EPAct/V2/E-89:
Testing, Results & Application in MOVES2013

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Background

Origins of "EPAct Program"

- Sec. 1506 of the Energy Policy Act of 2005 ("EPAct") directed EPA to produce an updated emissions model reflecting fuel property effects
  - Funding for RFS-related emission testing became available in 2007, at which point program design began

- ASD staff examined existing data together with requirements of EPAct 2005 and other regulatory needs going forward
  - Focus became LD Tier 2 vehicle fleet to address key data gaps for the following fuel properties:
    - Ethanol content
    - Aromatics content
    - Distillation parameters (T50, T90)
    - Vapor pressure

Addresses Key Data Gaps

- By 2017 Tier 2 will account for 80% of VMT, yet MOVES fuel effects were based on past studies of Tier 0-1
  - In RFS2, did not have enough data to analyze the impacts of ethanol
  - Also, could not analyze effect of fuel changes on PM and toxic emissions,
  - Lacked Tier-2 exhaust speciation profiles for air quality modeling

- Needed ability to assess interactions between fuel properties (e.g., changes in aromatics and T50 when ethanol is blended)
  - EPAct program design was optimized to allow modeling of multiple interactions, something not done since Auto/Oil AQIRP in early 1990s
  - *This is key to understanding effects of blending ethanol in the real world*

Other Data Gaps

- Sulfur
  - Requires a different program design
  - Covered by another EPA study, to be discussed later today

- Olefins
  - More fuels would have added cost
  - Didn't expect much impact on emissions
  - Examined later in CRC E-83, which confirmed little or no measureable impact

CRC & DOE Partners

- Program benefitted from collaboration with partners:
  - DOE (NREL) had resources to characterize effects of ethanol fuels, which led to an expanded fuel matrix covering E15 and E20 fuels.
  - CRC served as technical advisors to ensure industry concerns about study design and execution were addressed early. They also provided the E85 test fuel.

Overview of Phases

- Phases 1 & 2: Initial pilot phases (EPA)
  - Testing at 75°F (Phase 1) and 50°F (Phase 2) over LA92 (plus subset of FTP tests)
  - 3 fuels: E0, E10, E15 approximating typical market "match blends"
  - 19 high sales vehicles representing >50% of projected 2008 sales
  - Completed in mid-2008
  - Some concerns with fuel blending, plus dataset too small to model individual properties
- Phase 3 Main fuel matrix (EPA/DOE/CRC)
  - 27 fuels tested in 15 Tier 2 vehicles, E85 tested in 4 FFVs
  - LA92 test cycle at 75°F
  - Two replicates of each fuel/vehicle combination = ~60 tests/veh
  - Testing completed in mid-2010

Overview of Phases

- Phase 4: Temperature effects on normal emitters (DOE)
  - Collected 20°F and 95°F data for a subset of Phase 3 fuels (6) and vehicles (6)
  - Fuel effects modeling not possible; allows broad characterization of temperature effects
- Phase 5: High emitters (DOE)
  - SwRI sourced four actual high emitters from Houston, TX
  - Performed similar test matrix of fuels/temps as in Phase 4
  - Fuel effects modeling not possible; allows broad characterization of high emitter behavior
  - Since the failure modes were not characterized, it is difficult to extrapolate the results in fleet-wide modeling

Program Cost & Timeline

Initiated program design	Mid-2007
Phase 1	April-Aug 2008
Phase 2	Oct 2008 – Jan 2009
Phase 3	Mar 2009 – May 2010
Phase 4	May-June 2010
Phase 5	May-June 2010
Analysis and reporting	Mid-2010 – Mid-2012

Overall contract cost of $9.8 million for all phases (51% EPA)

Design

Program Overview

- Optimized matrix of 27 test fuels (plus E85 on FFVs)
- Test fleet of 15 high-sales cars and light trucks from 2008 MY
- Testing performed at 75°F over 3-bag LA92 cycle
  - 2+ replicates per vehicle-fuel combination
- Measured gaseous pollutants and PM for all tests and bags
  - Sec/sec data for THC, CH_4, CO, CO_2, NO_x in all tests
  - Alcohol, carbonyl, and HC speciation for a subset of tests/bags

- Vehicle handling and test procedures were highly specified to better isolate fuel effects from test-to-test variability and other artifacts that can erode statistical power

Fuel Matrix Overview

- Property ranges chosen to allow models to predict emissions for all in-use fuels found in U.S.
- Multiple levels of parameters to capture non-linear relationships between fuel properties and emissions
- Worked with a fuel study design expert to optimize fuel matrix to resolve interactions of interest while minimizing number of fuels (cost)

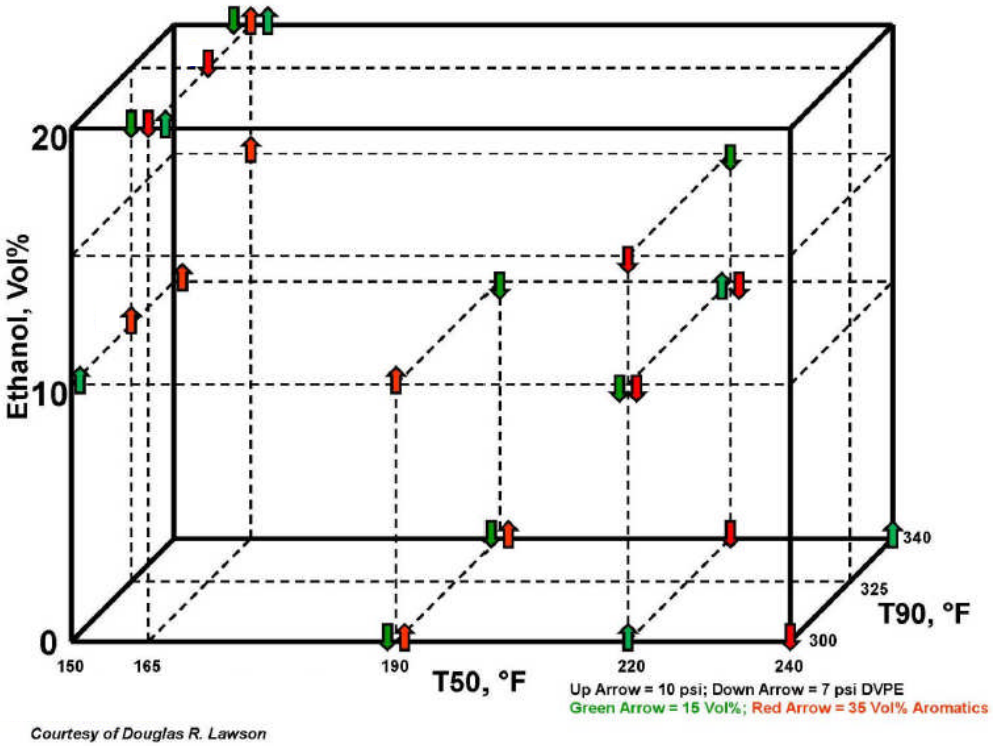
Fuel Parameter	Number of Levels	Target Values to Be Tested
Ethanol (vol%)	4	0, 10, 15, 20
T50 (°F)	5	150, 165 (E20 only), 190, 220, 240
T90 (°F)	3	300, 325, 340
Aromatics (vol%)	2	15, 35
RVP (psi)	2	7, 10

