Determining real world emissions effects of ethanol blends through measurement and modeling

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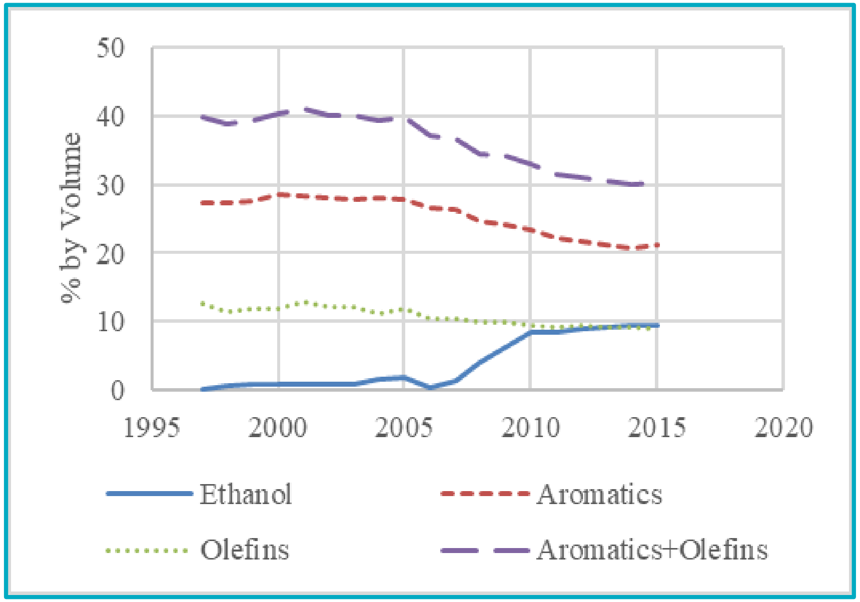
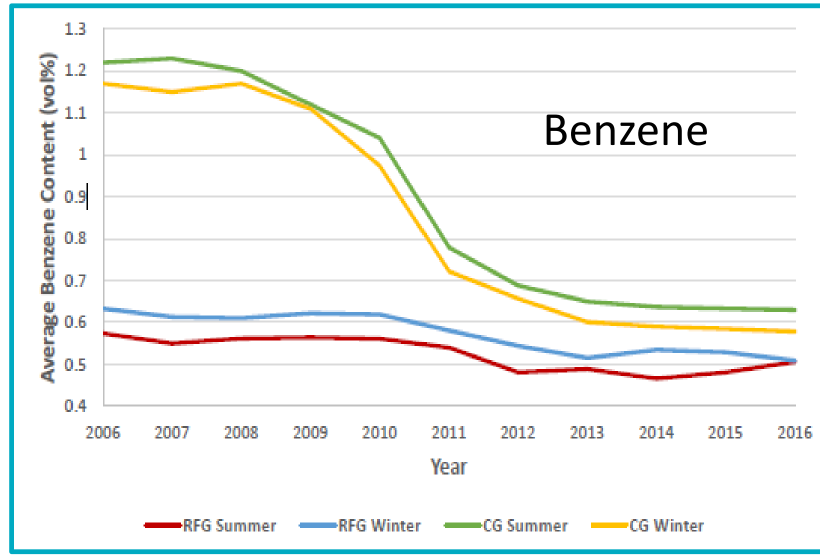
Abstract

US light-duty gasoline vehicles burn certification fuel to meet emissions standards, but studies and models show that the in-use fuel will have an effect on tailpipe emissions, and hence air quality. Advances in GDI technology affect the fuel-engine interaction, and so does the speed and load of the engine. Ethanol, as E10 (10% by volume) is blended into most US gasoline, and E15 is being considered for wider application. Determining the effect of ethanol concentration on tailpipe emissions is challenging, noting that the petroleum content varies widely in both composition and measured properties, and that the mixture behavior reflects nonlinear properties of blending. Typically studies have been constructed to explore the effect of ethanol along with major fuel properties such as aromatic content, but the limitation of variables challenges the extrapolation of resulting models to unseen blends. Employing composite variables such as the Particle Matter Index (PMI), itself a predictor, offers an important pathway, providing that the construct is true to the underlying chemistry and physics. Existing model predictions are compared for a variety of study and real-world fuel properties. New data allow a wider review of results and models, and an assessment of confidence in applying the data to real world fuel effect prediction. There are also more data that confirm the differences between the E0 to E10 step and the E10 to E15 step. It is challenging to choose a suite of study fuels that represent E0 and E10 equitably under constraint of real world production and economics.

