



# Utilizing Fuel Composition Data and Advanced Analytic Techniques in Routine Fuel Quality Assessments

Prepared By:

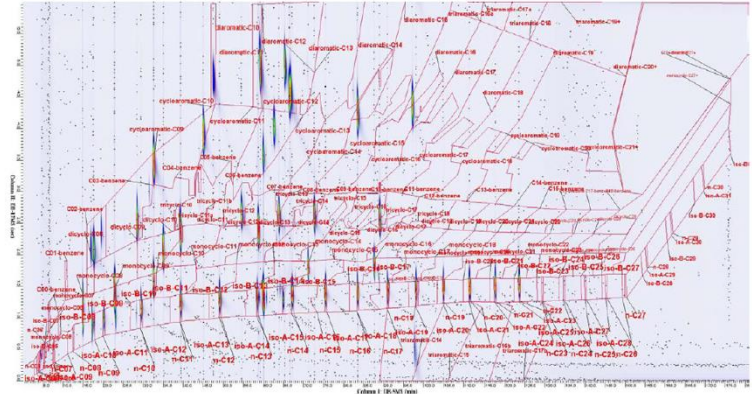
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# Background



- US DOW has developed and standardized analytical methods for measuring aviation and diesel fuel composition
  - “Production-ready”= High-throughput
  - Supplement traditional specification and fit-for-purpose level properties
  - Composition characterized in up to 108 fields
- Compositional information enables more robust fuel assessments and facilitates test method development
  - Fuel approvals– synthetic or commercial suppliers
  - Deployable test equipment
  - Contamination identification



Advanced analytical approaches and software solutions needed for recurring value

# Data Collection



- Three composition methods– hydrocarbon, extractable polar, and nitrogen species
  - Working towards publication in FED-STD-791
- Multiple on-going worldwide sampling programs
  - JP-5 and F-76 refinery samples
  - US Navy bases
  - Domestic and international marine gas oil (MGO) samples

Composition Component	Unique Compound Classes	Fuel Grades	Test Method
Hydrocarbon Composition	9 (tier 2) 108 (tier 3)	Aviation and Diesel	FED-STD- 791 Method 7508.0
Extractable Polar Compounds	14 (tier 2) 1 (tier 5)	Aviation and Diesel	DOW standardized SOP (Aviation)
Nitrogen Containing Compounds	14 (tier 2)	Aviation and Diesel	Navy In-house SOP
Sulfur Containing Compounds (Postponed)	5 (tier 2)	Aviation	Navy In-House SOP

## Tier Classifications

- Tier 0 – Specification and FFP testing (e.g. ASTM/IP test methods)
- Tier 1 – Chemical Family (paraffins)
- Tier 2 – Functional Group (e.g. isoparaffins)
- Tier 3 – Compound Sizing (e.g. mono-cycloparaffin C9)
- Tier 4 – Positional & Skeletal Isomerization (e.g. primary isoparaffin C9)
- Tier 5 – Individual Compound/Atom Identification (e.g. DiEGME)

# Navy Fuel Analysis & Characterization Tool

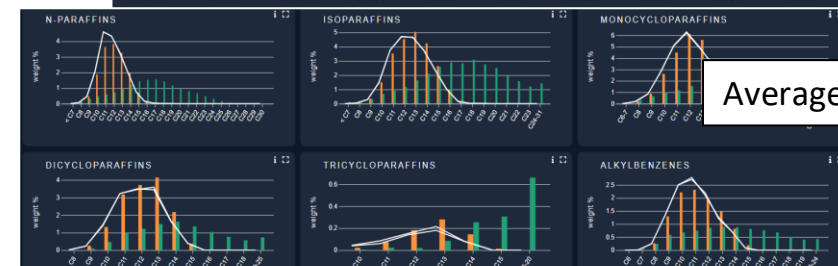
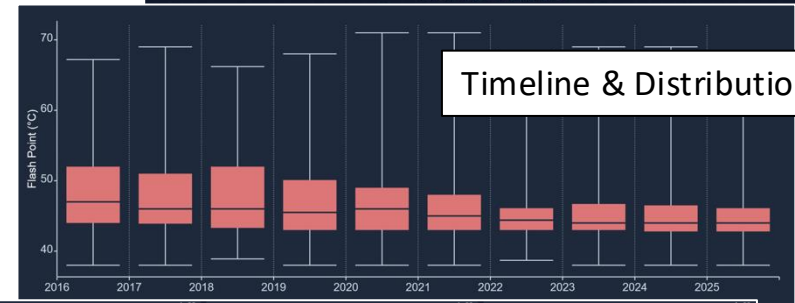
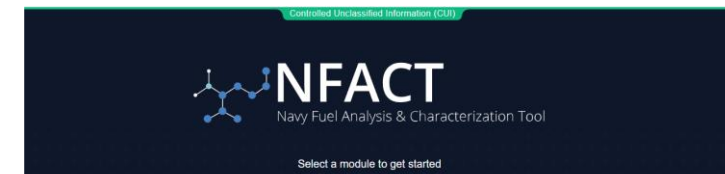