Fuel Matrix Summary

Fuel No.	T_{50}, °F	T_{90}, °F	EtOH, %	DVPE, psi	Aro, %
1	150	300	10	10	15
2	240	340	0	10	15
3	220	300	10	7	15
4	220	340	10	10	15
5	240	300	0	7	35
6	190	340	10	7	15
7	190	300	0	7	15
8	220	300	0	10	15
9	190	340	0	10	35
10	220	340	10	7	35
11	190	300	10	10	35
12	150	340	10	10	35
13	220	340	0	7	35
14	190	340	0	7	15
15	190	300	0	10	35
16	220	300	10	7	35
20	165	300	20	7	15
21	165	300	20	7	35
22	165	300	20	10	15
23	165	340	20	7	15
24	165	340	20	10	15
25	165	340	20	10	35
26	165	340	15	10	35
27	220	340	15	7	15
28	220	300	15	7	35
30	150	325	10	10	35
31	165	325	20	7	35

ETOH
ARO
T50
T90
RVP

$T50^2$
$ETOH^2$
ETOH*ARO
ETOH*T50
ETOH*T90
ETOH*RVP



Courtesy of Douglas R. Lawson

Aromatics Types in EPAct Fuels

- Market survey data were used to define aromatic carbon number ratios designed into EPAct fuels

		C7/C8/C9/C10 Aromatics Splits, %v	
		15% Aromatics Fuel	35% Aromatics Fuel
T90, °F	340	4/4/4/2	10/10/10/5
	300	4/4/4/2	13/13/7/2 or 14/14/5/2

Sizing of Test Vehicle Fleet

- Performed statistical power analysis consistent with approach used in Auto/Oil, based on
  - Estimates of test-to-test repeatability and vehicle-by-fuel variability taken from recent CRC, ARB, and EPA datasets
  - Smallest difference in emissions that should be detectable as significant being 25% as in Auto/Oil design (α = 90%)

- Results suggested a fleet size of 19 vehicles (Phase 1-2) with two test replicates for each fuel-vehicle combination
  - After iteration considering budget, speciation needs, etc., arrived at 15 vehicles for Phase 3 (later analyses showed power still >0.7)

Choice of Makes/Models for Test Fleet

- Based on MY and engine family sales data
  - Used data available for MY 04 – 06 Tier 2 sales
  - Usually multiple models to choose amongst for each engine family
  - High volume sellers are, by definition, representative, and should ease recruitment
- Most vehicles were Tier 2 Bin 5, some Bin 4 or 8
- All vehicles were new, leased vehicles
  - Dyno accumulation of ~4000 miles and oil conditioning of ~1000 miles prior to start of testing

Test Fleet Summary

Make	Brand	Model	Engine Size	Tier 2 Bin	LEVII Std	Odometer
GM	Chevrolet	Cobalt	2.2L I4	5	NA	4,841
GM	Chevrolet	Impala FFV	3.5L V6	5	L2	5,048
GM	Saturn	Outlook	3.6L V6	5	L2	5,212
GM	Chevrolet	Silverado FFV	5.3L V8	5	NA	5,347
Toyota	Toyota	Corolla	1.8L I4	5	U2	5,019
Toyota	Toyota	Camry	2.4L I4	5	U2	4,974
Toyota	Toyota	Sienna	3.5L V6	5	U2	4,997
Ford	Ford	Focus	2.0L I4	4	U2	5,150
Ford	Ford	Explorer	4.0L V6	4	NA	6,799
Ford	Ford	F150 FFV	5.4L V8	8	NA	5,523
Chrysler	Dodge	Caliber	2.4L I4	5	NA	4,959
Chrysler	Dodge	Caravan FFV*	3.3L V6	8	NA	5,282
Chrysler	Jeep	Liberty	3.7L V6	5	NA	4,785
Honda	Honda	Civic	1.8L I4	5	U2	4,765
Honda	Honda	Odyssey	3.5L V6	5	U2	4,850
Nissan	Nissan	Altima	2.5L I4	5	L2	5,211

*Caravan FFV was used only for E85 testing

Data Collection

LD Exhaust Emissions Data Collected

- Bag-level and composite emissions of THC, CH_4, NMHC, NMOG, CO, CO_2, NOx, NO_2 and PM
- Continuous and bag-integrated emissions of raw exhaust THC, CH_4, NMHC, CO, CO_2, NOx

- Alcohol, carbonyl, and hydrocarbon speciation was performed in >200 tests (including E85 tests)
  - Rigorous LOQ and QA procedures were applied to minimize effects of media and handling contamination, etc.
- Speciation dataset represents major upgrade in MOVES capabilities
  - Updated toxic:VOC ratios for Tier 2 vehicles
  - Besides ratios, now have fuel effects for several species of interest

Details of Speciation Schedule

Vehicle	Speciation Type	Replicate 1		Replicate 2+	
		Bag 1	Bags 2-3	Bag 1	Bags 2-3
CIMP, CSIL, F150, HCIV, TCOR	Alcohols, Carbonyls	All fuels	Subset	All fuels	-
	Hydrocarbons	Subset	Subset	-	-
All others	Alcohols, Carbonyls	All fuels	-	All fuels	-
	Hydrocarbons	Subset	-	-	-

Fuel Subset	Ethanol vol%	T50 °F	T90 °F	DVPE psi	Aromatics vol%
3	10.4	218	296	6.9	15.0
4	9.9	222	338	10.0	15.5
6	10.6	189	340	7.2	15.0
7	<0.10	193	298	7.2	17.0
10	9.8	217	340	7.1	34.0
13	<0.10	223	338	6.9	34.1
14	<0.10	193	339	7.1	16.9
21	20.1	168	305	7.1	35.5
23	20.3	163	338	6.8	15.9
27	14.9	222	340	7.0	14.9
28	15.0	217	299	6.9	34.5
31	20.1	167	325	7.0	35.5

Data Quality

- EPA, CARB, and industry best practices incorporated into program design
- Site visits
  - Detailed inspection of contractor's test facility performed by EPA personnel to identify any shortcomings prior to program launch
  - Periodic visits by EPA personnel to observe execution of test program details such as vehicle storage and refueling conditions, handling of exhaust speciation samples, etc.
- Data evaluation and processing
  - Data was delivered continuously to allow sponsors to perform quality control checks and identify any concerns quickly
  - Third replicate criteria implemented such that a wide spread in THC, NO_x or CO_2 would trigger a third replicate

Data Quality

- To better isolate fuel effects from test-to-test variability and other artifacts that can erode statistical power, vehicle handling and test procedures were highly specified
  - Fuel change preps required specific drive and idle behaviors to ensure fuel trim learning could occur (important for ethanol fuels)
  - Sulfur clean-outs were performed at each fuel change minimize drift in catalyst efficiency
  - Same driver performed all emission tests
  - Fuel change carryover was verified for each vehicle
  - Captured OBD and sampling system QA parameters with every test for review later if necessary (e.g., during outlier analysis)
  - Performed mid- and end-point replicate sets for all vehicles to screen for vehicle or site drift issues
  - Randomized order in which fuel/vehicle combinations were tested

Resulting Datasets & Reports

- 15 vehicles x 27 test fuels x 2+ replicates = 956 valid tests
- Databases
  - Available as individual test files (Excel) containing gaseous and PM by bag, plus modal and speciation data (~3 GB via DVD-ROM)
  - Single-file summary database (Excel) is also available for gaseous and PM by bag, as well as chemical speciation and fuel data (Tier 3 docket, OTAQ website)
- Reports
  - "Testing report" joint product between EPA, DOE/NREL, and CRC describing the program design and testing (Tier 3 docket, OTAQ website)
  - "Analysis report" presenting EPA's analysis of the dataset, including fuel effect models (Tier 3 docket, OTAQ website)
  - Peer review documents (Tier 3 docket, EPA science inventory website)

Analysis & Results

The Design

- GOAL: estimate fuel effects (free of confounding by vehicle variability)
  - Experimental Design
    - "Randomized Block"
      - "Block" = vehicles
      - "treatment" = fuels
- GOAL: minimize uncertainty (within budget)
  - Optimal design (generated by computer algorithm)
    - neutralizes correlations among properties, WHILE
    - maximizing precision of model terms
    - For a given "size" (n_{fuel}=27), AND
    - For a given set of fuel effects