Historical Changes in Fuel Composition

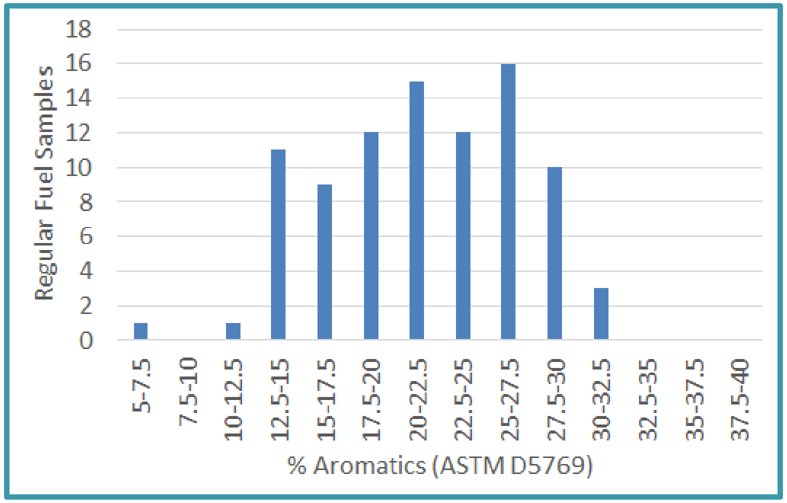


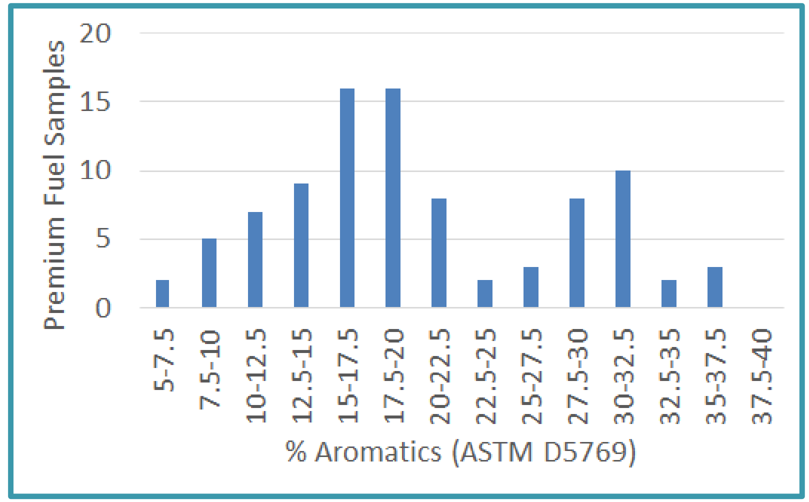
Data from the Fuel Trends Report, EPA-420-R-17-005, show reduction in aromatics with increase of ethanol use.



Not all historical trends are reversible or applicable to current fuel formulations. Benzene & Sulfur limits changed over the period of interest.