## System Design

- Started in 2018
- Python-based, fully custom design
- Hosted on US Navy secure server
- DOW access card required; admin granted permissions
- Standardized data entry via web form
- Data cleaning pipelines
- Three environments– development, staging, and production

## Database

- 1999 – Present
- 76.6 billion gallons represented
- JP-5, F-24 (Jet A), JP-8 (Jet A-1), F-76, MGO, synthetic fuels
- 66,000 samples w/full specification data (1999 - Present)
- 2,300 samples w/hydrocarbon composition
- Fit-for-purpose (FFP) and hardware data



# Let's Put Them to Use



## Case Studies

1. Fuel property assessments– Can I purchase the fuel?  
“Quality Assurance”
2. Property estimation– Should I use the fuel?  
“Quality Surveillance”
3. Contaminant identification- Is something wrong with the fuel?  
“Investigation”

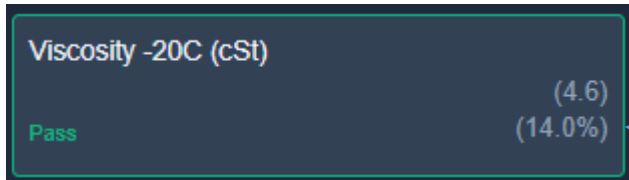
# Can I Purchase the Fuel?

## “Quality Assurance (QA)”

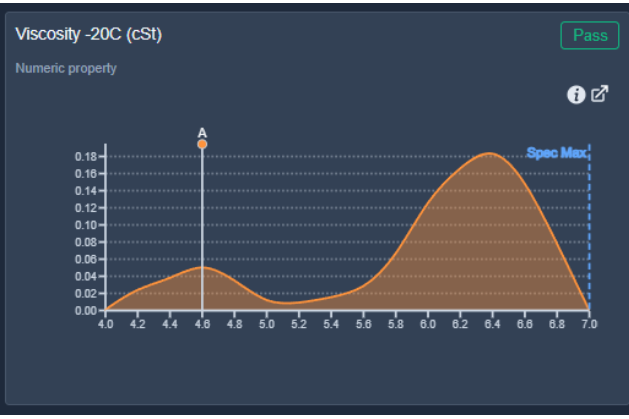
- Purchase requirements established by the fuel specification/purchase agreement
- New suppliers provide a Certificate of Quality (COQ) confirming properties meet specification

**Opportunity:** “Conforms or does not conform” decision, limited understanding of fuel’s uniqueness for purchaser or end user