Design Model: “Full Design”

- The “Full design” contained 27 fuels, measured on 15 vehicles
- The fuel set was optimized to estimate the following effects:
  - **Five** fuel properties (linear terms)
    - Ethanol (vol.%)
    - Aromatics (vol.%)
    - Reid Vapor Pressure (RVP, psi)
    - T50 (°F)
    - T90 (°F)
  - **Two** squared terms
    - etOH×etOH
    - T50×T50
  - **Four** interaction terms
    - etOH×Arom
    - etOH×RVP
    - etOH×T50
    - etOH×T90
- Applied to all species
  - THC, CO, NOx, PM, CH4, NMOG, NMHC
  - Selected Toxics in Bag 1 (Aldehydes, acrolein, ethanol)

Model Fitting started with this Set of 11 terms:
Include all at outset;
Not all necessarily kept

Design Model: “Reduced Design”

- The “Reduced” contained 11 fuels, measured on 5 vehicles
  - Reflecting speciation schedule
- The fuel set able to estimate the following effects:
  - **Four** fuel properties (linear terms)
    - Ethanol (vol.%)
    - Aromatics (vol.%)
    - T50 (°F)
    - T90 (°F)
- Applied to all species
  - Toxics in Bag 2

Approaches: Emissions

- Used natural logarithm of emissions (Y)
  - Rationale: Statistics
    - Normalized distributions
    - Stabilizes variances
  - Rationale: Interpretation
    - We are interested in relative differences
    - Differences in logarithms represent ratios

Approaches: “Standardization”

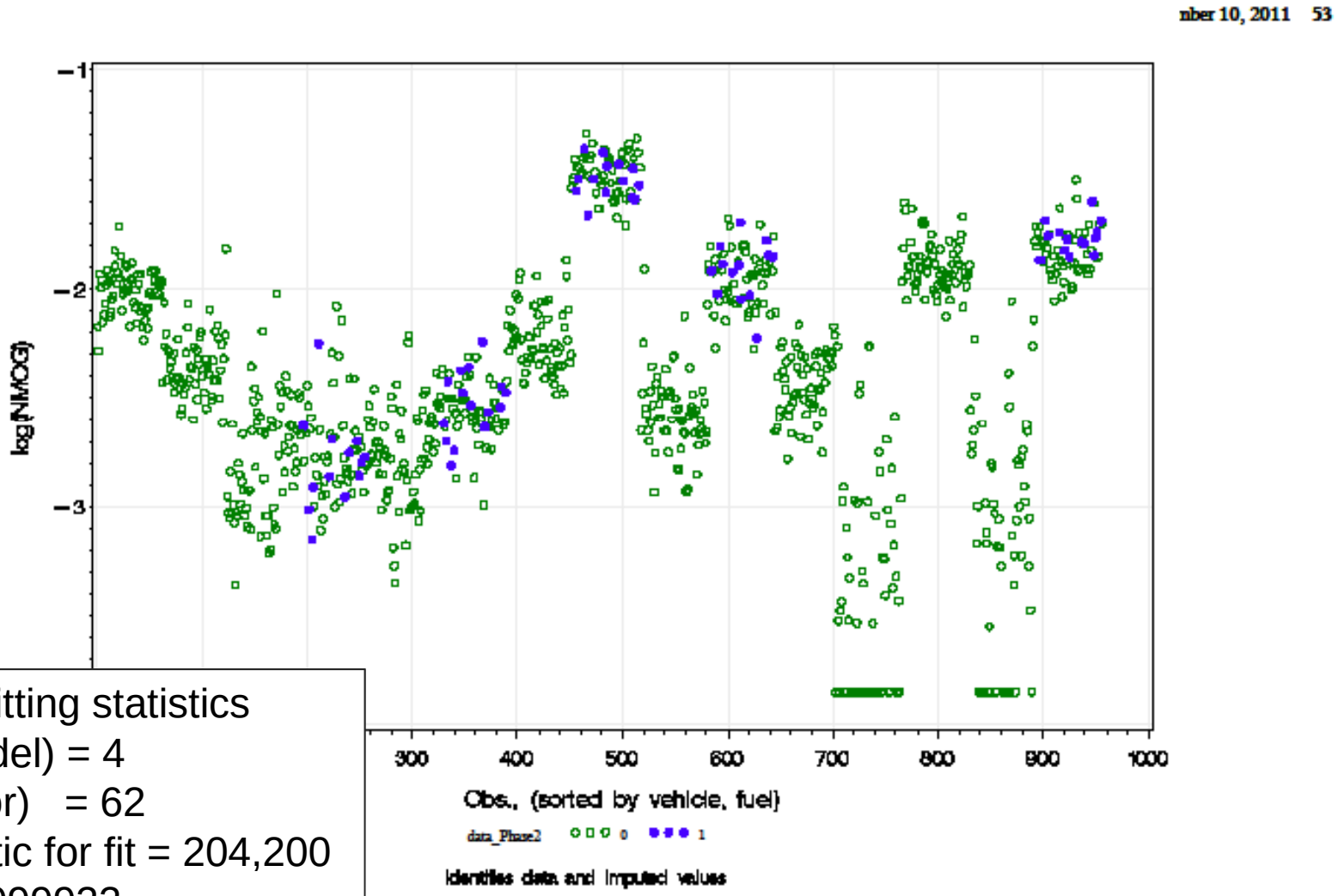
- “Standardized” fuel properties (*X*)
  - Subtracted mean from each measurement
  - Divided by standard deviation
  - Puts all five properties in “same space”

$$Z_{\text{etOH}} = \frac{x_{\text{etOH}} - \bar{x}_{\text{etOH}}}{s_{\text{etOH}}}$$

Approaches: “Imputation”

- “Imputed” NMOG, NMHC
  - These species calculated (not directly measured)
    - Using speciated HC results
    - Only available for subset of vehicles, fuels
      - For Bags 2, 3
  - But (very) strongly correlated to “NMHC by FID” ($NMHC_{FID}$)
    - Measured for all vehicles, fuels
- So, regressed on NMHC
  - response variables (Y) = NMOG, NMHC
  - Predictors (X) = NMHCFID, ethanol level (as class variable)
  - “Imputed” 2/3 of measurements in Bags 2, 3