Wide Distributions of Composition of Market Fuels



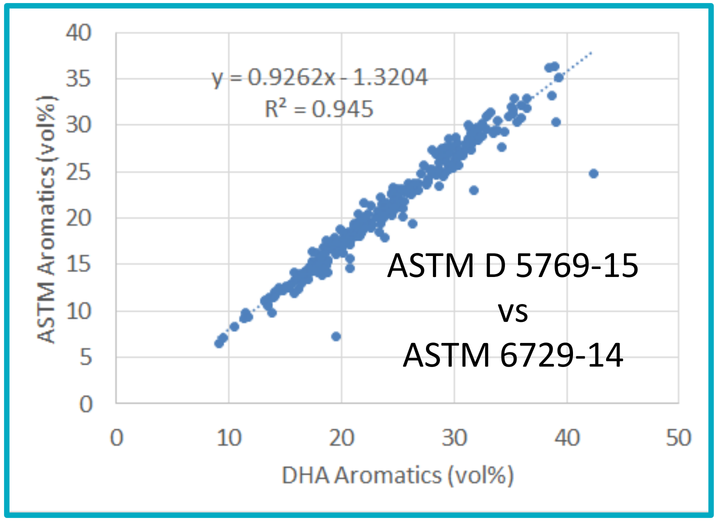


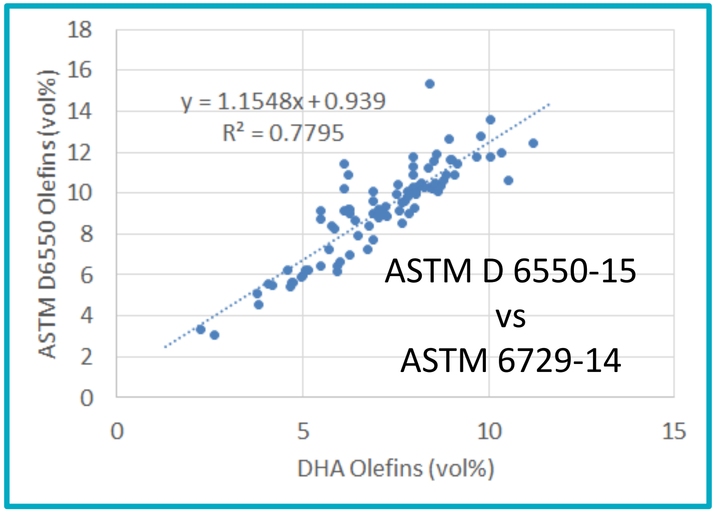
ASTM D5769 aromatic variation across regular and premium summer fuels.
Data from the 2020 ERG field survey of Texas finished E10 gasoline.
Other species also vary widely: e.g. olefins from about 2.5 to 10.1%.

Comparison of “Traditional” and DHA Composition Levels

