MICHIGAN DEPARTMENT OF ENVIRONMENT, GREAT LAKES, AND ENERGY

Fine Scale Modeling in Support of MOOSE

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Southeast Michigan Ozone Nonattainment Area

- Monitors in Southeast Michigan (SEMI) have exceeded O_3 National Ambient Air Quality Standard of 70 ppb.
- Seven counties (St. Clair, Macomb, Oakland, Livingston, Wayne, Washtenaw, Monroe) designated as SEMI ozone nonattainment area by U.S. EPA.
- Bump-up from “marginal” to “moderate” designation is possible based on 2018-2020 ozone data.
- A State Implementation Plan (SIP) and ozone attainment demonstration may be required for SEMI, if bumped up.


Port Huron
71 ppb
New Haven
71 ppb
Warren
68 ppb
Oak Park
72 ppb
Detroit East 7 Mile 71 ppb
Ypsilanti
67 ppb
Allen Park
67 ppb
Flint
Owosso
Sarnia
Waterford
Sterling Heights
Farmington Hills
Southfield
Novi
Livonia
Westland
Ann Arbor
Lake St Clair
Walpole Island No. 46
Leamington
Point Pelee National Park
Adrian

Michigan-Ontario Ozone Source Experiment (MOOSE)

- International / intergovernmental collaboration:
  - **United States:** Michigan EGLE, U.S. EPA, NASA, NSF, U.S. Forest Service, U.S. Department of Energy
  - **Canada:** Environment and Climate Change Canada (ECCC), Ontario Ministry of Environment, Conservation, and Parks (MECP)
- 2021 campaign (May 20 – Sep 30) deploys:
  - Advanced ground and airborne remote sensing and mobile real-time monitoring techniques
  - Very high spatial and temporal resolution regional and micro-scale chemical transport models

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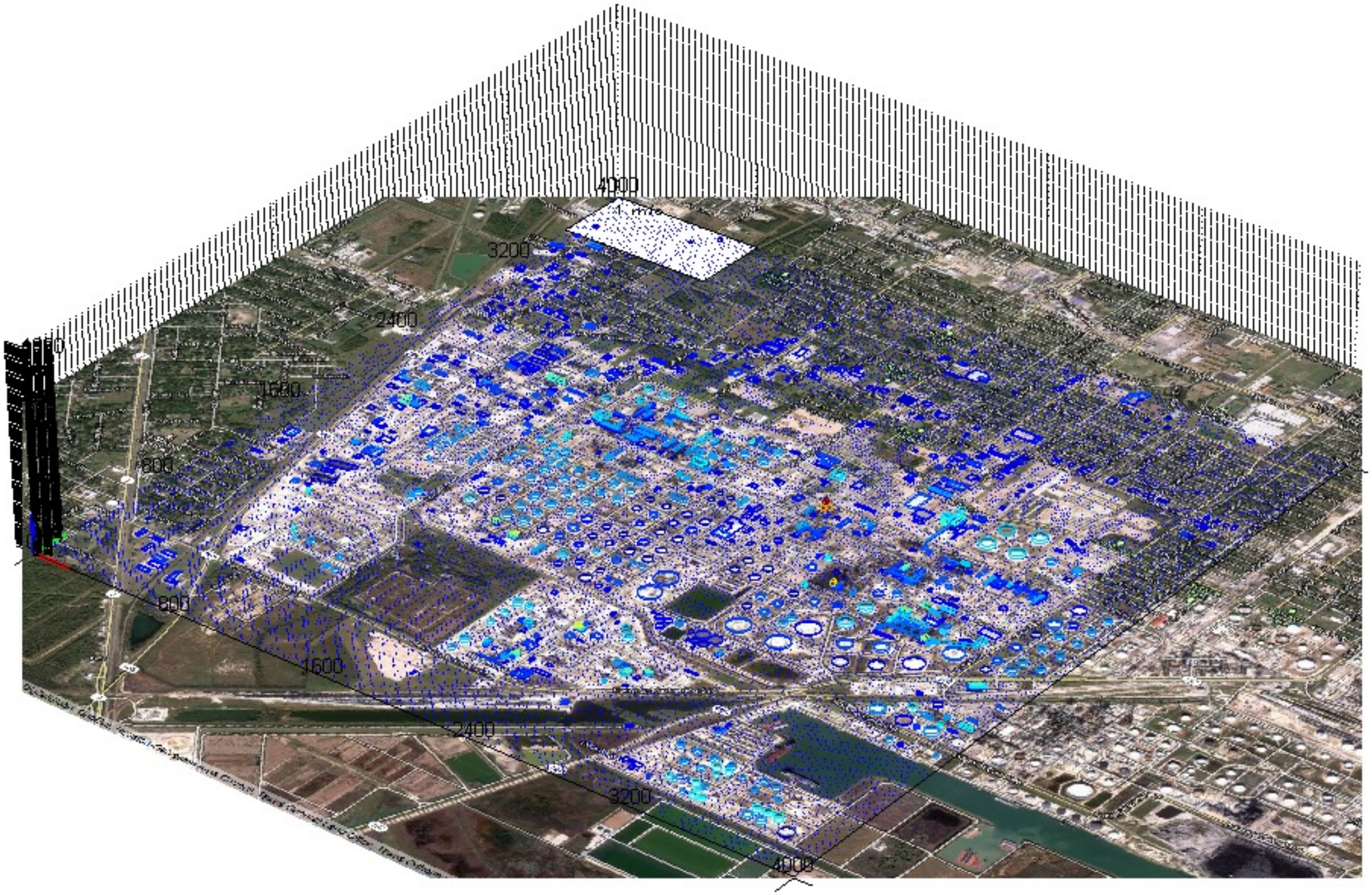
High Resolution Urban Wind Model



QUIC model used to simulate wind based on 3D LIDAR building morphology
Olaguer et al. (2013), *J. Geophys. Res.-Atmos.*, *118*, 11,317–11,326.