Bag 2: log(NMOG), Data + Imputed

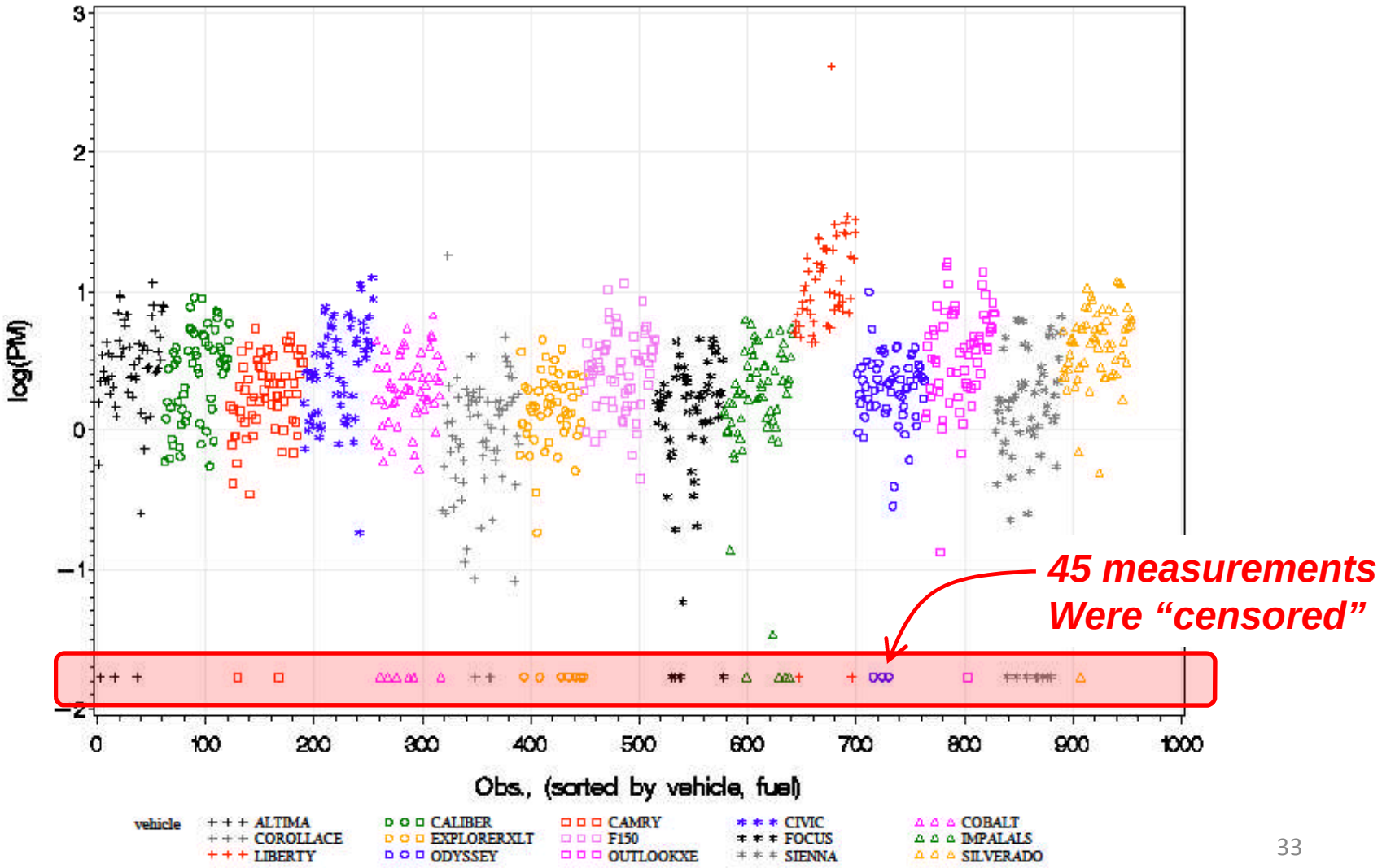


Model fitting statistics
d.f.(model) = 4
d.f.(error) = 62
F statistic for fit = 204,200
R^2 = 0.999922

Approaches: “Censoring”

- Measurements “censored” if
  - No value present, because
  - Measurement not quantified by technique used
    - Below “limit of quantitation”
    - Effectively below background levels
  - Assumption: small but positive measurement was present, but not quantified.
- Approach
  - “minimal” (≤ 5 measurements) substitute minimum value
  - “severe” (> 5 measurements) , use “Tobit regression”
    - Compensates model estimation for absence of measurements “that should be there”

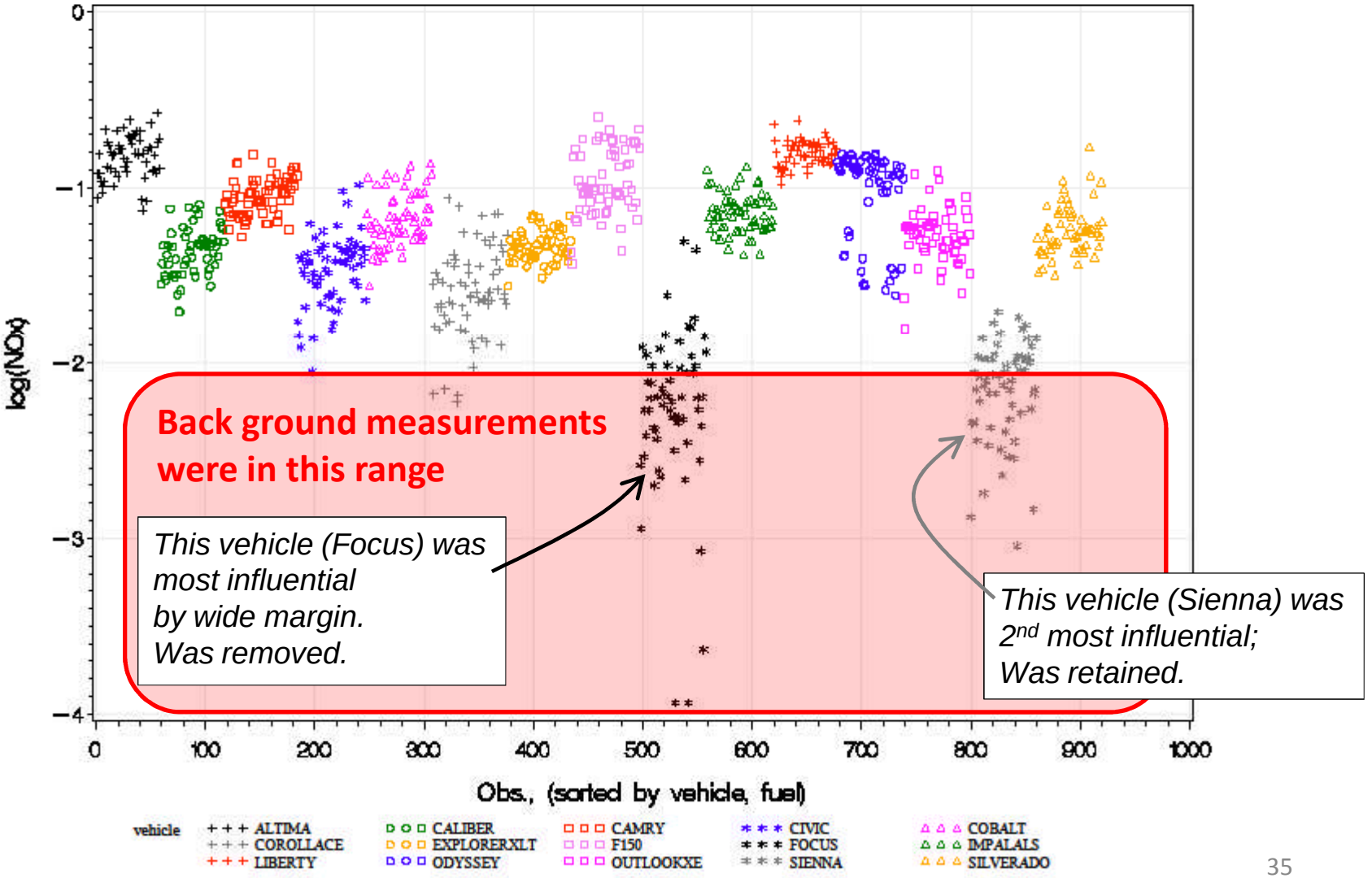
Example of “censoring”: log(Particulate Matter) (Bag 1)



Rounds of Modeling

- Round 1
  - Identify influential observations
  - Result: several obs. removed (all for PM)
- Round 2
  - Identify influential vehicles
  - Result: several vehicles removed
    - For NOx, NMOG
- Round 3
  - Fit final models ("Playing for keeps")