- Aromatic content is a parameter employed by most emissions models
- Measured aromatic levels vary between laboratories and between test methods
- Uncertainty over composition propagates to uncertainty in model predictions
- A 1% aromatic change produces a 3.9% change for Bag 1 PM in EPAct model

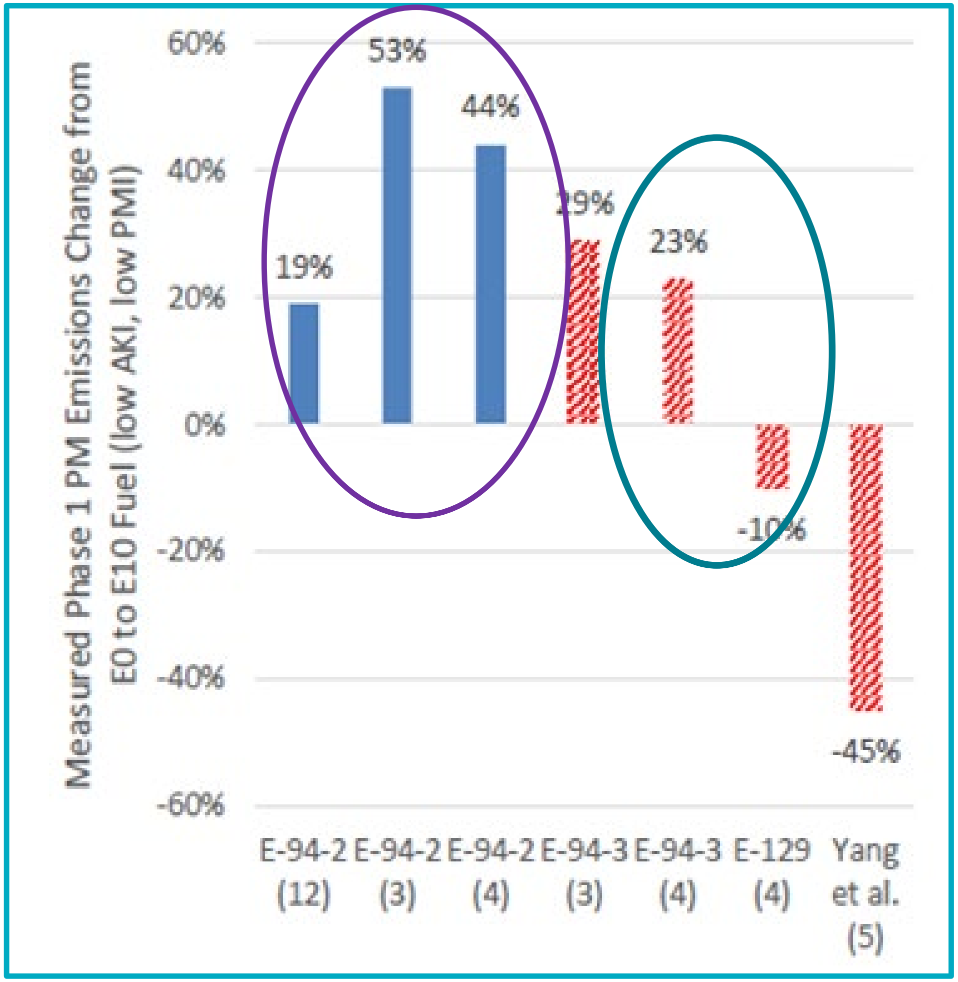
Data in plots from ERG Texas 2020 Summer Fuel Field Study. DHA data are summed across constituent species