**Solution:** Quantification of properties relative to history (percentiles)



Value  
 Percentile



Required Properties				
Total Sulfur (mg/kg) Pass (1800.0) (91.0%)	Vis Appearance (pass/fail) Pass (PASS)	Saybolt Color (color) Pass (22.0) (11.0%)	Jet Acid Nbr (mg/KOH/g) Pass (0.0) (0.0%)	Mercaptan Sulfur (mass%) Pass (0.001) (56.0%)
Distill - Inl Bol Pt (°C) Pass (179.0) (48.0%)	Distill - 10% (°C) Pass (182.0) (29.0%)	Distill - 20% (°C) Pass (185.0) (16.0%)	Distill - 50% (°C) Pass (204.0) (6.2%)	Distill - 90% (°C) Pass (224.0) (4.0%)
Distill - End Point (°C) Pass (241.0)	Distill - Residue (vol%) Pass (1.0) (0.0%)	Distill - Loss (vol%) Pass (1.0) (88.0%)	Distill T50-T10 (°C) Fail (12.0) (3.0%)	Distill T90-T10 (°C) Fail (32.0) (2.0%)
Flash Pt (°C) Pass (83.0) (22.0%)	Density 15C (kg/L) Pass (0.788) (5.0%)	API Gravity (MM) Pass (45.8) (93.0%)	Viscosity -20C (cSt) Pass (4.6) (14.0%)	Viscosity -20C (cSt) Pass (4.6) (14.0%)
Net Heat of Combustion, Mass (MJ/kg) Pass (43.28) (78.0%)	Celane Idx Pass (49.2) (95.0%)	Celane Idx (calc 4 var) Pass (47.0) (94.0%)	Hydrogen Content (mass%) Pass (13.9) (43.5%)	Smoke Pt (mm) Pass (25.0) (85.0%)
Naphthalenes (vol%) Pass (1.0) (37.0%)	Copper Strip Corrosion Pass (1a)	TS DT 260C (mm) Fail (No Data)	Existent Gums (mg/100 mL) Pass (1.0) (8.5%)	MSEP Additives Pass (88.0) (17.0%)
Calc FSII Conc (vol%) Pass (0.09) (8.0%)	Particulate Contamination (mg/L) Pass (0.5) (85.0%)	Filtration Time (min/5gal) Pass (3.0) (0.0%)	FAME Content (mg/kg) Fail (No Data)	AO Chem Fail (No Data)
AO Conc (mg/L) Pass (15.0) (2.0%)	Calc CILI Conc (mg/L) Pass (18.0) (0.0%)	CILI Chem Fail (No Data)		

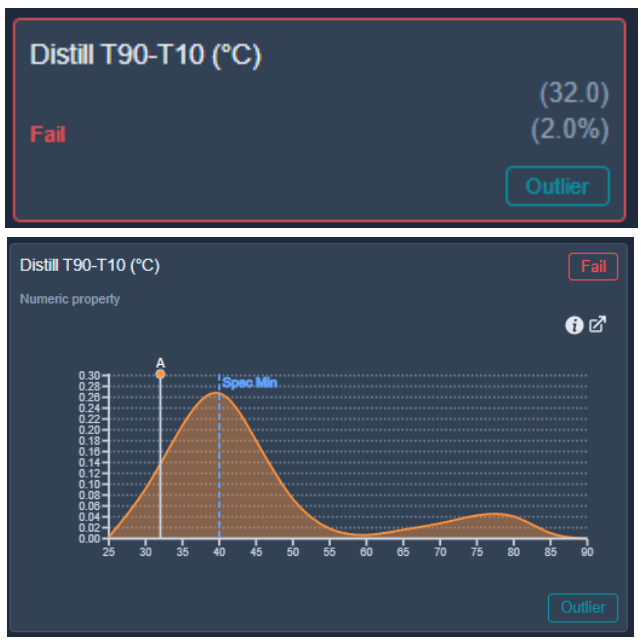
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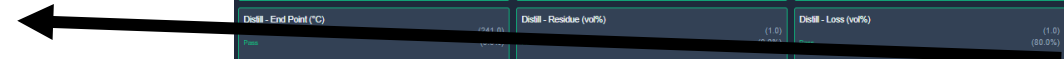
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Flash Pt (°C) Pass (83.0) (22.0%)	Density 15C (kg/L) Pass (0.788) (5.0%)	API Gravity (MM) Pass (45.8) (93.0%)	Freeze Pt (°C) Pass (-49.0) (24.0%)	Viscosity 20C (cSt) Pass (4.0) (14.0%)	
Net Heat of Combustion, Mass (MJ/kg) Pass (43.29) (78.0%)	Celane Idx Pass (49.2) (95.0%)	Celane Idx (calc 4 var) Pass (47.0) (94.0%)	Hydrogen Content (mass%) Pass (13.9) (43.0%)	Smoke Pt (mm) Pass (25.0) (85.0%)	
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## Key Takeaways

- Natural distributions exist for fuel properties
- Fuels at extremes of experience may warrant additional investigation to assure fit-for-purpose



# Should I Use the Fuel?



## “Quality Surveillance (QS)”

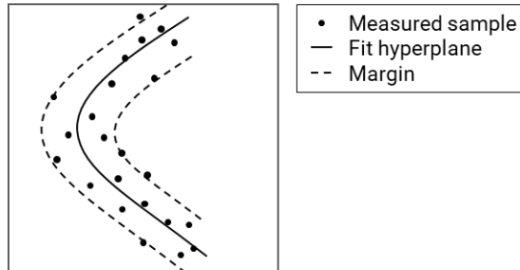
- Quality surveillance testing performed in accordance with MIL-STD-3004-1 and NATOPS 00-80T-109
- Up to 21 properties measured based on delivery scenario