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Microscale Forward and Adjoint Chemical Transport (MicroFACT) Model

- 3D Eulerian model simulates transport of 35 species by **advection** and **turbulent diffusion**
- **Chemistry** is simulated by 116 gas-phase and 5 heterogeneous reactions
- **Very fine resolution** (10 s, 400 m horizontal)
- Model has both **forward and adjoint** modes
- Can **infer emissions at fine scale** from MOOSE measurements (inverse modeling)

Olaguer, E.P., *Atmosphere* **2021**, *12*, 877. https://doi.org/10.3390/atmos12070877

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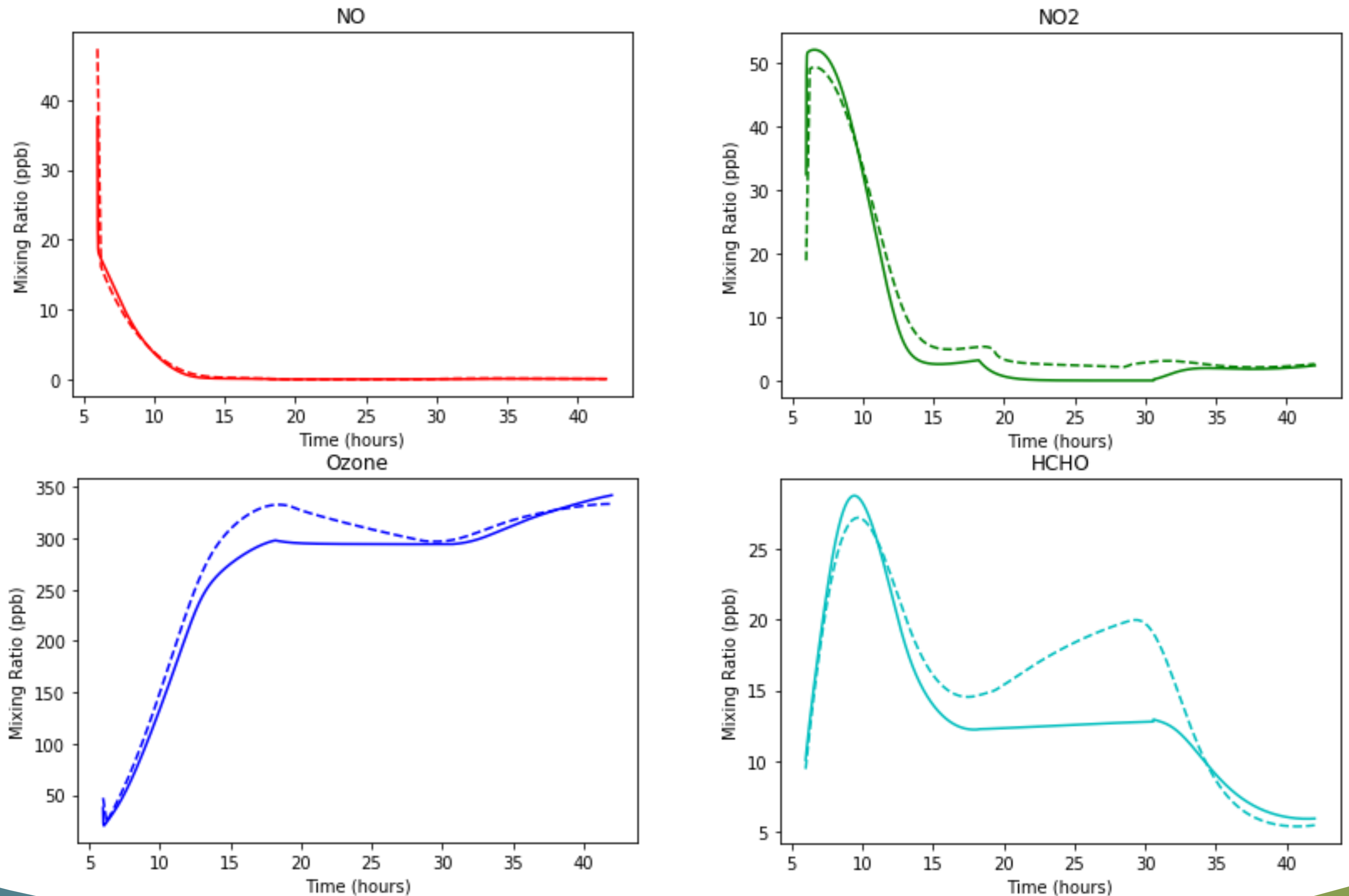
Chemical Mechanism: MCM vs MicroFACT



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Policy Questions

- **Where does the ozone during an exceedance come from?**
  - How critical are lake breeze effects in transporting ozone?
  - Is local chemistry significantly impacted by fine-scale dynamical features? Which sources are most affected?

- **Which set of ozone precursors need control?**
  - VOC or NOx-limited? Transitional?
  - If VOCs, which species/sources? Are there significant under-estimated sources?
  - Are primary sources of radicals (e.g., HCHO, HONO) under-estimated? How much does this impact ozone productivity and control strategy efficacy in models?
  - Does methane (CH_4) contribute significantly to ozone?