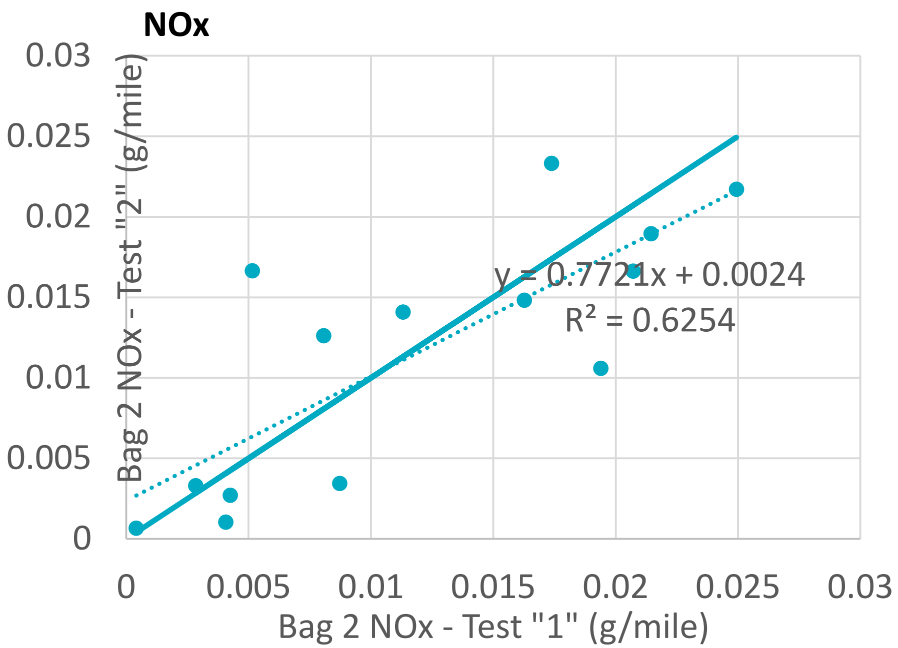


Individual Vehicle Responses Vary

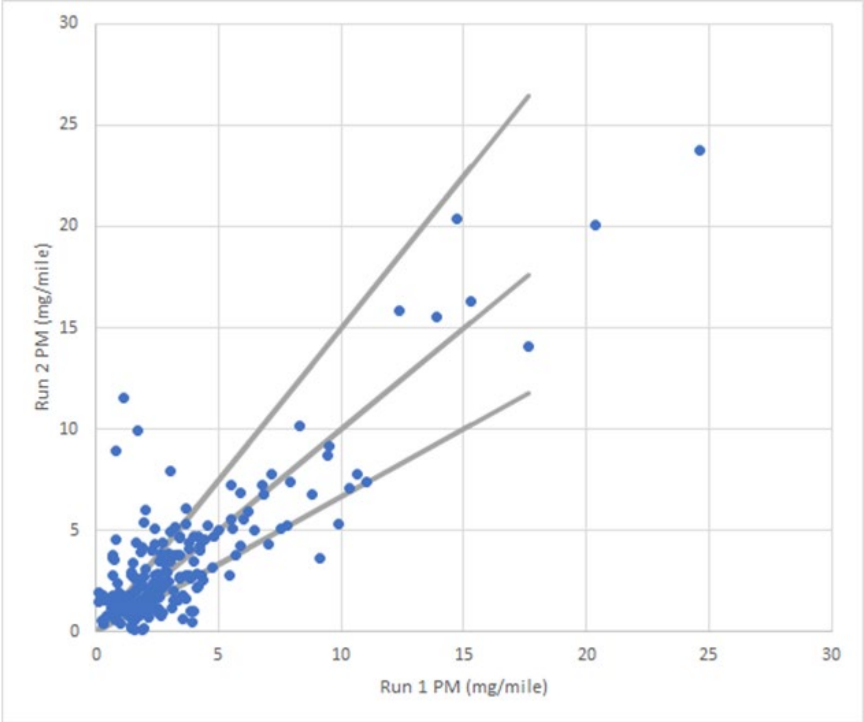
- E-94-2 emissions differences between E0 and E10 differ between 3, 4 and 12 GDI vehicle cohorts. Aromatics and PMI were held fairly constant.
- E-129 and E-94-3 compared: emissions changes between splash blended E0 and E10 differed between two different vehicle cohorts. E-129 used a re-blend of the E-94 fuel.
- Variability between limited runs could appear as vehicle variability.
- Yang et al. (UCR) data were for an E0 30% aromatic versus an E10 20% aromatic.
- All vehicles were GDI.



Low Emissions and Emissions Differences Require a High Count of Replicate Runs



EPAct Fuel 13 on Bag 2 LA92 - NOx



First two runs of LA92 – EPAct - PM

- Repeat test runs valuable, but limited by resources
- Emissions levels low and difficult to measure accurately
