter Blocking Tendency	CAN/CGSB-3.52	1.8		1.1 *
Total Contamination	EN 12662	24 max	mg/kg	< 10 *
Oxidation Stability	EN 15751	3 min **	hours	5.35
Visual/Haze	ASTM D4176	2 max	scale	1
Specific Gravity	ASTM D1298	Report***	@ 60 F	0.884 g/cm³
Specific Gravity	ASTM D1298	Report***	@ 15 C	883.130 kg/m³
Kinematic Viscosity, 40°C	ASTM D445	1.9-6.0	mm²/s	4.003 *
Cetane Number	ASTM D613	47 min		48.0 *
Sulfated Ash	ASTM D874	0.02 max	% mass	n.d. *
Carbon Residue	ASTM D4530	0.05 max	% mass	n.d. *
Phosphorus Content	ASTM D4951	0.001 max	% mass	n.d. *
Sodium / Potassium	EN 14538	5 max	ppm (μ g/g)	<1.0 *
Calcium / Magnesium	EN 14538	5 max	ppm (μ g/g)	<0.5 *
Distillation Temperature	ASTM D1160	360 max	° C	351.4 *
Copper Strip Corrosion	ASTM D130	# 3 max		1a *
Nace Corrosion	TM -0172	B +		B+ *

This product is derived from plant based oils and meets current ASTM D6751 specifications.

* typical results based on most recent full specification analysis by an outside qualified lab.

** or per customer specifications

*** typical result based on historical data

"n.d." indicates none detected.

Country of Origin: USA

Additive: None

Prepared By:

Kelly Samuelson

F8-2 03/12 Rev. 3

Fuel certificate for the biodiesel fuel used in this work.