Bag 1: log(NOx) by Vehicle, Fuel



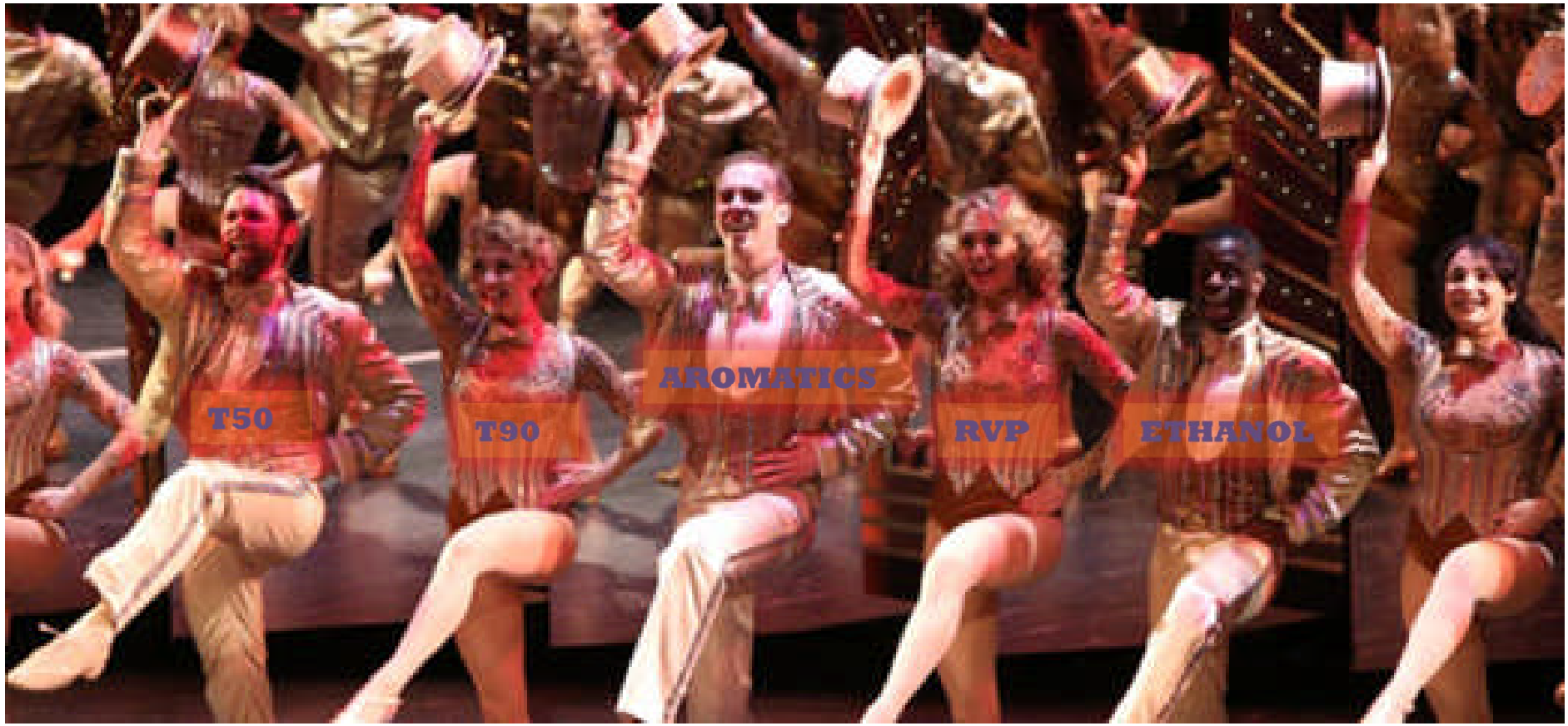
Summary

- Outcome:
  - effects do exist
  - are measurable
    - **Even for hot-running emissions**!
- CAUTION !
  - Coefficients represent fuel effect as though all other factors could be held constant
    - Doesn't work this way for real fuels!
    - But *very, very useful*
- **Bottom Line**
  - **Coefficients cannot be taken individually**
  - **Must be taken as a full set**

… You may be tempted to take one of the coefficients and run with it …

… but DON'T…

… Because all the coefficients need to work together as a team …



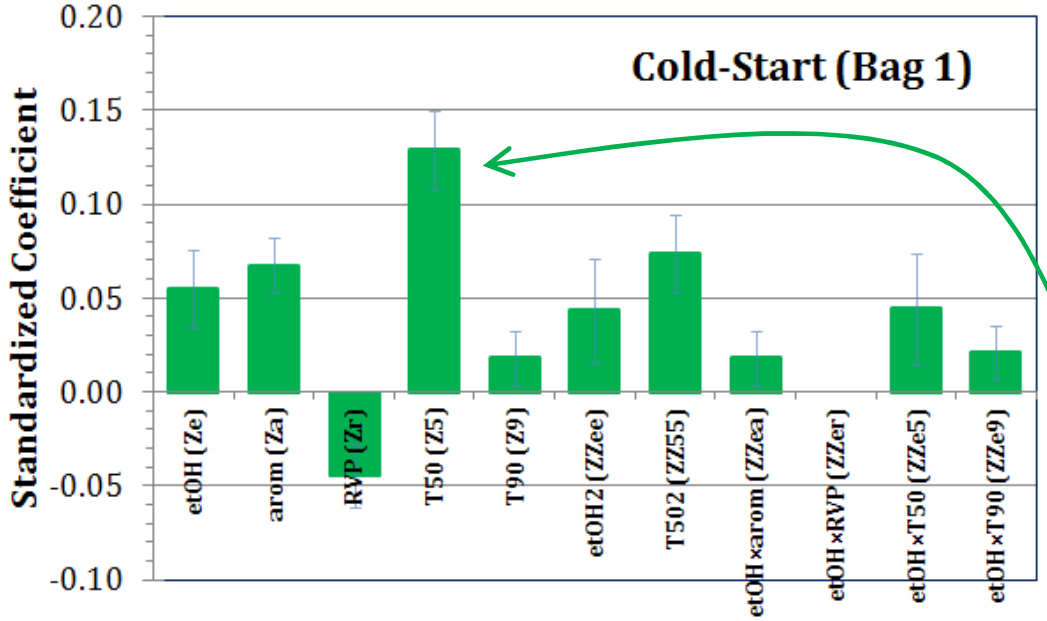
… and all the members of the cast have to dance together …

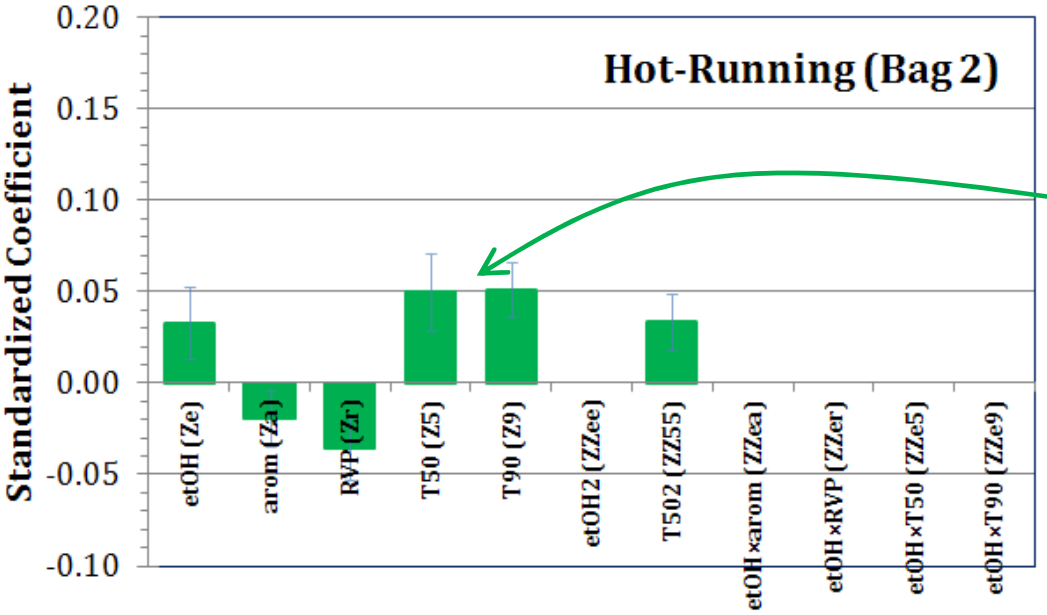
Sets of Model Coefficients

RESULTS

What we're looking at

- Sets of "Standardized" coefficients
  - With 90% confidence intervals
- What do they mean?
  - $\Delta \ln(\text{Emission})/\sigma$ change in fuel property
- CON: abstract, arcane
- PRO: can compare coefficients
  - For different properties
  - Between start and running, etc.
- Positive coefficient
  - Emission increases if property increases
  - Emission decreases if property decreases
- Negative coefficient
  - Emission decreases if property increases
  - Emissions increases if property decreases