- Emissions differences often small or distributed

Market Fuel Variability Is Dictated by Refinery Economics

	RVP psi	Octane (R+M)/2	Aromatics Vol%	T50 °F	Share %
FCC Gasoline	5	85.0	27	225	31
Reformate	4	90.5	50	265	27
Alkylate	5	92.5	0	218	13
Isomerate	14	81.5	0	125	5
Aromatic by-product	1	105.0	95	250	1
Butane	60	92.0	0	100	3
Other	12	77.0	7	138	20

Typical streams – FFS report

EPA Fuel Trends 2006 & 2016
Aromatics 5 to 95%

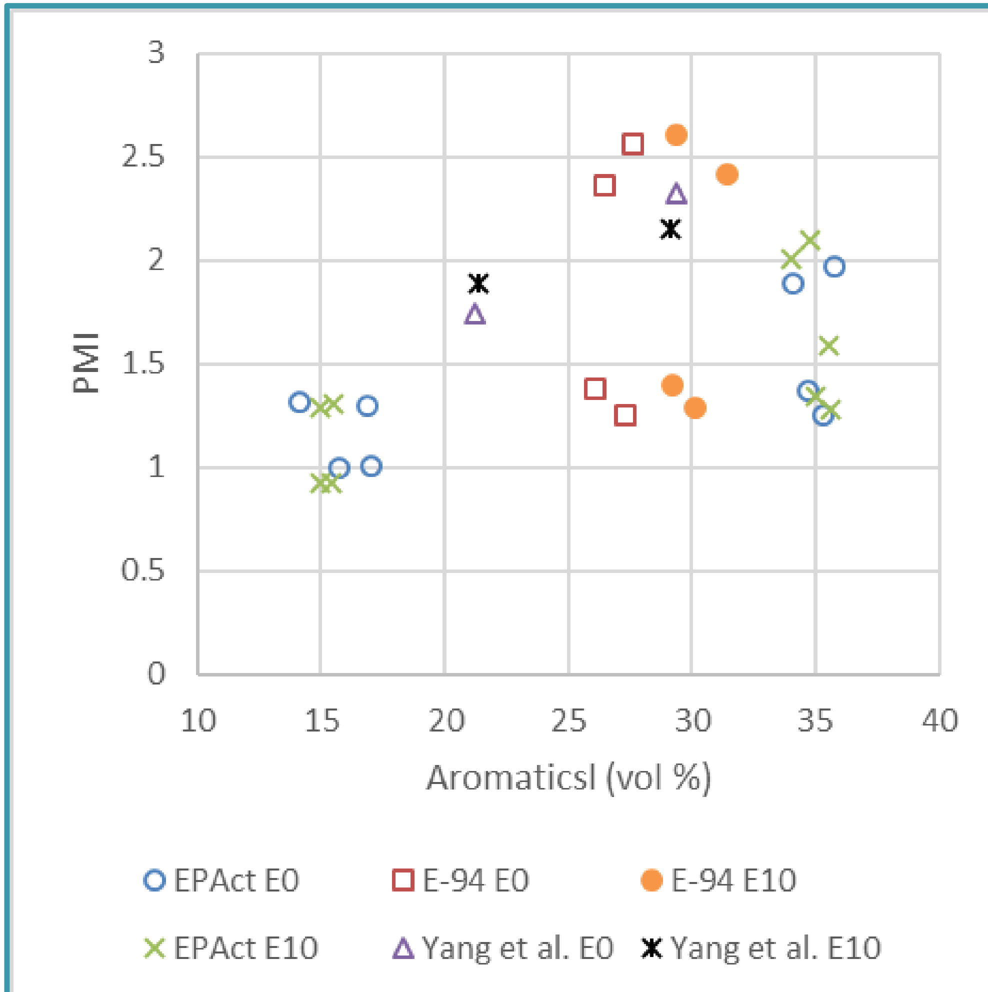
- FCC/reformate >50% of total production
- Reformate octane and percentage volume can be varied
- Aromatic and iso-paraffin content increase octane rating
- Overall refinery economic constraints dictate that octane is seldom “given away”
- Commercial gasoline must meet regulations (RVP, RFG) and ASTM specifications
  - Seasonal, Conventional, RFG, CARB
- Large variations over time and by refinery (EPA Fuel Trends report)