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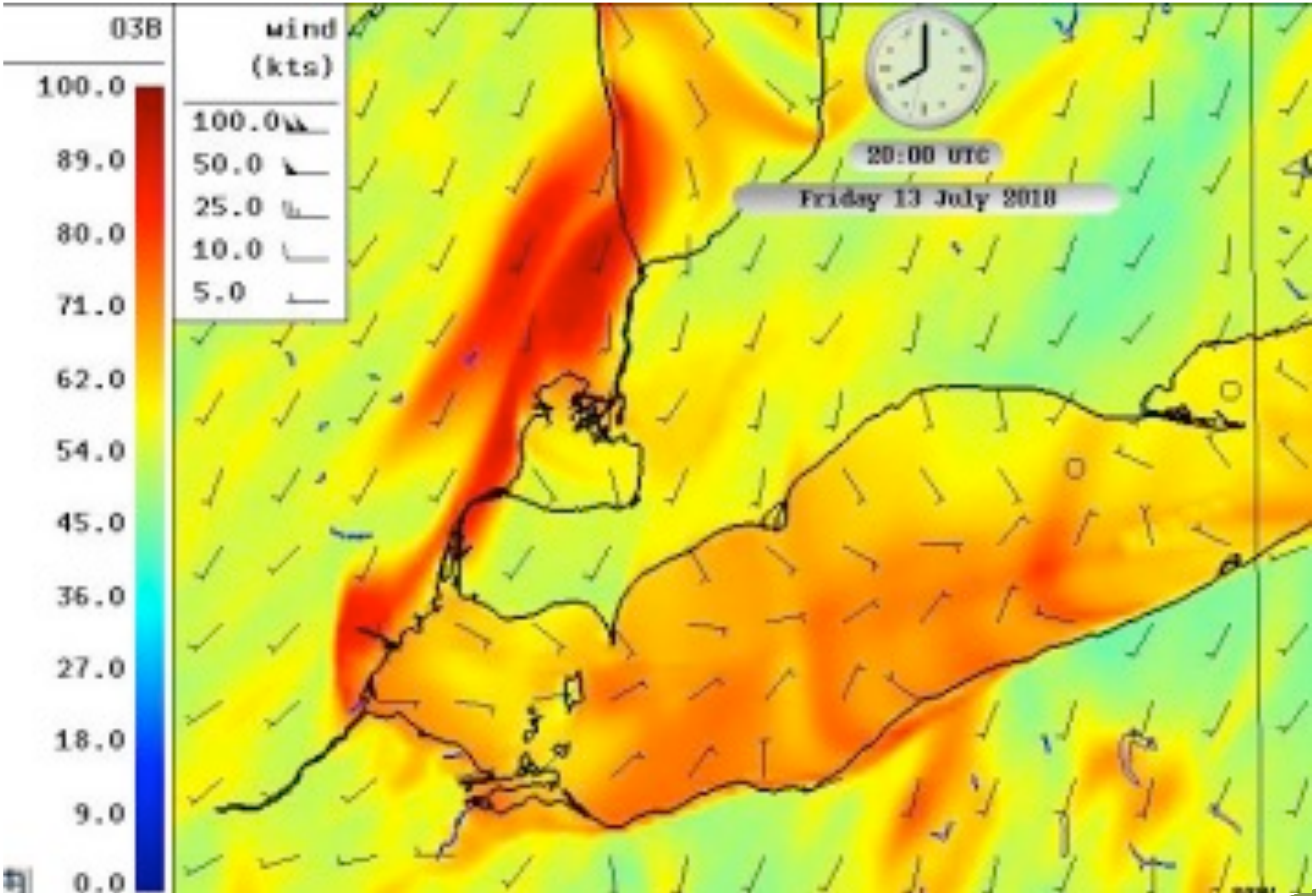
GEM-MACH 2.5-Δkm Ozone Simulation