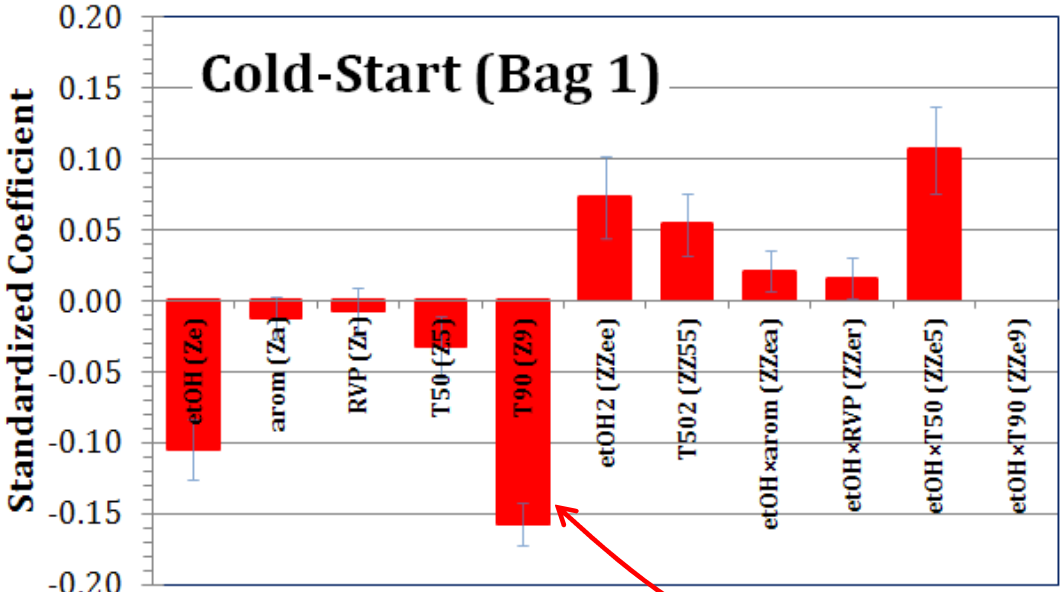


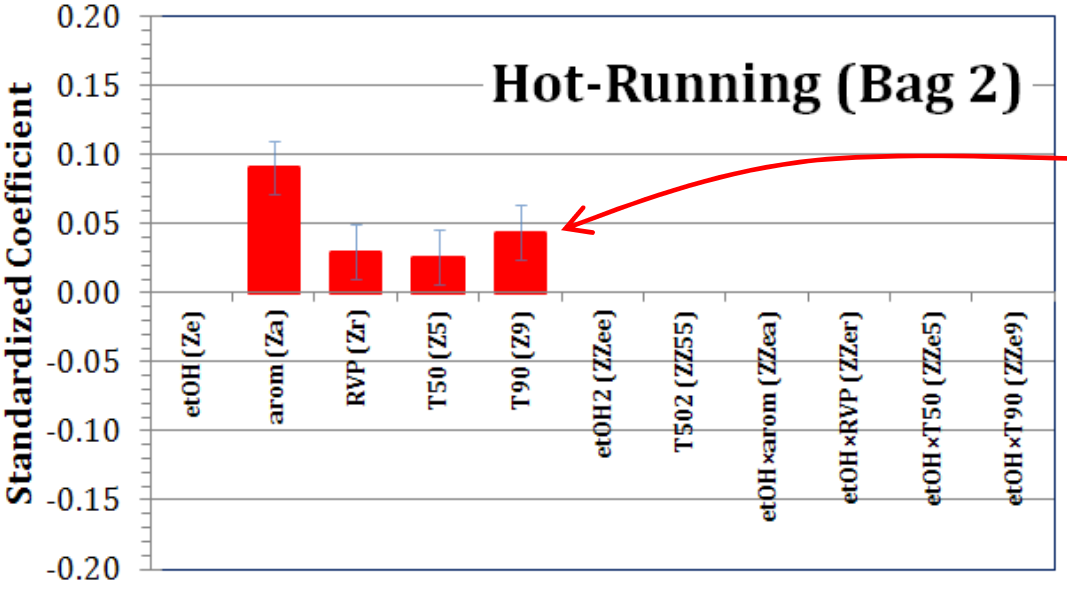
Model-o-gram

THC

Distillation parameters are the primary driver:
Heavier fuels have higher (unburned) HC during starts (T50),

and also during running (T50, T90)





Model-o-grams

CO

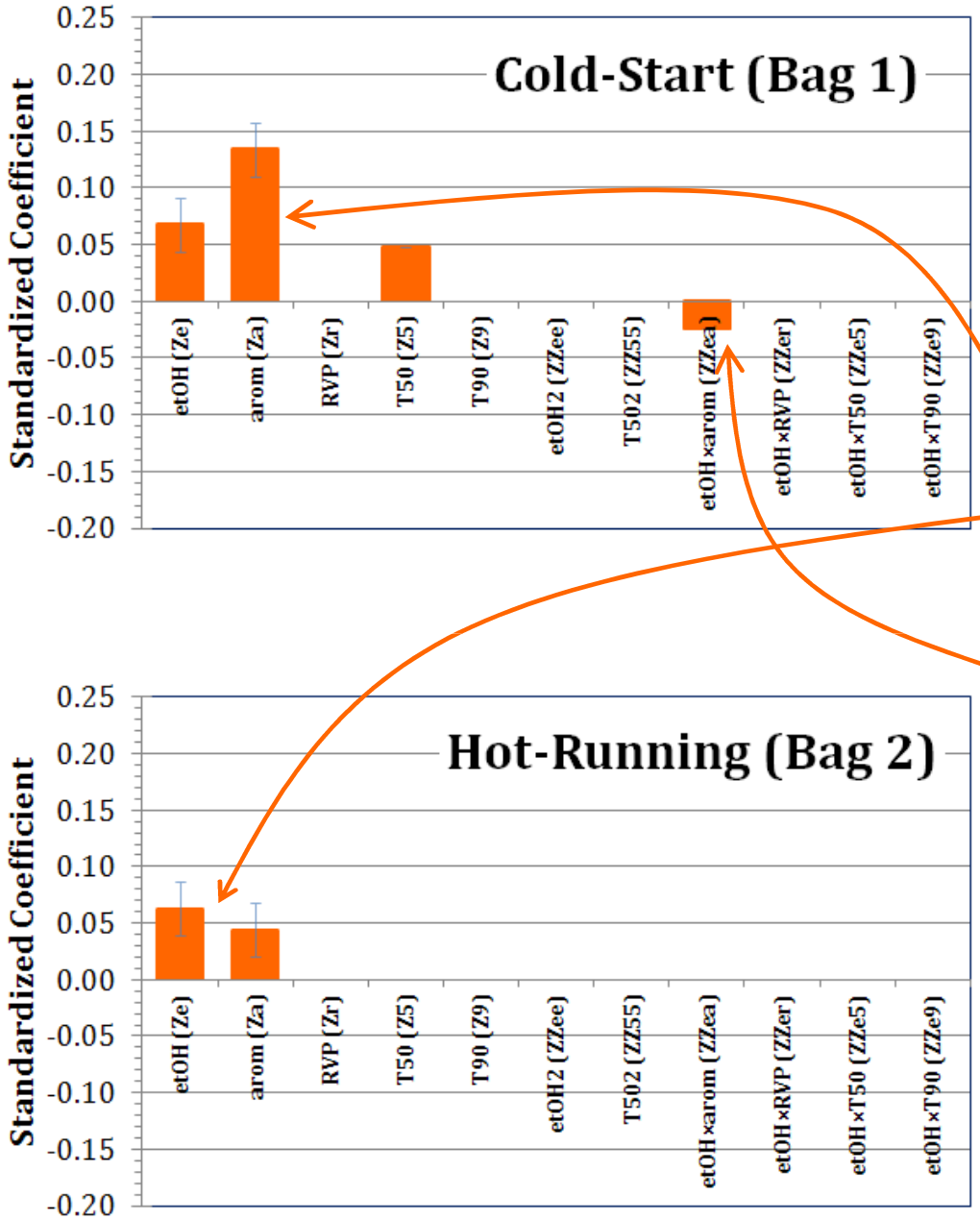
Patterns for start and running differ;