Varied Approaches for Determining Ethanol Influence on Gasoline Engine Emissions

- Current market fuel effects (e.g. fuel pairs)
  - Applicability to real world
  - Requires study fuel composition based on known fuels
- Proposed market effects (e.g. fuel pairs)
  - Requires estimating future fuel compositions
  - Requires study fuel choice based on estimations
- Influence of chosen properties (e.g. parametric studies)
  - Requires model / translation/ detail for real world application
  - Parameters identified as study variables
  - Study fuel choice based on parameters
- Splash blending
  - Simple definition, requires baseline fuels choice only
  - Applicable to real world in some circumstances
    - e.g. some E10 to E15 splash

PM Parameters

- PM mass and number are of of heightened interest for GDI vehicles
- Aromatic content is a parameter traditionally associated with exhaust PM
- Spectrometry now enables enabled quantification of hydrocarbon species in gasoline
- PMI (PM Index) is calculated from the detailed analysis as a PM predictor
- The relationship between PMI and aromatics differs between studies



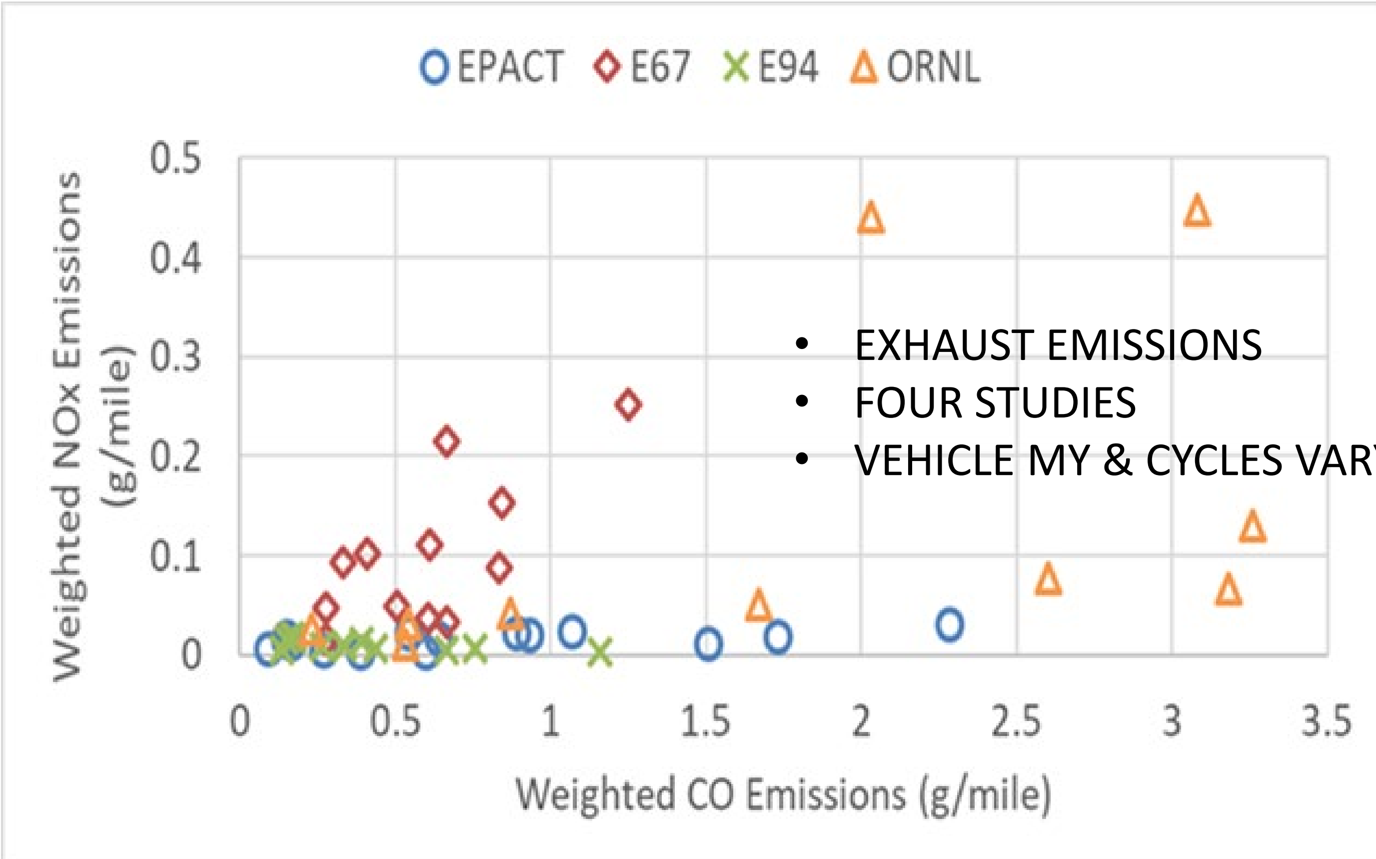
Nonlinearity and Interdependence

- Nonlinear behavior exists between different hydrocarbon groups
- Nonlinear behavior exists with ethanol – petroleum blends
- Ethanol boosts gasoline AKI far more than its own AKI would suggest
- Ethanol boosts AKI more with high olefin / low aromatic BOB
- Vapor versus liquid compositions are affected by ethanol
- Permeation behavior is not proportional, and influenced by other species
- Enthalpy of vaporization of ethanol is affected upon blending

(Foong et al., Kar et al., Chupka et al., Anderson et al., Ghosh et al., Aulich et al., API data)

- Both nonlinear behavior and correlation between variables are difficult to capture quantitatively with a limited data set
- Property changes in the E0 to E10 range usually do not reflect changes above E10.
- PMI and PM production are raised by aromatics, but more so by heavy aromatics
- C10+ aromatics and T90 typically correlate

