

# OP-FTIR Weekly Report (10-5-16 through 10-12-16)

Prepared for the U.S. Department of Energy  
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy  
Office of River Protection under Contract DE-AC27-08RV14800



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Date Published

October 2016

WRPS

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**APPROVED**  
*By Janis Aardal at 1:48 pm, Nov 08, 2016*

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Release Approval

Date

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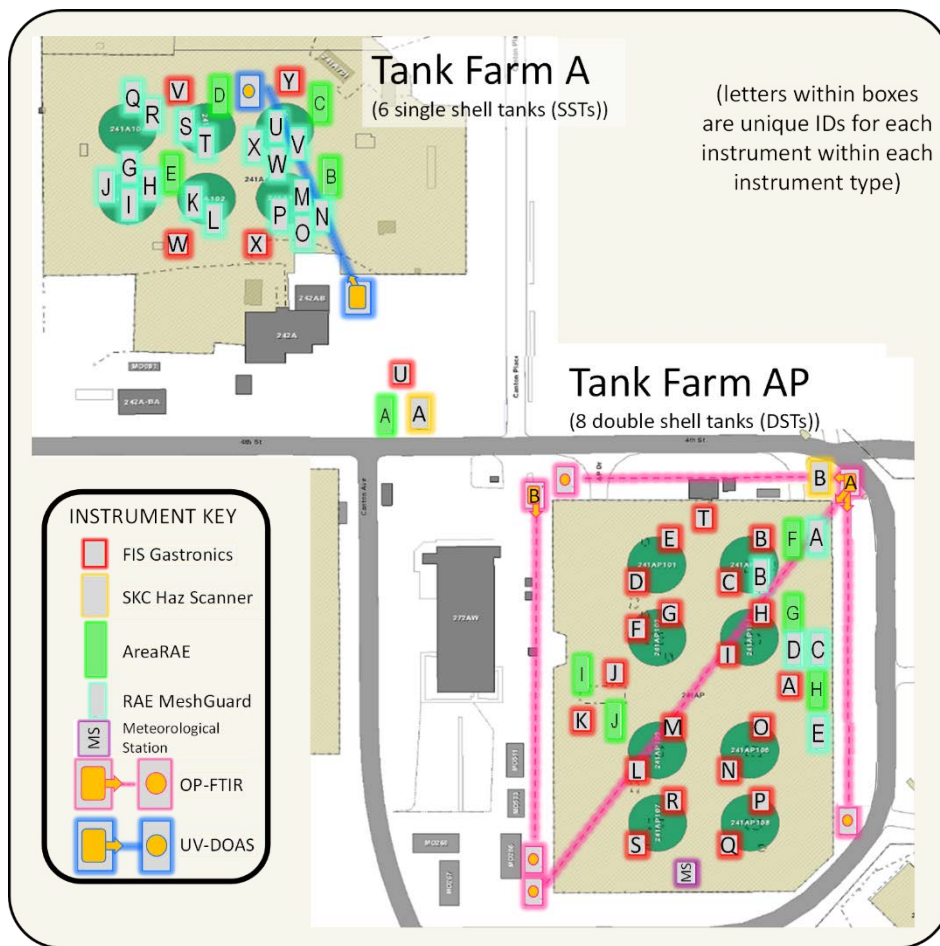
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# OP-FTIR Weekly Summary

10/5/16 6:00 – 10/12/16 6:00



The following information is for the time period from October 5<sup>th</sup> at 6:00 a.m. through October 12<sup>th</sup> at 6:00 a.m. This summary contains Vapor Monitoring and Detection System (VMDS) pilot-scale data collected over one week for the open path Fourier transform infrared spectrometer (OP-FTIR). Pilot-scale testing is focused on evaluating component integration and functionality. Data shown may include results from calibration and bump tests performed verify instruments function; these tests result in data spikes.

Abbreviations:

- CH<sub>4</sub> = methane
- NH<sub>3</sub> = ammonia
- NO = nitric oxide
- N<sub>2</sub>O = nitrous oxide
- NO<sub>2</sub> = nitrogen dioxide
- OEL = occupational exposure limit
- OP-FTIR = Open Path Fourier Transform Infrared Spectrometer
- R<sup>2</sup> = R-squared
- VMDS = Vapor Monitoring and Detection System

# OP-FTIR Weekly Summary

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## Weekly Summary:

The OP-FTIR spectrometer provides real-time multi-gas measurement (qualitative and quantitative) of gases<sup>1</sup>. Even though the instrument is very accurate regarding the quantification of compounds, reported results cannot be directly calculated into a concentration for a specific location, this is due to its sample size – an open path between two points. The sample path is defined by the location of the emitter and the reflector which may be 10s to 100s of meters apart. Therefore data from these instrument types will not be directly compared to Occupational Exposure Limits (OELs) and Action Levels, but used to determine concentrations of compounds along the path of the instrument's beam.