Courtesy of Craig Stroud, ECCC

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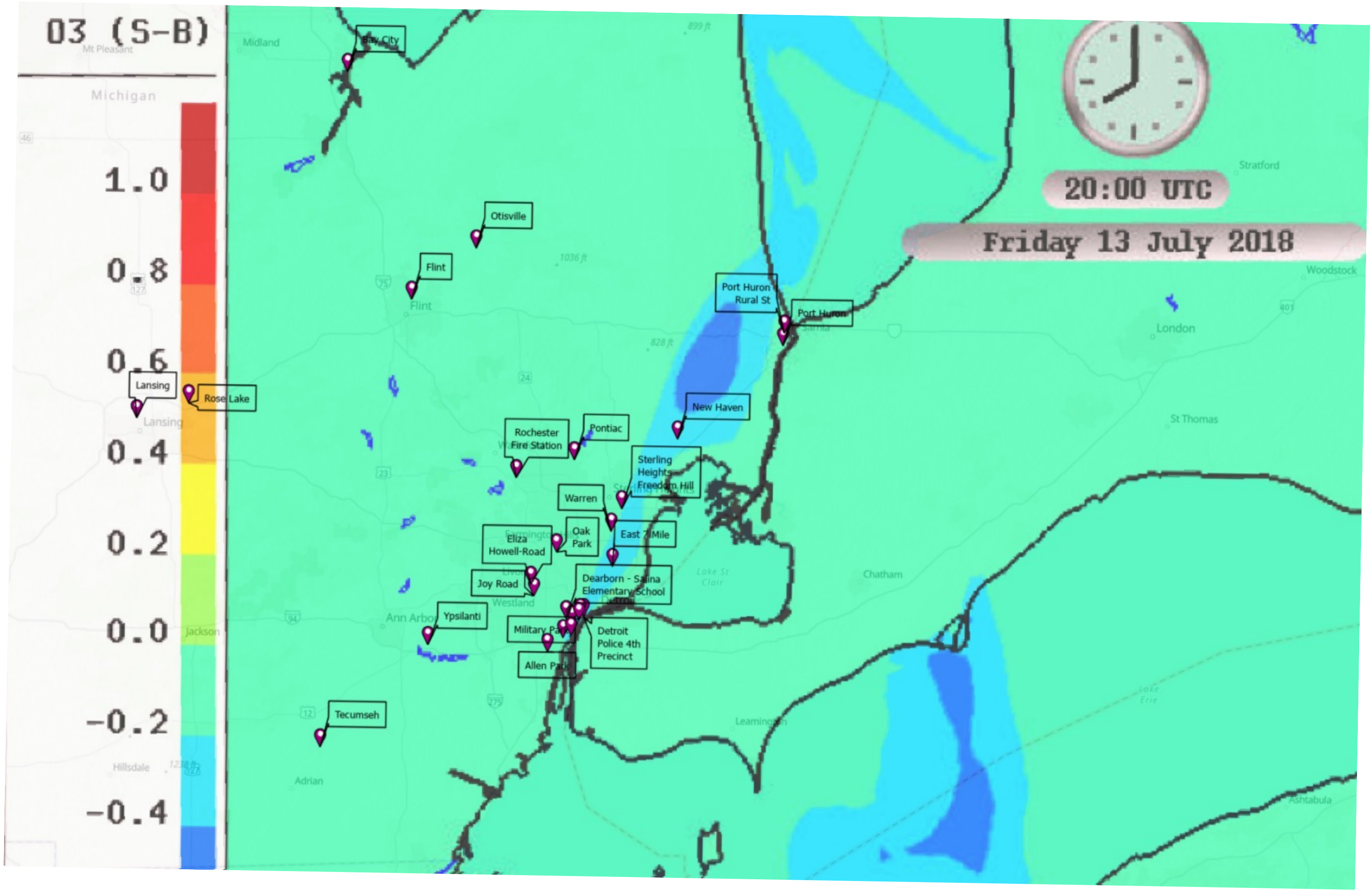
10% VOC solvent use emission reduction



Blue areas are VOC sensitive, high in NOx

S-B is sensitivity run minus base run (in ppbv)

Courtesy of Craig Stroud, ECCC

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Volatile Chemical Products

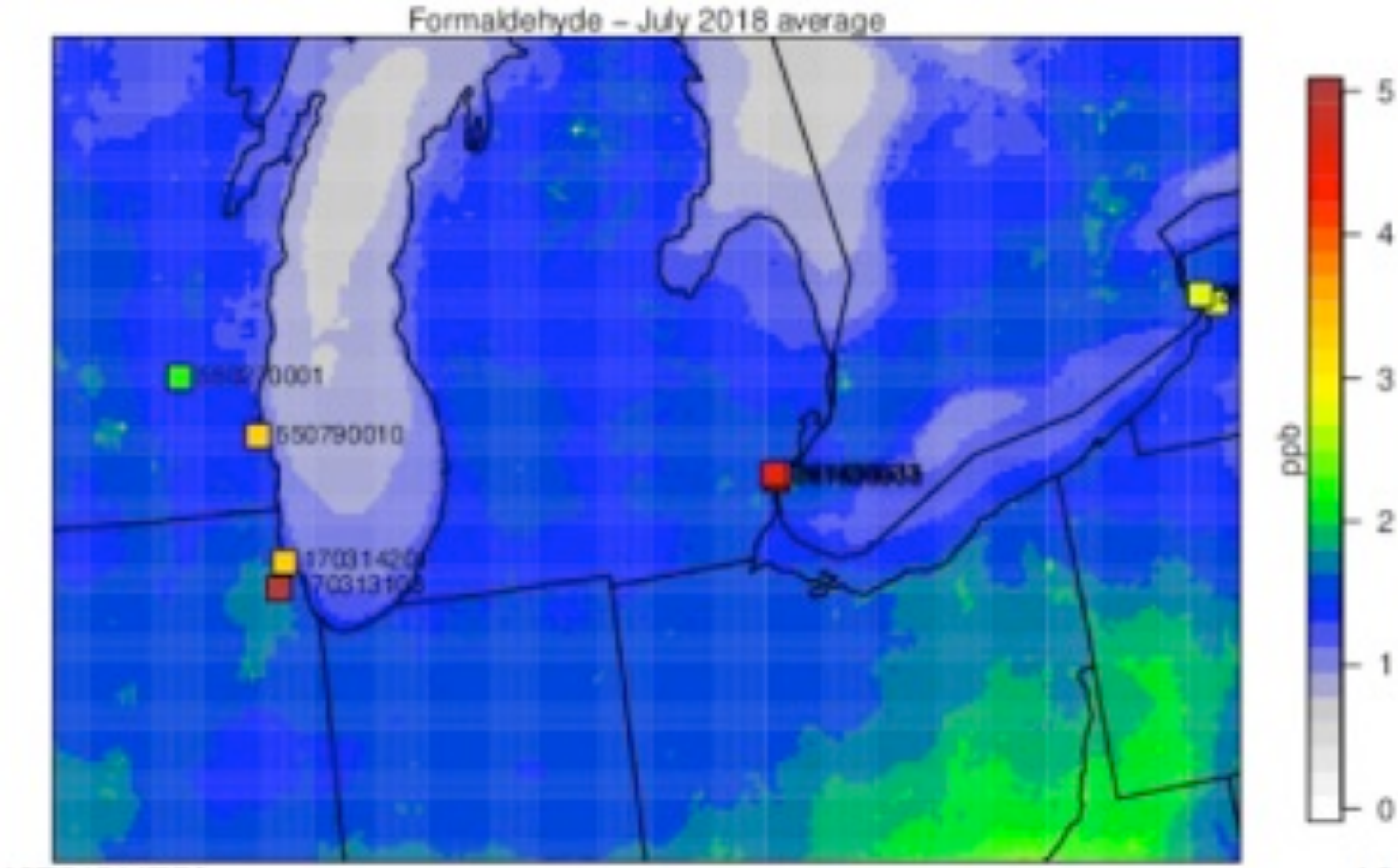
- McDonald et al. (2018) found that volatile chemical products (VCPs)—including pesticides, coatings, printing inks, adhesives, cleaning agents, and personal care products—now constitute half of fossil fuel VOC emissions in industrialized cities.