heavier fuels produce less CO during starts

but more CO during running (?)

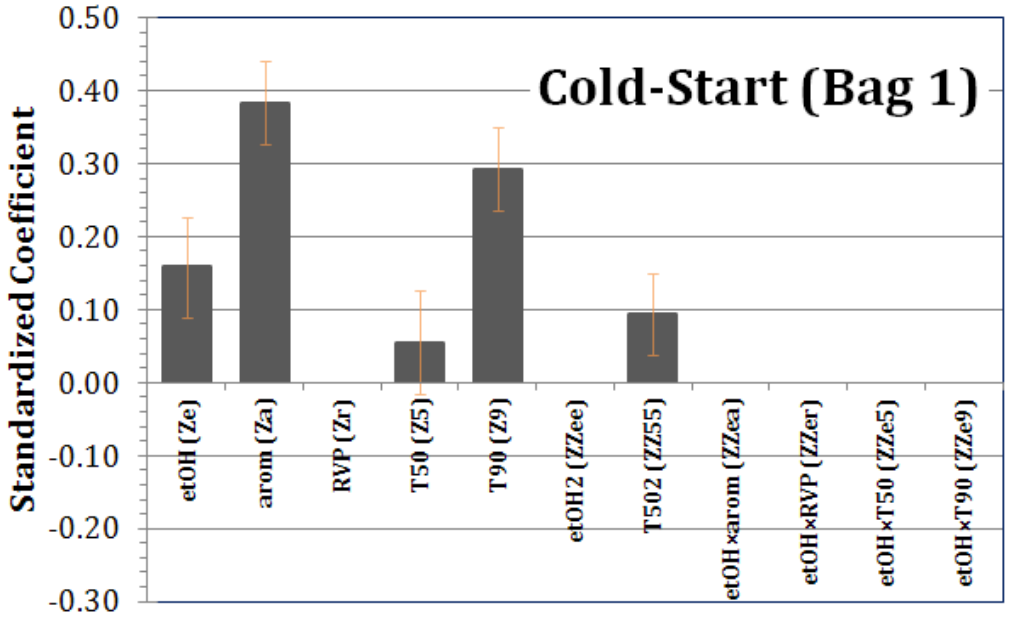
Model-o-grams

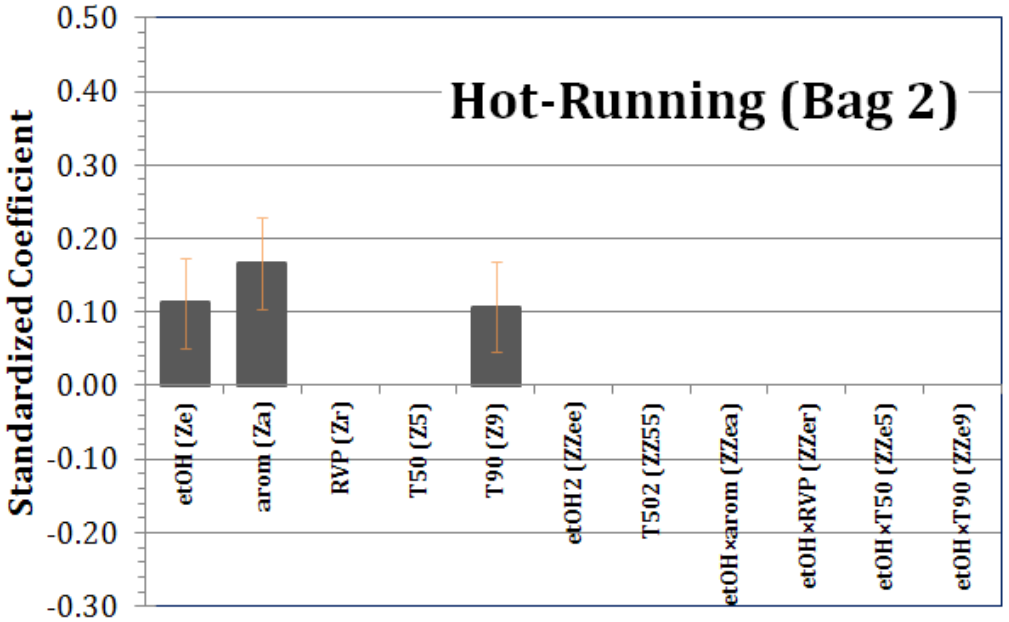
NO_x



Ethanol and aromatics are the primary drivers,

although they interfere with each other (slightly) during starts





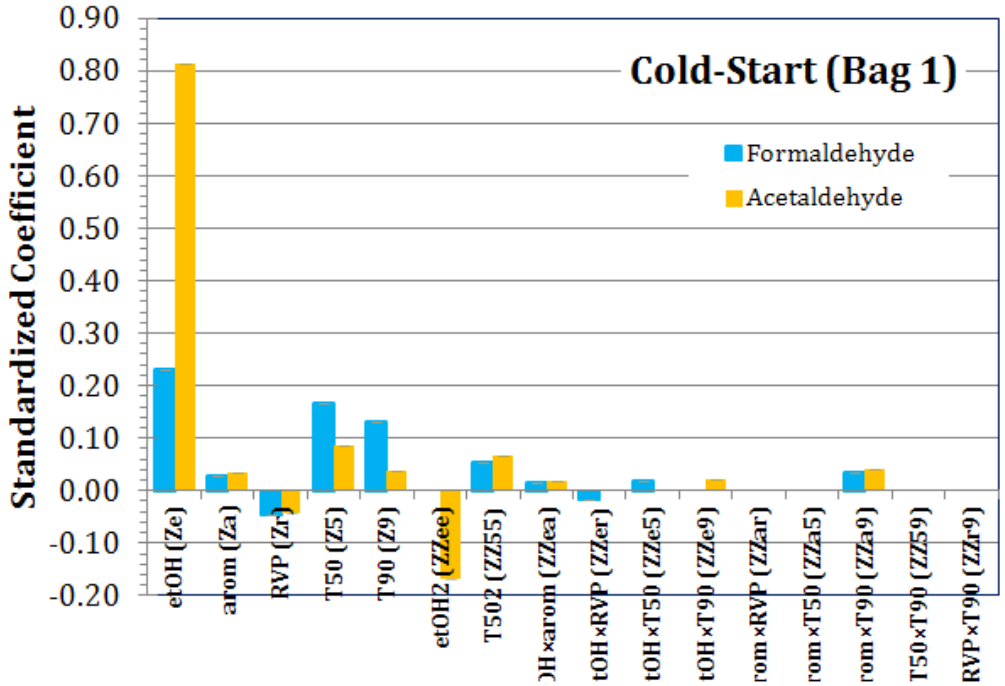
Model-o-grams

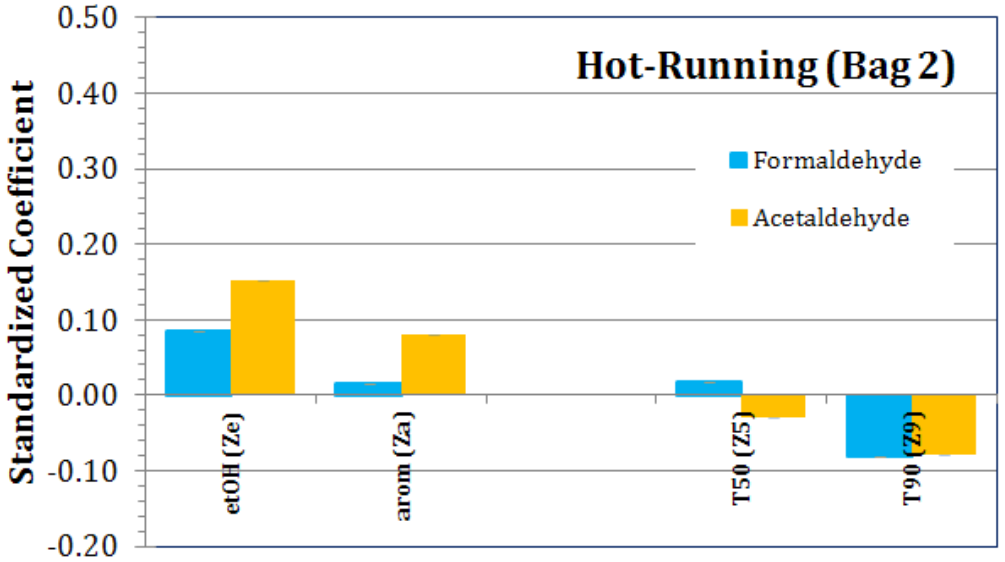
PM

Aromatics and T90 are the primary drivers,

For both starts and running

Heavy components in the fuel contribute to PM





Model-o-grams

Aldehydes

Starts: fit with full design

Running: fit with reduced design

Calculation of Fuel Adjustments

APPLICATION TO MOVES

Scope of Application

- Fuels
  - Gasoline (fuelTypeID = 1)
  - Ethanol (fuelTypeID = 5)
    - **Blends from 0 – 20% vol.%**
- Model Year Groups
  - MY 2001 and later
- SourceTypes
  - Applies to all
- Emission Processes
  - Running Exhaust (processID =1) (uses Bag-2 models)
  - Start Exhaust (processID =2) (uses Bag-1 models)
- Database Table:
  - GeneralFuelRatioExpression
    - Expressions up to 32,000 characters

Scope of Application

Pollutants

pollutantID	pollutantName	Acronym
1	**Total Gaseous Hydrocarbons**	THC
2	**Carbon Monoxide**	CO
3	**Oxides of Nitrogen (NOx)**	NOx
111	**Primary PM2.5 – Organic Carbon**	PM (OC)
112	**Primary PM2.5 – Elemental Carbon**	PM (EC)

Fuel Adjustments

using Cold-start NOx (Bag 1) as an example

To start, we modeled the logarithm of NOx for a given fuel,

$$\ln(\mathrm{NO}_x) = \beta_0 + \beta_e Z_e + \beta_a Z_a + \beta_5 Z_5 + \beta_{ea} ZZ_{ea}$$

so we can estimate NOx be reversing the transformation.

$$\mathrm{NO}_x(\mathrm{g/mi}) = \exp(\beta_0 + \beta_e Z_e + \beta_a Z_a + \beta_5 Z_5 + \beta_{ea} ZZ_{ea}) \exp(0.5\sigma^2)$$

A fuel adjustment is a ratio representing a difference in emissions
between an "in-use" fuel and
a MOVES "base" fuel.

$$\mathrm{Adj.} = \frac{\mathrm{NO}_x^{in\text{-}use}}{\mathrm{NO}_x^{base}} = \frac{\exp(\beta_e Z_e^{in-use} + \beta_a Z_a^{in-use} + \beta_5 Z_5^{in-use} + \beta_{ea}^{in-use} ZZ_{ea})}{\exp(\beta_e Z_e^{base} + \beta_a Z_a^{base} + \beta_5 Z_5^{base} + \beta_{ea}^{base} ZZ_{ea})}$$

Calculation of Toxic Fractions

APPLICATION TO MOVES

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  - Applies to all
