future fuel strategies

A Fuel Blending Guide for Ethanol

Identifying Sound Practices for Acquiring or Blending Fuels for Studies of Emissions Changes

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Objective & background

- ***Purpose of Blending Guide***
  - Develop a uniform approach for future programs
    - Avoid uncertain predictions of real world outcomes
  - Encourage use of anticipated market fuels for studies
    - Focus on a precise question
  - Emphasize tailpipe and evaporative emissions studies
    - Can be applied to other predictive study objectives
  - Emphasize gasoline-ethanol blends
    - Can be applied to other fuel formulations
- ***Guide draws on prior findings***
  - SAE Paper 2019-01-0997
  - JAWMA Paper (doi: 10.1080/10962247.2020.1754964)
  - Future Fuel Strategies Report

Essential understanding

- Ethanol varies as percent volume, but is a single component
- The gasoline (BOB) chemical composition varies
  - BOB = “Blendstock for oxygenate blending”
- The ethanol-BOB blend at the terminal must satisfy constraints
  - Anti-knock index, Reid Vapor Pressure, Distillation temperature
- Petroleum components and ethanol blend in a nonlinear fashion
  - Blend properties depend on the precise components
- Refinery economics and constraints influence the BOB composition strongly

Refinery constraints

- Light Straight Run Naphtha (LSR)
  - high volatility, low octane
- Reformate
  - Low volatility, high octane / aromatics
- Alkylate
  - Moderate volatility, isoparaffins
  - Regular <octane < premium
- Isomerate
  - High volatility, moderate octane
- FCC
  - Olefins feed alkylation unit

Blended BOB composition must reflect product stream availability, balance and value

Parameter	Units	2006	2016
Ethanol	Vol%	2.91	9.57
Sulfur	PPM	49.2	23.1
Benzene	Vol%	1.04	0.58
Aromatics	Vol%	24.5	19.3
Olefins	Vol%	1.1	8.6
E200	Vol%	49.1	54.4
E300	Vol%	83.7	85.9
T40*	°F	177	155
T50*	°F	202	181

*Estimated, not reported by EPA

Finished Gasoline Historical change, EPA Fuel Trends report
Note aromatic reduction in response to ethanol blending:
Aro %change = 0.78*(EtOH %change)

Principles to guide fuel selection

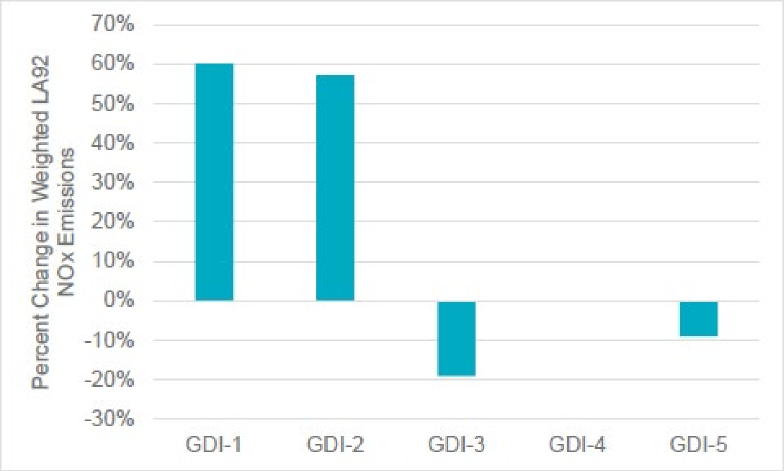
- Targeted studies seek to predict influence of fuel composition on inventory
  - Emissions from late model year vehicles are very low and difficult to measure
  - Differences in emissions between two fuels are typically small
- For predictive accuracy, fuels expected in the market should be used
  - Exploring a broader matrix of fuel composition change yields broader information, but less specificity
  - Interpolation in a broad matrix of fuel composition may not explore nonlinear effects accurately

Composition versus properties

- **Guide: “Fuels expected in the market should be used”**
  - Use only fuels with the ethanol levels of interest
  - Use BOB compositions that are expected in the market at those ethanol levels
  - Market fuels reflect both refinery stream composition and profitable blending of those streams
- **Guide: “Fuel composition is preferred for defining fuels”**
  - Properties ultimately depend on chemical composition
  - Several different compositions may yield the same set of properties
  - Some properties (RVP, Octane) are market constraints
- **Multivariate studies differ from Guide**
  - Several prior studies measured effects of multiple properties on emissions
  - Formulations blended to match chosen properties may not represent market fuels in chemical composition
  - “Aromatics” and “Paraffins” are each highly variable in behavior