- Seltzer et al. (2020) predicted larger VCP emissions than the 2017 NEI for approximately half of all U.S. counties, with 5 % of all counties featuring increases > 60%. This will be reflected in the 2020 NEI.

Formaldehyde (HCHO)

- Formaldehyde (HCHO) is a **Volatile Organic Compound (VOC)** that is very reactive (lifetime of a few hours). Like other VOCs, it reacts with already available hydroxyl radical (OH).
- HCHO is a powerful ozone precursor due to its ability to generate **new, unrecycled radicals** that fuel $NO \rightarrow NO_2 \rightarrow O_3$.
- HCHO is also a **Hazardous Air Pollutant (HAP)** with both cancer and non-cancer (e.g., airway irritation and asthma) health effects.
- **Secondary HCHO** is the by-product of the chemical degradation of other VOCs already in the atmosphere, including biogenic VOCs.
- **Primary HCHO** is emitted by human activities, mostly incomplete combustion, where **HCHO/CO molar ratio is likely between 2-10%**.
- HCHO is likely **underrepresented in official emission inventories** (Olaguer et al., *J. Geophys. Res. Atmos.*, 119:2597-2610, 2014).

CMAQ Model Formaldehyde versus Observations



Courtesy of Kirk Baker, USEPA

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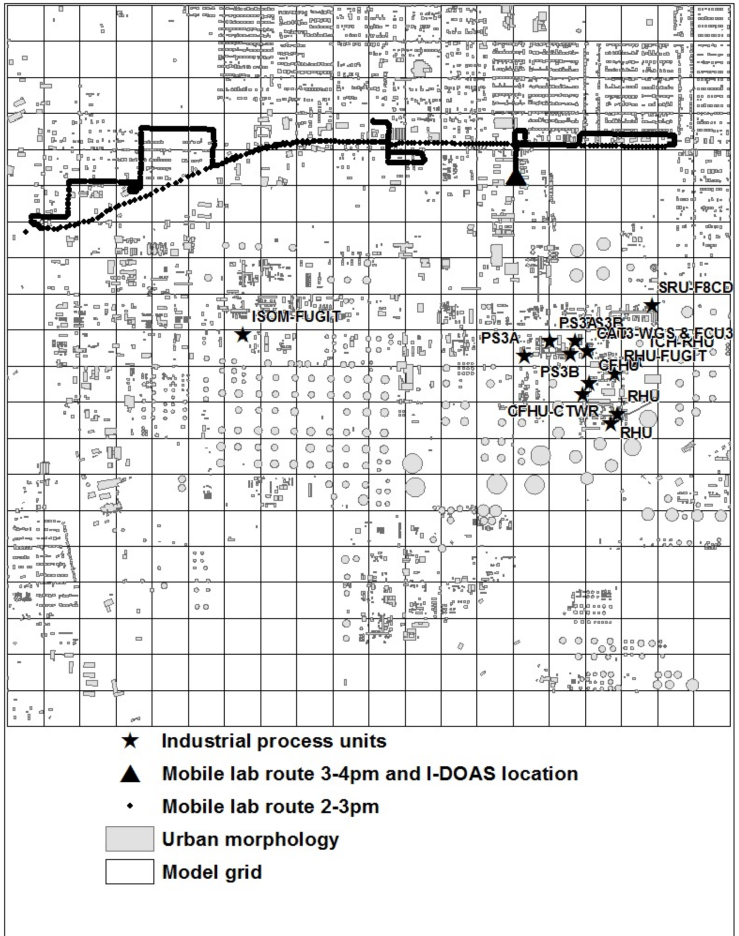
Formaldehyde Source Attribution for a Texas City Refinery



- Winds from QUIC model
- Inverse modeling based on mobile QCL measurements
- Emissions attributed primarily to fluidized cat cracking and desulfurization operations
- Formaldehyde emissions agree with I-DOAS remote sensing measurements (18 kg/hr)
- HCHO/CO molar ratio = 3%

Olaguer et al. (2013), *J. Geophys. Res.-Atmos.*, *118*, 11,317–11,326.

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OXIDATION CATALYSIS OF NG ENGINES

Engine	CO Emissions (lb/hr)	Average CO Emissions (lb/hr)	HCHO Emissions (lb/hr)	Average HCHO emissions (lb/hr)	Heat input (MMbtu/hr)
Engine 1 (oxidation catalyst)	.13	.15	.024	.030	17.5
Engine 2 (oxidation catalyst)	.17		.026		16.1
Engine 3 (oxidation catalyst)	.07		.019		16.7
Engine 4 (oxidation catalyst)	.24		.049		17.1
Engine 5 (no catalyst)	7.31	7.08	.71	.72	18.1
Engine 6 (no catalyst)	6.94		.74		17.1
Engine 7 (no catalyst)	7.03		.75		16.8
Engine 8 (no catalyst)	7.03		.69		16.9

Data from 8 4-Stroke Lean Burn NG Engines at a New Jersey natural gas processing facility; 4 of the engines have been equipped with oxidation catalysis. The results demonstrate a 98% reduction in CO emissions, and a 96% reduction in HCHO emissions.

