

Publication Citations
AQRP Projects
FY 2010-2011

10-006

Johansson, J., Johan Mellqvist, Jerker Samuelsson, Brian Offerle, Jana Moldanova , Bernhard Rappenglück, Barry Lefer, and James Flynn (2014) , Formaldehyde Quantitative Measurements and Modeling of Industrial Formaldehyde Emissions in the Greater Houston Area during Campaigns in 2009 and 2011, *Journal of Geophysical Research: Atmospheres*, 119, DOI: 10.1002/2013JD020159

Johansson, J. K. E., J. Mellqvist, J. Samuelsson, B. Offerle, B. Lefer, B. Rappenglück, J. Flynn, and G. Yarwood(2014), Emission measurements of alkenes, alkanes, SO₂, and NO₂ from stationary sources in Southeast Texas over a 5 year period using SOF and mobile DOAS, *J. Geophys. Res. Atmos.*, 119, doi:10.1002/2013JD020485.

10-008

Digar, A., D.S. Cohan, X. Xiao, K.M. Foley, B. Koo, and G. Yarwood (2013). Constraining ozone-precursor responsiveness using ambient measurements. *Journal of Geophysical Research*, 118(2), 1005-1019, [doi:10.1029/2012JD018100](https://doi.org/10.1029/2012JD018100).

10-009

The following papers were submitted to *Industrial & Engineering Chemistry Research* for a Special Issue on Industrial Flaring:

Torres, V.M., Herndon, S., Wood, E., Al-Fadhli, F.M., Allen, D.T., Emissions of Nitrogen Oxides from Flares Operating at Low Flow Conditions, *Industrial & Engineering Chemistry Research*, 51, 12600-12605, DOI: 10.1021/ie300179x (2012)

Pavlovic, R.T., Al-Fadhli, Kimura, Y., Allen, D.T., and McDonald-Buller, E.C. Impacts of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area, *Industrial & Engineering Chemistry Research*, 51, 12593-12599, DOI: 10.1021/ie203052w (2012).

Knighton, W.B., Herndon, S.C., Franklin, J.F., Wood, E.C., Wormhoudt, J., Brooks, W., Fortner, E.C., and Allen, D.T. Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy, *Industrial & Engineering Chemistry Research*, 51, 12674-12684, DOI: 10.1021/ie202695v (2012)

Torres, V.M., Herndon, S., Kodesh, Z., Nettles, R., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research*, 51, 12559-12568, DOI: 10.1021/ie202674t (2012).

Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research*, 51, 12569-12576, DOI: 10.1021/ie202675f (2012)

Herndon, S.C., Nelson, D.D., Wood, E.C., Knighton, W.B., Kolb, C.E., Kodesh, Z., Torres, V.M., and Allen, D.T., Application of the carbon balance method to flare emissions characteristics, *Industrial & Engineering Chemistry Research*, 51, 12577-12585, DOI: 10.1021/ie202676b (2012)

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research*, 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

The following presentations were given at the Air & Waste Management Association June 2012 Conference, and papers were published in the Conference Proceedings:

Torres, V.M., Allen, D.T., Herndon, S. and Kodesh, Z., Overview of the Texas Commission on Environmental Quality 2010 Flare Study, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-437-AWMA, San Antonio, June, 2012.

Torres, V.M., Al-Fadhli, F.M., Allen, D.T., Herndon, S., and Wood, E., NOx Emissions from Industrial Flaring, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-315-AWMA, San Antonio, June, 2012.

10-015

The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models

J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood

In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride

J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood

In preparation for Journal of Geophysical Research

10-020

Several papers are expected to be published based on this Project. Their titles and current status are below:

Accepted in Journal of Geophysical Research:

The Effects of NOx Control and Plume Mixing on Nighttime Chemical Processing of Plumes from Coal-Fired Power Plants.

Steven S. Brown, William P. Dubé, Prakash Karamchandani, Greg Yarwood, Jeff Peischl, Thomas B. Ryerson, J. Andrew Neuman, John B. Nowak, John S. Holloway, Rebecca A. Washenfelder, Charles A. Brock, Gregory J. Frost, Michael, Trainer, David D. Parrish, Frederick C. Fehsenfeld and A. R. Ravishankara

In preparation for Journal of Geophysical Research:

Biogenic VOC Oxidation and Organic Aerosol Formation within an Urban Nocturnal Boundary Layer – Aircraft Vertical Profiles in Houston, TX.

Steven S. Brown, William P. Dubé, Roya Bahreini, Ann M. Middlebrook, Charles A. Brock, Carsten Warneke, Joost A. de Gouw, Rebecca A. Washenfelder, Elliot Atlas, Jeff Peischl, Thomas B. Ryerson, J. Andrew Neuman, Jonathan B. Nowak, Michael Trainer, David D. Parrish, Frederick C. Feshenfeld and A. R. Ravishankara

In preparation for Atmosphere:

Reactive Plume Modeling to Investigate NO_x Reactions and Transport at Night

Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:

Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique

Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021

The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the submitted abstract was *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, "CFD Modeling of Laboratory Flames and an Industrial Flare," manuscript submitted to Journal of the Air & Waste Management Association (under revision).