- Emission Processes
  - Running Exhaust (processID =1) (uses Bag-2 models)
  - Start Exhaust (processID =2) (uses Bag-1 models)
- Database Table:
  - GeneralFuelRatioExpression
    - Expressions up to 32,000 characters

$$fraction = \frac{\text{toxic}}{\text{VOC}}$$

Scope of Application

Pollutants

pollutantID	pollutantName	Start	Running
26	Acetaldehyde	complex	complex
25	Formaldehyde	complex	complex
27	Acrolein	complex	simple
21	Ethanol	complex	complex
20	Benzene	complex	simple
24	1,3-Butadiene	complex	No emissions

Fractions calculated using model; change with fuel properties

Fractions uniform; do not change with fuel properties

Toxic Fractions

using Hot-Running Acetaldehyde (Bag 2) as an example

To start, we model the Acetaldehyde, NMOG and Ethane for a given fuel,

$$\text{Acet. (g/mi)} = \exp\left(\beta_0 + \beta_e Z_e + \beta_a Z_a + \beta_5 Z_5 + \beta_9 Z_9\right)\exp\left(0.5\sigma^2\right)$$

$$\text{NMOG (g/mi)} = \exp\left(\gamma_0 + \gamma_e Z_e + \gamma_a Z_a + \gamma_5 Z_5 + \gamma_9 Z_9\right)\exp\left(0.5\sigma^2\right)$$

$$\text{Ethane (g/mi)} = \exp\left(\varphi_0 + \varphi_e Z_e + \varphi_a Z_a + \varphi_5 Z_5 + \varphi_9 Z_9\right)\exp\left(0.5\sigma^2\right)$$

A toxic fraction represents the toxic emission as a fraction of total VOC, for a single fuel.

$$\text{Fraction} = \frac{\text{Acetaldehyde}}{\text{VOC}} = \frac{\text{Acetaldehyde}}{\text{NMOG - Ethane}}$$

Post-Hoc Adjustments

- Address limitations in EPAct design
  - Benzene:
    - Design includes aromatics as class,
      - not benzene in particular
    - But how account for benzene in exhaust
      - Without accounting for benzene in fuel?
    - Developed post-hoc adjustment
      - Applied to EPAct results
      - Same for start, running
  - 1,3-Butadiene
    - Design did not include olefins
    - But olefins considered important for 1,3-butadiene
    - Developed post-hoc adjustment
      - Applied to EPAct result
      - Start only (no running emissions)

Summary

- EPAct analysis complete
  - Reports now available on OTAQ website at http://www.epa.gov/otaq/models/moves/epact.htm
- Results to be applied in MOVES2013
  - Fuel adjustments
  - Toxic fractions
- Questions?

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