After Ratzman (2018)

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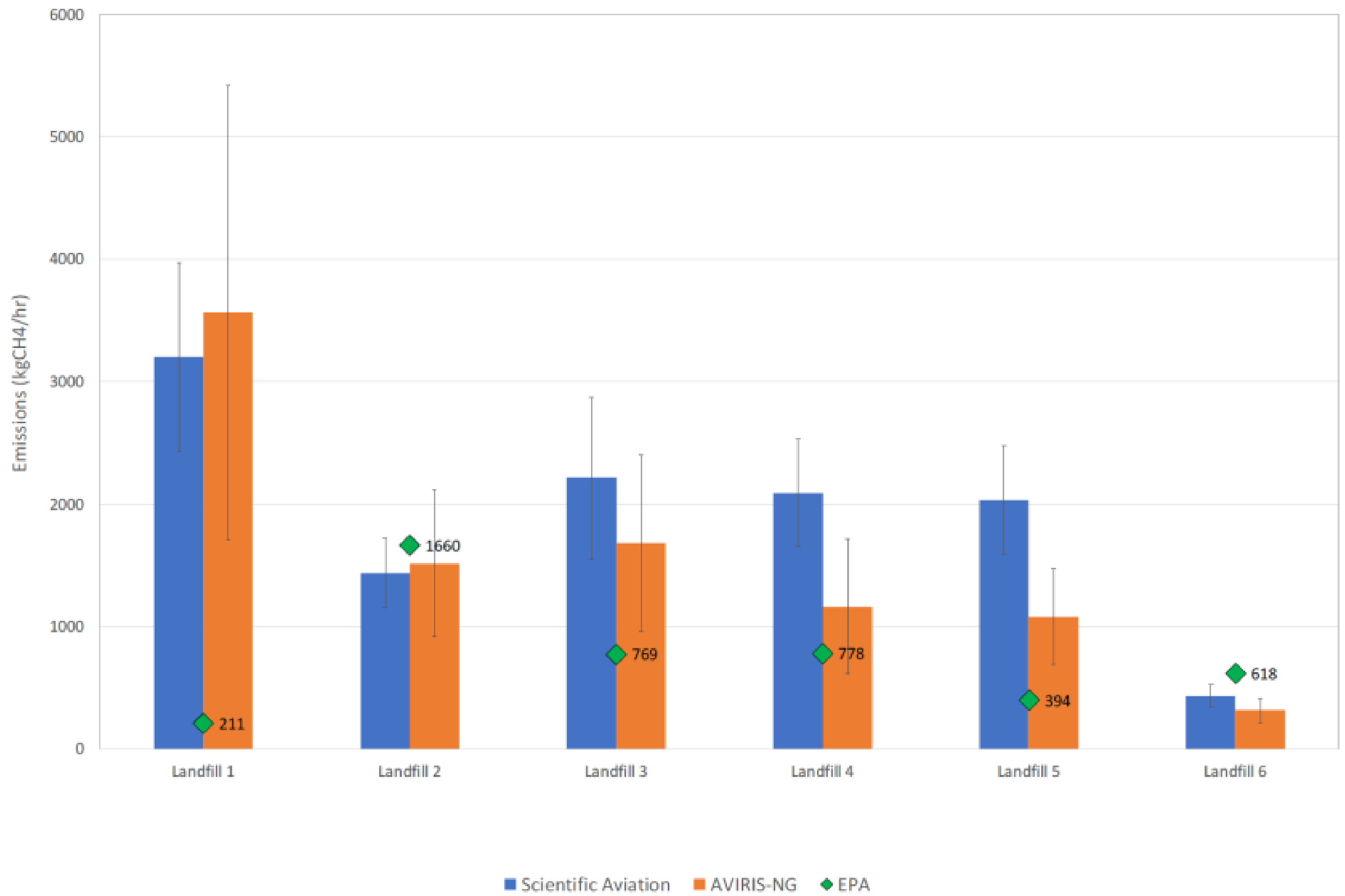
California Methane Survey: Landfills



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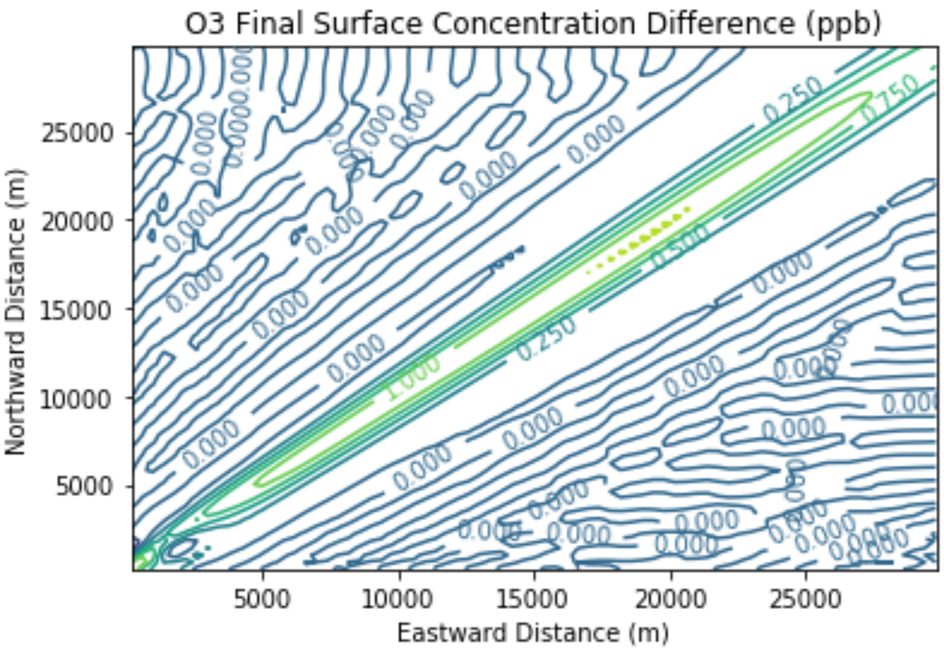
Hypothesis: Landfills Create Significant Ozone Plumes