Additional guide recommendations

- ***Recognize influence of vehicle technology***
  - Vehicles in a cohort react differently to the same fuel change
  - More thorough classification than PFI or GDI is desirable
  - Understanding engine control strategy helps to interpret data
- ***Cover real-world driving for real-world effects***
  - Low-power and high-power engine operation differs
  - At least employ one low power cycle (e.g. FTP) graphs
  - At least employ one higher power cycle (e.g. US06)



Vehicle differences: Change in NOx for GDI vehicles (20% and 30% aromatic fuels compared) Yang et al. (2019): Growth Energy Study

Guide recommended steps 1-5

Core fuel steps in green

- *Step 1: Identify the mission and study purpose. Present the types or species of emissions, efficiency or performance to be characterized, the applicable fuel source or geographic region, restrictions or rules related to fuel composition, climatic and fleet limitations, and contemplated fleet activity.*

- *Step 2: Identify resources and consider allocation. Quantify and resolve tradeoffs between assigning resources to acquisition of fuels, acquisition of vehicles, data collection (typically on a dynamometer), and data analysis and reporting.*

- *Step 3: Determine representative fuel properties. Identify a pathway for precise definition of the target fuel or suite of fuels. This will require estimation of the range of parameters (properties and composition) for the one or more BOBs to be used in the study.*

- *Step 4: Define the fuels. Sample baseline fuels to determine how the composition varies. Determine best estimate compositions for target fuels from expert consultation, modeling or existing refinery data. Determine whether a single fuel or a suite of fuels will represent each ethanol level. Set the composition of the baseline and target fuel(s) to represent two composition distributions.*

- *Step 5: Procure the fuels. It is possible to use market fuels, but generally the fuels must be blended to a specification. It is preferred that blending targets many parameters, typically expressed as composition, and employs streams with refinery DHA.*

Recommended steps 6-10

- *Step 6: Determine representative vehicles*. Vehicle count should be balanced with tests per vehicle. Study duration suggests bias to newer technology if inventory projection is the objective. Recognize differences between vehicles and develop a plan for in-test vehicle data logging.

- *Step 7: Procure and prepare the vehicles*. Vehicles may be procured in a variety of ways, should be inspected for malfunction, and evaluated during conditioning runs. A lubrication change usually precedes the start of the testing.

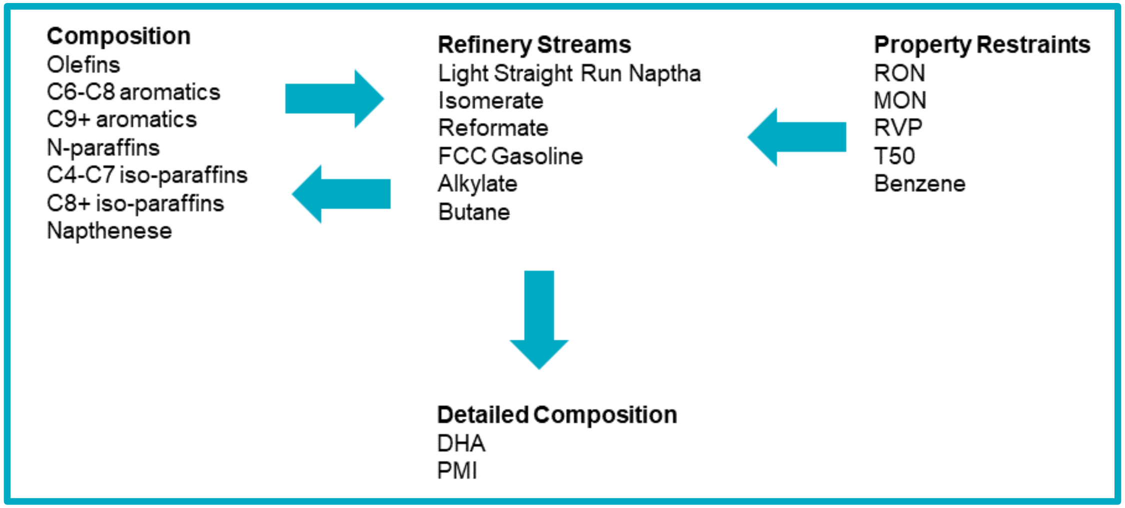
- *Step 8: Determine representative vehicle activity*. Either existing driving schedules may be used, or a cycle may be customized to satisfy the objective. Use of continuous emissions data is valuable

- *Step 9: Choose test protocols and schedules*. Vehicle operation or activity should reflect the study objectives. A low power schedule such as the LA92 and a high power schedule such as the US06 may be chosen. Other schedules are available, and wide open throttle (WOT) operation may be of interest.