**Opportunity:** Reduced time, cost, and equipment

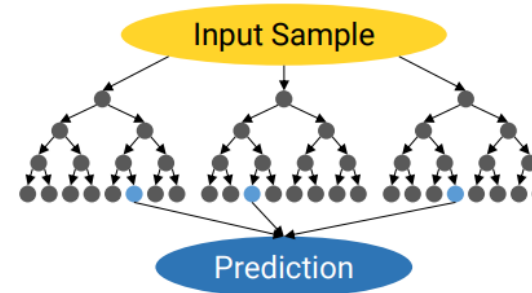
**Solution:** Property estimation via fuel composition

## Step 2: Modeling

### Support Vector Regression (SVR)



### Random Forest (RF)



Unsupervised training with a 5-fold cross validation  
Sample set split-- 75% for training & 25% for testing

# Model Results



- 18 properties modeled
  - Stability related properties deferred until models trained w/ heteroatom composition
- Random forest models performed slightly better than support vector regression models
- 14 models w/RRMSE less than ~3%
- <5 mL of fuel required for property estimations

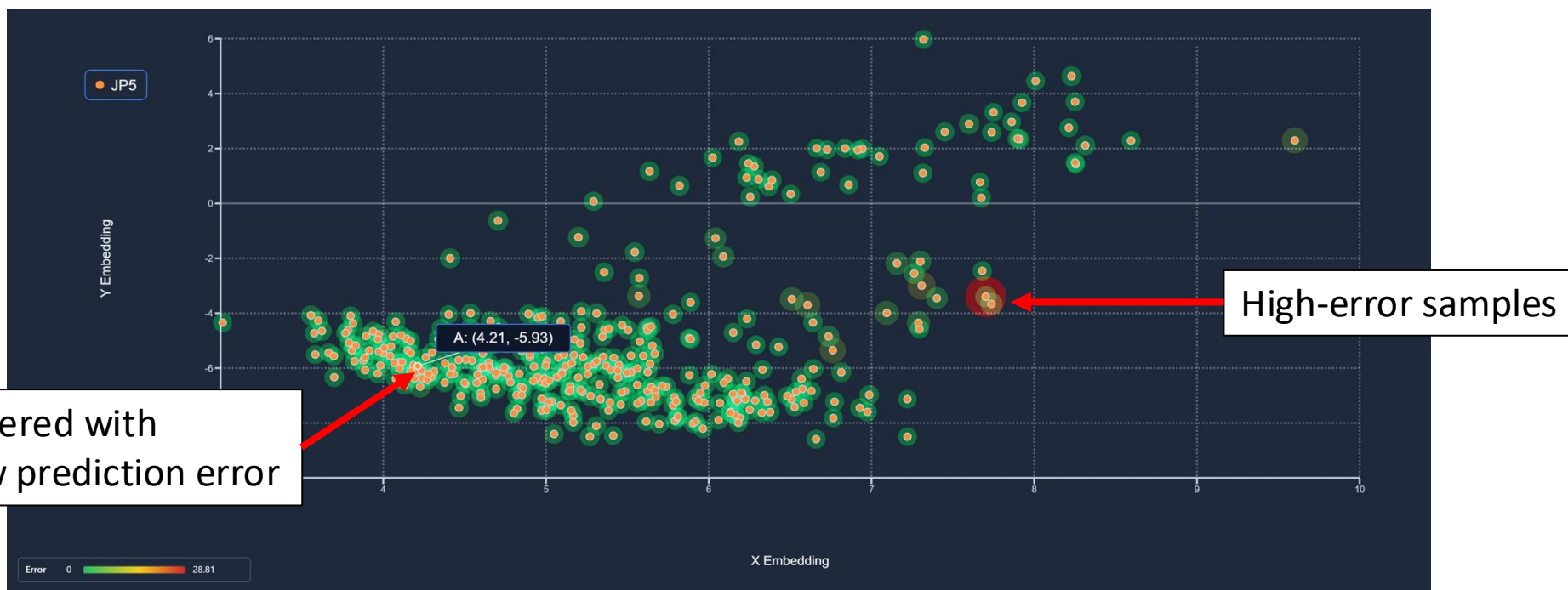
Aromatic Concentration	Best Model	Root Mean Square Error (RMSE)	Relative RMSE (RRMSE)
Density at 15°C	SVR=RF	0	N/A
Flash Point	RF	1.0	1.7%
Freeze Point	RF	1.3	2.5%
Hydrogen %	RF	0.2	1.2%
Naphthalene Concentration	RF	0.1	15.9%
Net Heat Value	RF	0.04	0.1%
Viscosity at -20°C	RF	0.2	3.1%
Cetane Index	RF	0.5	1.2%
Distillation Initial	RF	1.8	1.0%
Distillation 10%	RF	1.4	0.7%
Distillation 20%	RF	1.2	0.6%
Distillation 50%	RF	1.2	0.5%
Distillation 90%	RF	1.2	0.5%
Distillation End	RF	2.1	0.8%
Distillation T50 - T10	RF	1.3	6.1%
Distillation T90 - T10	RF	1.6	3.4%
Existent Gum Content	RF	0.5	44.9%
Smoke Point	RF	0.5	7.0%