- Landfills emit large amounts of **methane (radical extender)**.
- Landfills also can emit significant amounts of **formaldehyde (radical precursor)** from on-site gas-to-energy conversion facilities (engines and flares)**.**
- Landfill activities also produce **NOx** and other ozone precursors**,** including **VOC from landfill gas**.
- The combination of these emissions result in significant ozone plumes that **may add at least 1 ppb to ozone design values in Southeast Michigan**.

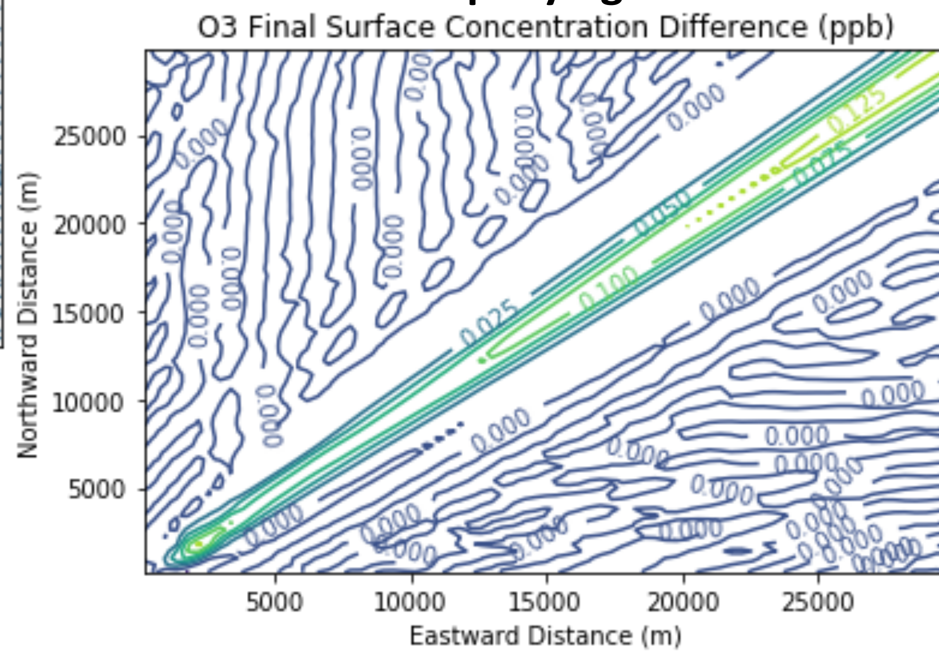
Landfills in SE Michigan

MicroFACT Simulation of Ozone Impact of a Hypothetical Landfill



Additional Ozone over Background due to Combustion Emissions from Flares and Engines

Ozone Enhancement due to Landfill Gas Fugitive Emissions of 3000 kgCH_4/hr Plus Accompanying NMOC



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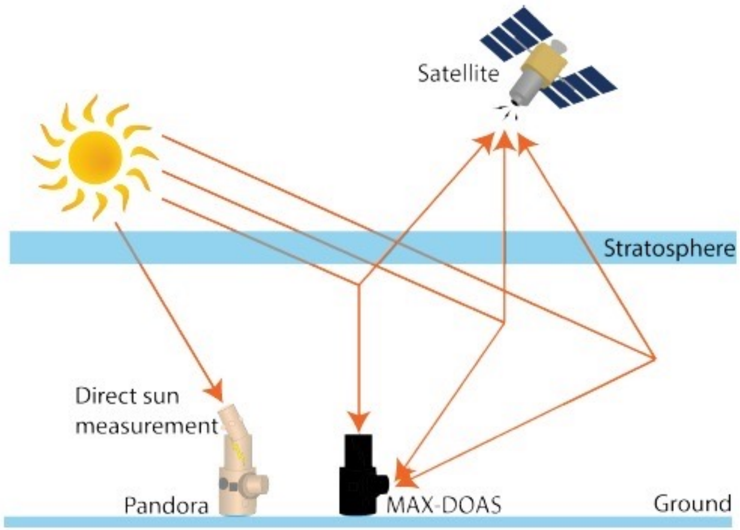
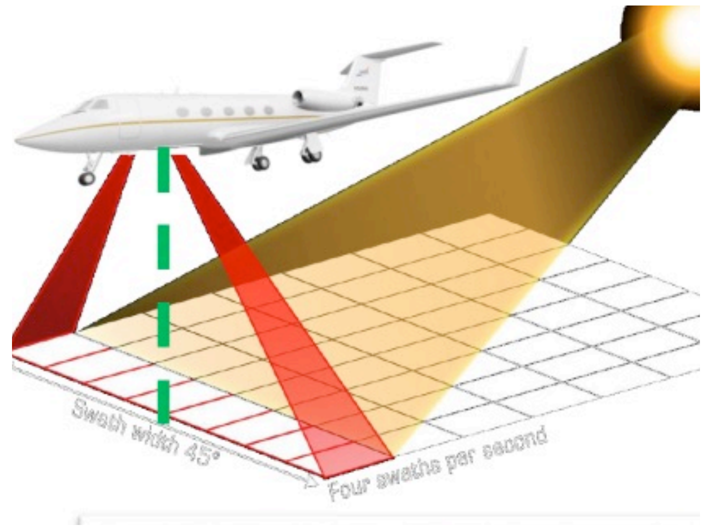
MOOSE Instrument Platforms