- *Step 10: Address quality control and statistical confidence*. Develop a statistical plan that includes rejection of outliers and anticipates most eventualities before measuring emissions. Develop a data management plan. Define statistical analysis to be employed: simple analysis is possible for addressing basket blends or averages of suites.

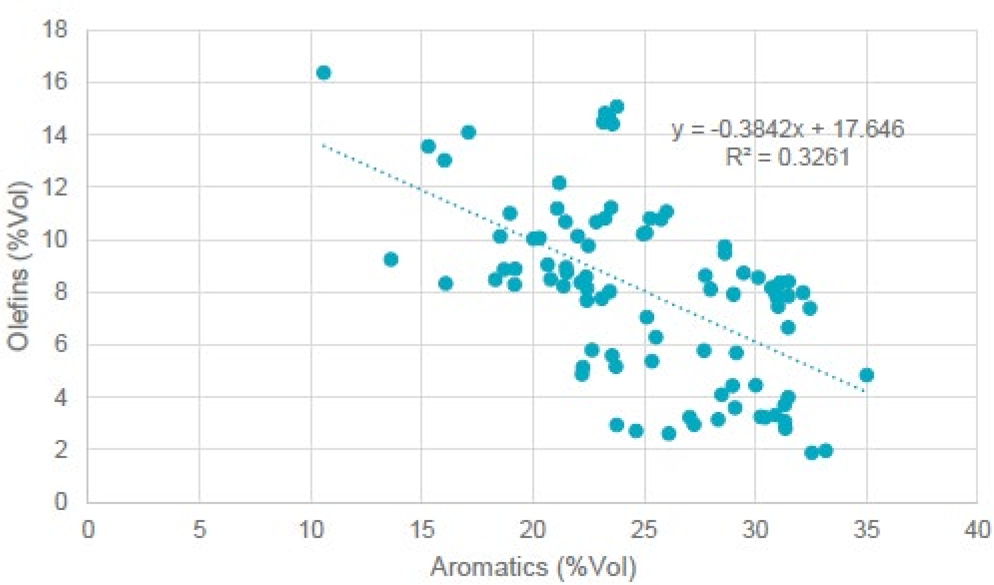
Guide example 1: tailpipe emissions study
E10 vs. E15 with common BOB

- E10 BOB must meet specifications (e.g. RVP, octane)
- Identify important hydrocarbon groupings
- Gather samples and analyze composition by groups
- Determine one or more representative BOBs for study
  - Consider most important independent variables
- Procure fuels
  - Blend to suit considering refinery streams, or
  - Acquire diverse market fuel stocks, or
  - Consider a basket blend



Guide example 2: PM study
E10 versus E20

- Same finished specifications, different BOB
- Identify resources (BOB variation effects)
- Consult with refiners & experts on BOB compositions
- Look to existing E10 DHA data for guidance on BOB variability (e.g. available data from Texas gasoline survey)
- Consider effects of ethanol octane boost on BOB differences



Example: Aromatic content does not predict E10 olefin content reliably, so olefins must have an average value in the study or be a separate independent variable from aromatics

Gasoline survey data

- Determine whether to use an average content, or several concentrations of a species
  - Consider E10 DHA composition variability to determine constituents that vary widely
  - Consider components believed to influence the emissions (PM)

	Average (% Vol)	StDev (% Vol)
Paraffin	13.30	2.41
I-Paraffins	34.93	5.13
Aromatics	25.17	5.04
Mono-Aromatics	23.58	5.18
Naphthalenes	0.49	0.20
Naphtheno/Olefino-Benzs	1.09	0.35
Indenes	0.01	0.01
Naphthenes	7.44	1.81
Mono-Naphthenes	7.44	1.81
Di/Bicyclo-Naphthenes	0.00	0.00
Olefins	7.98	3.39
n-Olefins	2.82	1.26
Iso-Olefins	4.43	1.83
Naphtheno-Olefins	0.73	0.35
Di-Olefins	0.00	0.00
Oxygenates	9.70	0.46
Unidentified	1.48	0.56

Content and standard deviation of content, by hydrocarbon group for the Texas survey regular gasoline.