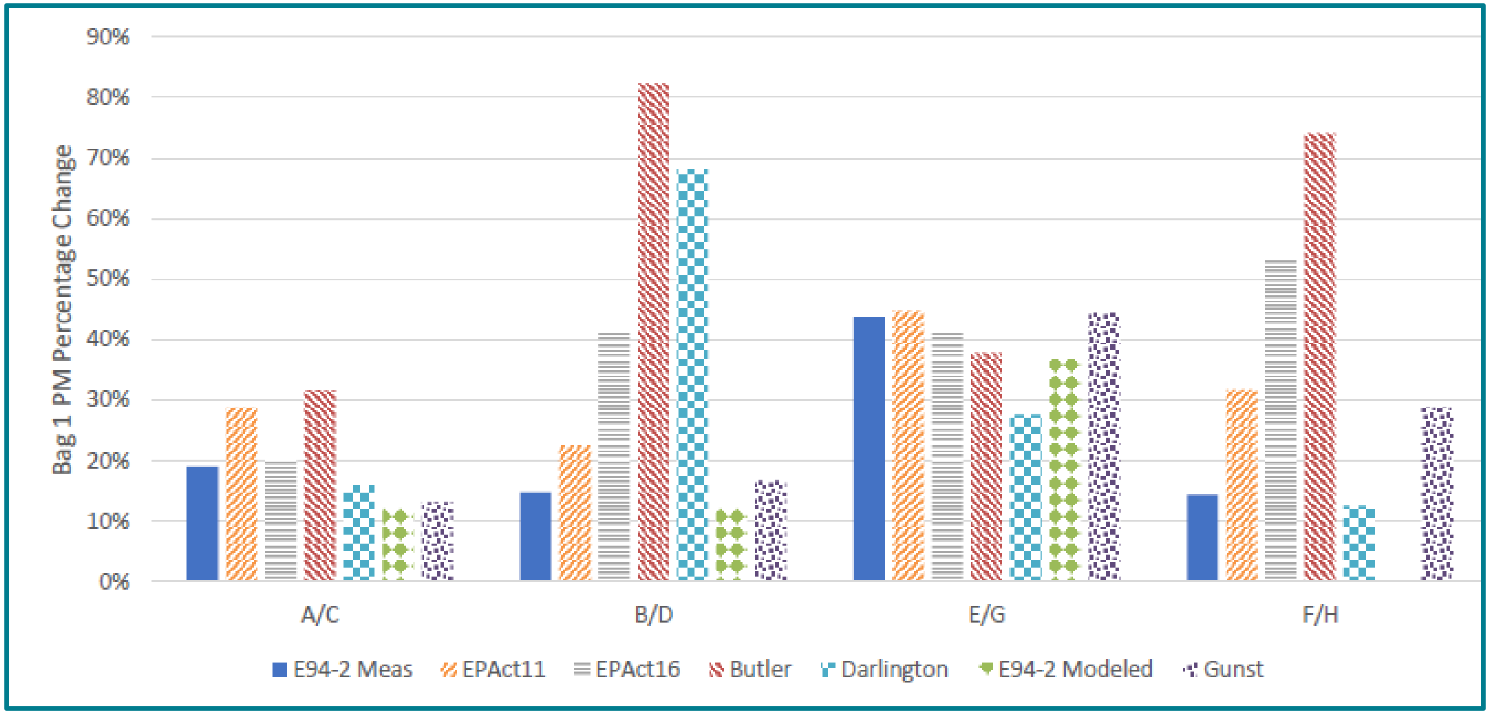
Tightening Standards & Changing Technology



- EXHAUST EMISSIONS
- FOUR STUDIES
- VEHICLE MY & CYCLES VARY

- Fleet turnover with changing engine and road load technology require periodic studies
- Advancing materials / regulations influence evaporative emissions
- Changes in refinery practice and product demand influence emissions inventory

Modeling, Interpolation and Extrapolation



- E-94-2 represents unseen fuel and new vehicle technology relative to EPAct study
- Bag 1 E10/E0 PM ratios for four E-94-2 fuel pairs
- Various EPAct fit models differ predictively for new engines and unseen fuels
- E94-2 targeted PMI as a measure for blending, rather than aromatics

Summary Thoughts

- Too few replicate runs reduce confidence of statistical conclusions
- Nonlinear behavior of blended fuels is difficult to characterize with a small data set or with simple models
- Strong influence of species in the fuel calls for accurate analysis of fuel properties and composition
- Uncertainty in study fuel analysis propagates into the reliability of models
- Models derived from study fuel matrices may not extrapolate well in predicting unseen fuel behavior
- Using market fuels, or likely future fuel compositions, accounts directly for nonlinear effects of inventory

Additional analysis available in:
CLARK, N.N., McKAIN, D.L., KLEIN, T., and HIGGINS, T., "Quantification of Gasoline-Ethanol Blend Emissions Effects," Journal of the Air & Waste Management Association, Vol. 71, 2021, Issue 1, pp. 3-22, https://doi.org/10.1080/10962247.2020.1754964

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