Each analyte has a specific predetermined infrared (IR) trace which represents the model for that chemical. The detection and reporting of that chemical is based on evaluation of the R-squared ( $R^2$ ) values (coefficient of determination) calculated by comparing the detection trace to the model trace for that chemical.  $R^2$  is a statistical value representing the "percent of variance explained" by evaluating the detected trace with the model trace, or an estimate of how well the two traces match.  $R^2$  values range from 0 to 1 with higher values indicating a better fit.  $R^2$  values for OP-FTIR data are dependent on sample concentration, chemical compounds [chemicals present can interfere/overlap with each other at key locations; typically those having the same functional groups (e.g., methane or ketone groups)], and many other factors. Results presented here are for compounds having an  $R^2$  value of greater than or equal to 0.5.

During the week in review, instrument 506A detected nitrous oxide ( $N_2O$ ), methane ( $CH_4$ ), and 1-3 butadiene. The butadiene  $R^2$  value is typically below the reporting threshold of 0.5, but in three instances the  $R^2$  value was 0.5 or above and detected concentrations of butadiene ranged from about 0.175 to 0.210 ppm. A recurring pattern of simultaneous  $N_2O$  and  $CH_4$  spikes was noted again this week. However, no detections were found which would indicate that an OEL was exceeded.

Instrument B also detected  $N_2O$  and  $CH_4$ . Concentrations are consistent with values reported by instrument A for the week. No strong correlation between the two instruments was observed this week.

Compounds detected by both instruments are typically present in air at detectable levels (including 1-3 butadiene<sup>2</sup>). This information indicates that the OP-FTIR units are effectively measuring composition of the gas components within its path. Specific instrument information is reported below.

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<sup>1</sup> OP-FTIR Fact Sheet: <http://hanfordvapors.com/wp-content/uploads/2016/10/OP-FTIR-fact-sheet.pdf>

<sup>2</sup> EPA: <https://www.epa.gov/sites/production/files/2016-08/documents/13-butadiene.pdf>

# OP-FTIR Weekly Summary

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## October 5<sup>th</sup> – October 12<sup>th</sup> 2016 Instrument Notes:

**Table 1. Chemical Species Detected on Open Path FTIRs at AP Tank Farm.**

Chemical (ALL PM)	506A: OP-FTIR Multipath	506B: OP-FTIR Single
Nitrous Oxide*	0.21 – 0.46 ppm	0.18 – 0.42 ppm
Ammonia*	ND – 0.024 ppm	ND
Methane	1.2 - 2.6 ppm	0.84 – 1.8 ppm
1-3-Butadiene*	ND - 0.21 ppm	ND
1-Butanol*	ND	ND
2-Hexanone*	ND	ND
3-Buten-2-one*	ND	ND
Acetaldehyde*	ND	ND
Acetonitrile*	ND	ND
Benzene*	ND	ND
Butanal*	ND	ND
Butyl Nitrite*	ND	ND
Ethylamine*	ND	ND
Formaldehyde*	ND	ND
Furan*	ND	ND
Methanol*	ND	ND
Methyl Isocyanate*	ND	ND
Methyl Nitrite*	ND	ND
N-Nitrosodiethylamine*	ND	ND
N-Nitrosodimethylamine*	ND	ND
N-Nitrosomorpholine*	ND	ND
Propanenitrile*	ND	ND
Pyridine*	ND	ND
Tributyle Phosphate*	ND	ND