Using resources

DHA correlation matrix

	Paraffin	I-Paraffins	Aromatics	Mono-Aromatics	Naphthalenes	Naphtheno/Olefino-Benzs	Indenes	Naphthenes	Mono-Naphthenes	Olefins	n-Olefins	Iso-Olefins	Naphtheno-Olefins	Di-Olefins	Oxygenates
Paraffin	1.00	-0.59	0.50	0.55	-0.45	-0.68	-0.58	0.15	0.15	-0.46	-0.44	-0.48	-0.42	-0.52	-0.52
I-Paraffins	-0.59	1.00	-0.76	-0.75	-0.12	0.16	0.17	-0.22	-0.22	0.08	0.04	0.11	0.08	0.33	0.22
Aromatics	0.50	-0.76	1.00	0.99	-0.07	-0.28	-0.28	0.05	0.05	-0.57	-0.51	-0.60	-0.58	-0.61	-0.43
Mono-Aromatics	0.55	-0.75	0.99	1.00	-0.16	-0.37	-0.36	0.07	0.07	-0.62	-0.56	-0.64	-0.62	-0.65	-0.46
Naphthalenes	-0.45	-0.12	-0.07	-0.16	1.00	0.83	0.82	-0.04	-0.04	0.49	0.50	0.48	0.46	0.37	0.34
Naphtheno/Olefino-Benzs	-0.68	0.16	-0.28	-0.37	0.83	1.00	0.85	-0.28	-0.28	0.65	0.66	0.62	0.65	0.59	0.45
Indenes	-0.58	0.17	-0.28	-0.36	0.82	0.85	1.00	-0.08	-0.08	0.50	0.52	0.48	0.47	0.53	0.25
Naphthenes	0.15	-0.22	0.05	0.07	-0.04	-0.28	-0.08	1.00	1.00	-0.28	-0.31	-0.27	-0.22	-0.40	-0.28
Mono-Naphthenes	0.15	-0.22	0.05	0.07	-0.04	-0.28	-0.08	1.00	1.00	-0.28	-0.31	-0.27	-0.22	-0.40	-0.28
Olefins	-0.46	0.08	-0.57	-0.62	0.49	0.65	0.50	-0.28	-0.28	1.00	0.99	0.99	0.96	0.80	0.57
n-Olefins	-0.44	0.04	-0.51	-0.56	0.50	0.66	0.52	-0.31	-0.31	0.99	1.00	0.96	0.94	0.80	0.55
Iso-Olefins	-0.48	0.11	-0.60	-0.64	0.48	0.62	0.48	-0.27	-0.27	0.99	0.96	1.00	0.94	0.79	0.57
Naphtheno-Olefins	-0.42	0.08	-0.58	-0.62	0.46	0.65	0.47	-0.22	-0.22	0.96	0.94	0.94	1.00	0.74	0.55
Di-Olefins	-0.52	0.33	-0.61	-0.65	0.37	0.59	0.53	-0.40	-0.40	0.80	0.80	0.79	0.74	1.00	0.53
Oxygenates	-0.52	0.22	-0.43	-0.46	0.34	0.45	0.25	-0.28	-0.28	0.57	0.55	0.57	0.55	0.53	1.00

Correlation coefficients (r) between component groups from Texas 2017 DHA survey (91 regular AKI fuel samples)

E10 vs E20: Expert input & analysis
Hypothetical Market Compositions

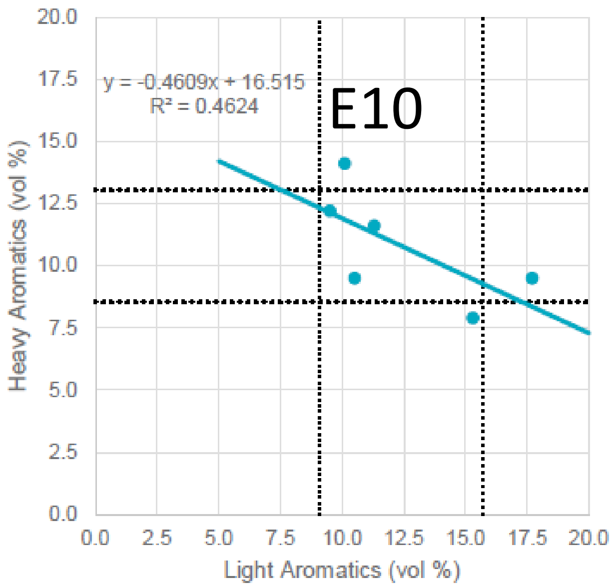
- Study planner (hypothetically) confers with six experts (refiners, blenders) and receives suggested future market E10 and E20 compositions from each
  - E10 to E20 step is assumed to reduce aromatics (reformate)
  - Planner may use current E10 data to test credibility
  - All twelve fuels are too great in number for resources
  - Aro %change = 0.74*(EtOH % change)