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, " Parametric Study of Ethylene Flare Operations and Validation of a Reduced Combustion Mechanism," Engineering Applications of Computational Fluid Mechanics, Vol. 8, No. 2, pp. 211–228 (2014).

Hitesh S. Vaid, Kanwar Devesh Singh, Helen H. Lou, Daniel Chen, Peyton Richmond, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale CFD Simulations," International Journal of Numerical Methods for Heat and Fluid Flow, Vol. 24 No. 1, 2014, pp. 21-35.

K. Singh, T. Dabade, H. Vaid, P. Gangadharan, D. Chen, H. Lou, X. Li, K. Li, C. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Ind. & Eng. Chem. Research, 51 (39), 12611-12620, October, 2012.

H. Lou, D. Chen, C. Martin, X. Li, K. Li, H. Vaid, K. Singh, P. Gangadharan, "Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, " Industrial & Engineering Chemistry Research, Industrial flares special issue, 51 (39), 12697-12705, October, 2012.

H. Lou, C. Martin, D. Chen, X. Li, K. Li, H. Vaid, A. Tula, K. Singh, "Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, Volume 14, Issue 4, pp 737-748, August 2012, DOI 10.1007/s10098-011-0441-6.

Helen H. Lou, Christopher B. Martin, Daniel Chen, Xianchang Li, Kyuen Li, Hitesh Vaid, Anjan Tula Kumar, Kanwar Devesh Singh, & Doyle P. Bean, "A reduced reaction mechanism for the simulation in ethylene flare combustion," Clean Technologies and Environmental Policy, Volume 14, Issue 2, pp 229-239, April 2012, doi:10.1007/s10098-011-0394-9.

10-024

The Project Investigators have submitted articles to the following journals:

J. Geophysical Research (in revision)

Atmospheric Environment (in review)

10-032

Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhan, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappengluck, K. W. Wong, C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke and P. Kelley (2013), Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *Journal of Geophysical Research-Atmospheres*, 118, 5770-5780, doi:10.1002/jgrd.50342.

10-042

Heo, G., McDonald-Buller, E.C., Carter, W.P.L., Yarwood, G., Whitten, G.Z. and Allen, D.T. "Modeling Ozone Formation from Alkene Reactions using the Carbon Bond Chemical Mechanism, *Atmospheric Environment*, 59, 141-150, DOI: 10.1016/j.atmosenv.2012.05.042 (2012).

Heo, G. Y. Kimura, E. McDonald-Buller, D. T. Allen, G. Yarwood, G. Z. Whitten Evaluation of a New Toluene Mechanism For Carbon Bond 05 Using Environmental Chamber Data and Ambient Data, Air and Waste Management Association Annual Meeting, Paper #154, Detroit, June 2009

In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate NOx removal and recycling represented in atmospheric mechanisms for air quality modeling*
Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen

In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial NO_x*

Gookyoung Heo, William Carter, Greg Yarwood

10-045

Olga Pikelnaya, James H. Flynn, Catalina Tsai, and Jochen Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, *Journal of Geophysical Research*, [Volume 118, Issue 15](#), pages 8716–8728, 16 August 2013, DOI: 10.1002/jgrd.50643

The following papers were submitted to *Industrial & Engineering Chemistry Research* for a Special Issue on Industrial Flaring. The paper edition of this special edition will come out in Fall 2012, but the online versions are available now.

Knighton, W.; Herndon, Scott; Wood, Ezra; Fortner, Edward; Onasch, Timothy; Wormhoudt, Joda; Kolb, Charles; Lee, Ben; Zavala, Miguel; Molina, Luisa; Jones, Marvin, “*Detecting fugitive emissions of 1, 3-butadiene and styrene from a petrochemical facility: An application of a mobile laboratory and a modified proton transfer reaction mass spectrometer – NO + PTR-MS*”

Status: Published Online

Wood, E.; Herndon, S.; Fortner, E.C.; Onasch, T.; Wormhoudt, J.; Kolb, C.E.; Knighton, W.B.; Lee, B.; Zavala, M.; Molina, L.; Jones, M., “*Combustion and Destruction/Removal efficiencies of in-use chemical flares in the greater Houston area*”.

Status: Published Online

This project has also resulted in the following publications:

Olga Pikelnaya, Jochen Stutz, Scott Herndon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuete, Evan Couzo, “*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview*”, in preparation for *Journal of Geophysical Research*

Olga Pikelnaya, Scott Herndon, Ezra Wood, and Jochen Stutz, “*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign*,” under development.