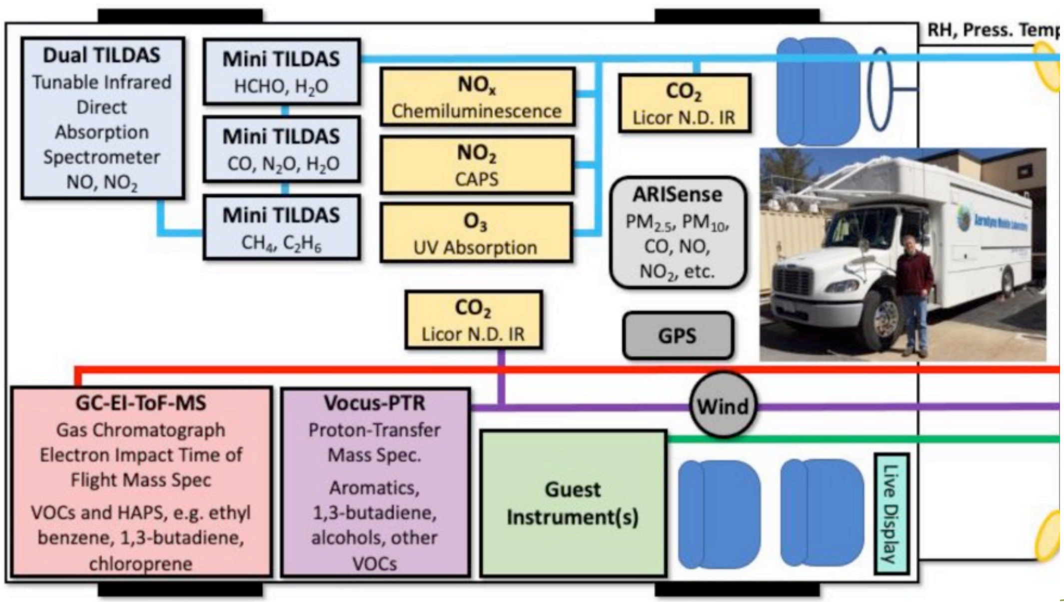
HCHO, NO_2



HCHO, NO_2

HCHO, NO_x, CH_4, CO, O_3

VOCs



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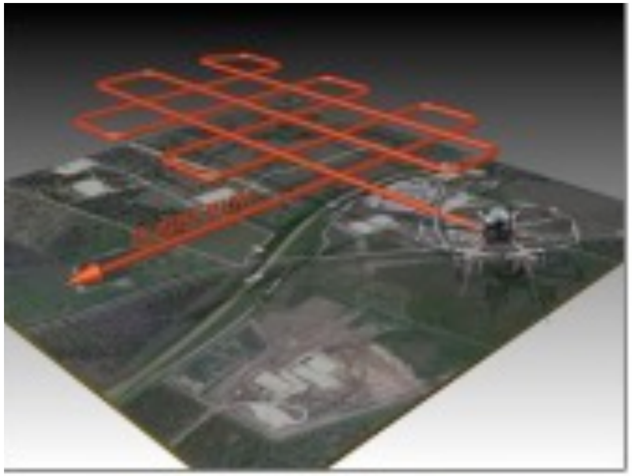
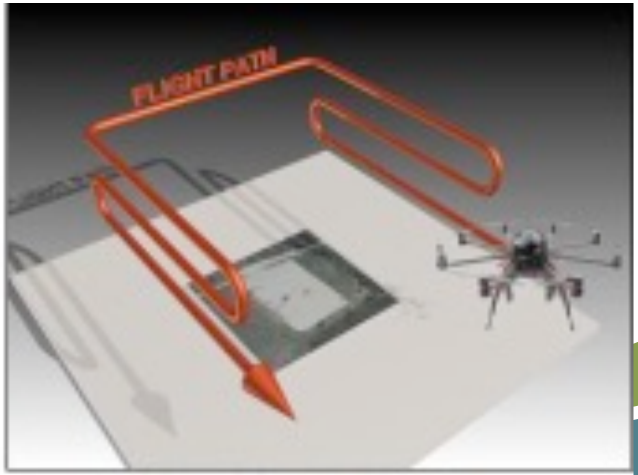
Drone Measurements at Landfills

- Negotiated access to 2 landfills in SE Michigan
- Two drone measurement platforms:
  - ❑ Aegis IEV2 drone with BlueHalo WP-V2 UAS Weather Payload
  - ❑ DJI M600 heavy-lift drone with a Scentroid DR1000 and a CH_4 Tunable Diode Laser Absorption Spectrometer (TDLAS)
- Gaussian plume/complex terrain inverse model





Issues to be Investigated with Fine Scale Air Quality Modeling

- How much is NO_x diluted and O_3 productivity enhanced by uplift at lake breeze frontal boundaries?
- How much does flaring by steel mills and other large industrial combustion activities contribute to HCHO emissions and nearby community exposure to HCHO?
- Are there large, undocumented emissions of solvents and other VCPs from point sources? What impact do these emissions have on ozone formation downwind?
- Do large urban pipeline leaks of natural gas (CH_4 and other hydrocarbons) significantly enhance the O_3 productivity of co-located VOC and NO_x emissions?


Questions?