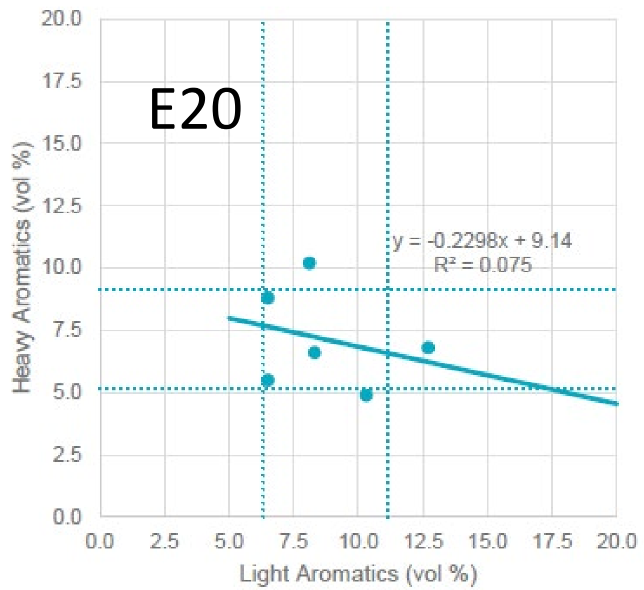
Component	E10-1	E10-2	E10-3	E10-4	E10-5	E10-6	E10-Ave
Olefins	7.5	13.0	10.8	8.0	12.8	14.8	11.2
C6-C8 aromatics	10.1	11.3	15.3	17.7	10.5	9.5	12.4
C9+ aromatics	14.1	11.6	7.9	9.5	9.5	12.2	10.8
n-paraffins	15.5	7.6	16.7	15.3	12.9	10.6	13.1
iso-paraffins	34.8	39.8	31.0	33.8	38.7	34.6	35.5
Napthenes	8.1	6.9	8.3	5.7	5.5	8.4	7.2
Ethanol	9.9	9.8	10.0	10.0	10.1	9.9	10.0

Component	E20-1	E20-2	E20-3	E20-4	E20-5	E20-6	E20-Ave
Olefins	6.9	11.5	10.0	8.0	10.8	12.6	10.0
C6-C8 aromatics	8.1	8.3	10.3	12.7	6.5	6.5	8.7
C9+ aromatics	10.2	6.6	4.9	6.8	5.5	8.8	7.1
n-paraffins	14.4	10.1	16.7	16.1	11.5	10.9	13.3
iso-paraffins	31.7	35.6	30.0	30.8	38.2	32.8	33.2
Napthenes	8.7	7.9	8.3	5.7	7.5	8.4	7.8
Ethanol	20.0	20.0	19.8	19.9	20.0	20.0	20.0

E10 vs E20: Selecting fuels

Some fuel trends considered



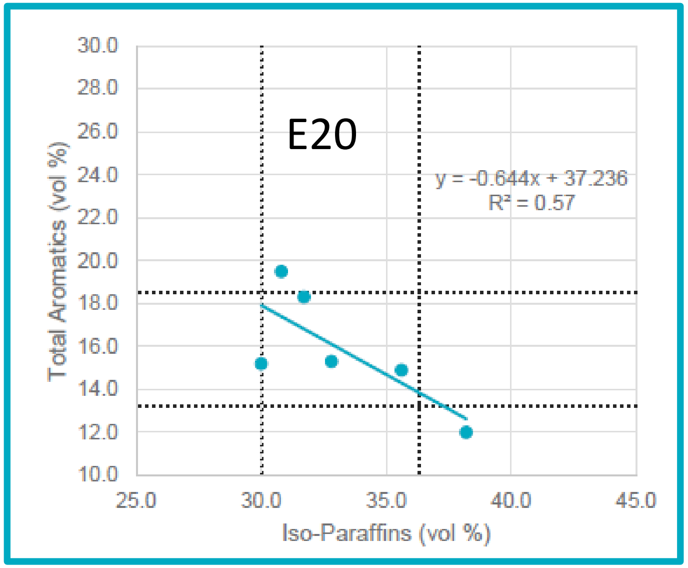


- E10 and E20 are major independent variables
- Light and heavy aromatics are each potential independent variables
  - Correlation between light and heavy aromatics is poor
- Iso-paraffin content (or alkylate species) may also be a candidate

E10 vs E20: Selecting fuels

Example study employing two E10 and two E20

- Using sum (Light Aro + Heavy Aro) as second variable
- Two E10 fuels
  - Total Aromatics 21.4% and 25.0%
- Two E20 fuels
  - Total aromatics 13.9% and 17.9%
- Other species chosen to best match these four fuel compositions
- Other variable options possible



As an example, iso-paraffin content should differ between the high and low aromatic E20 study fuels. Iso-paraffin composition should reflect an appropriate mix of species

Questions?

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