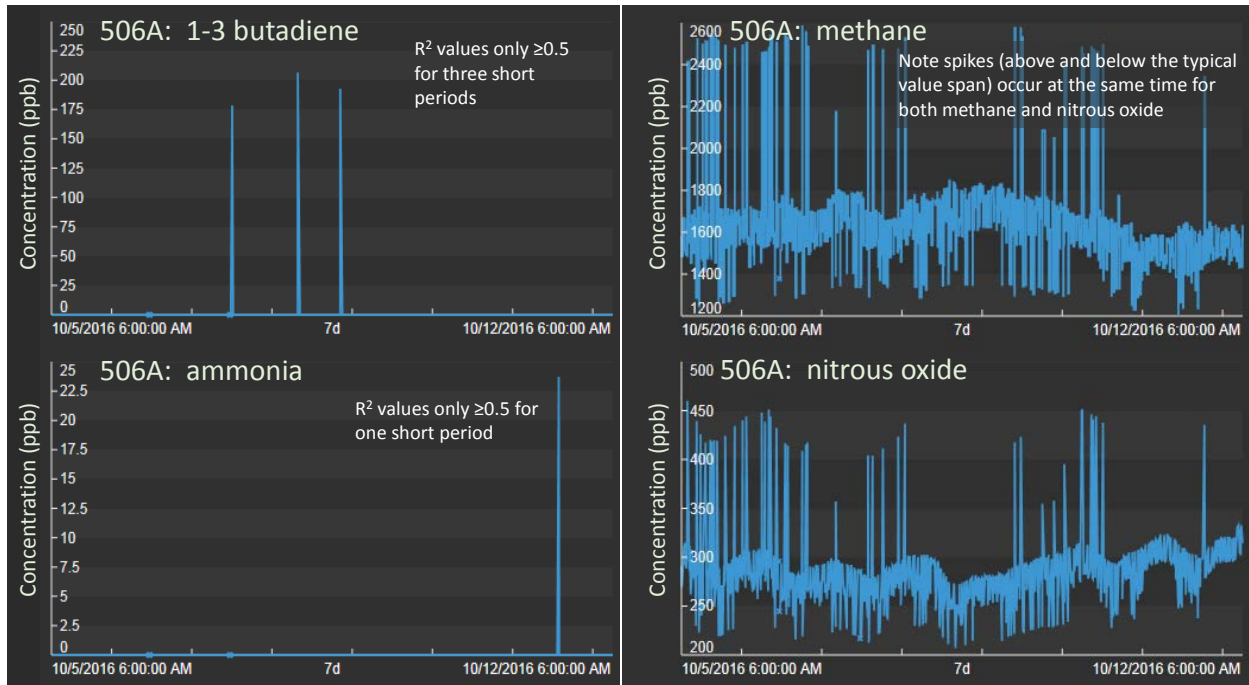
\*Chemical is on COPC list

Notes: ND – Not detected by instrument (i.e., either value reported was 0 or R<sup>2</sup> value is <0.5)

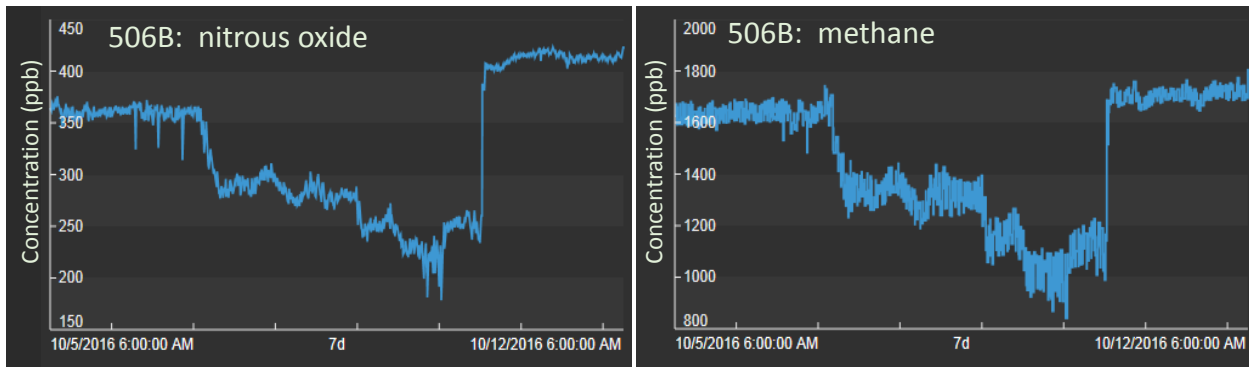
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**Figure 1. OP-FTIR A (506A) Review.**  
(Note that concentration units are ppb)



**Figure 2. OP-FTIR B (506B) Review.**  
(Note that concentration units are ppb)



**Table 2. OP-FTIR Instrument Time Reporting<sup>a</sup>.**

Instrument	Comments
506A	The instrument was reported 100% of the time.
506B	The instrument was reporting 100% of the time.

Notes: a) % down is based on review of graph data from OSI PI<sup>3</sup>

<sup>3</sup> OSI PI is a data visualization software package from [OSIsoft](http://OSIsoft.com).