# Model Results



## Implementation Challenges:

- 1) Routine use-- standard practiced needed for determining when a target sample should or shouldn't be used with models
- 2) Expansion
  - GCxGC-FID systems are expensive and more complex to operate than current methods
  - Continuous, in-situ measurements aren't feasible



Target sample clustered with Samples having low prediction error

High-error samples

# What's Wrong with the Fuel?



## “Investigation”

- Triggered by a failing fuel property, atypical performance, or hardware inspection
- Identify, contain, and correct

**Opportunity:** Improved root-cause determination

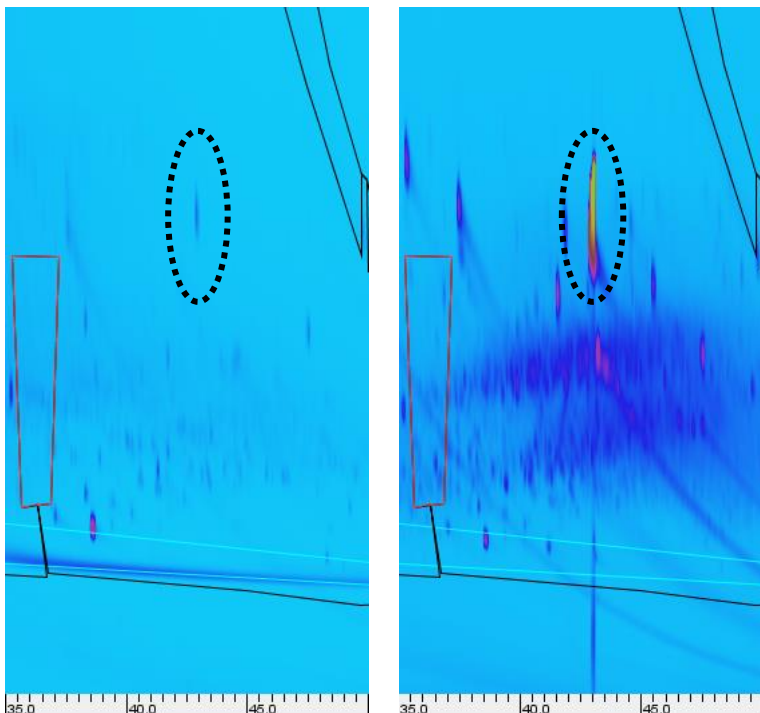
**Solution:** Compositional analysis + artificial intelligence

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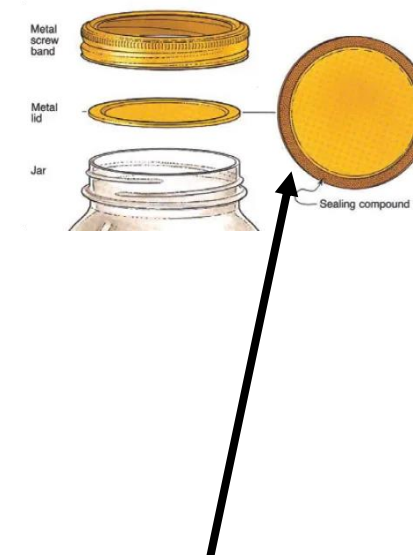
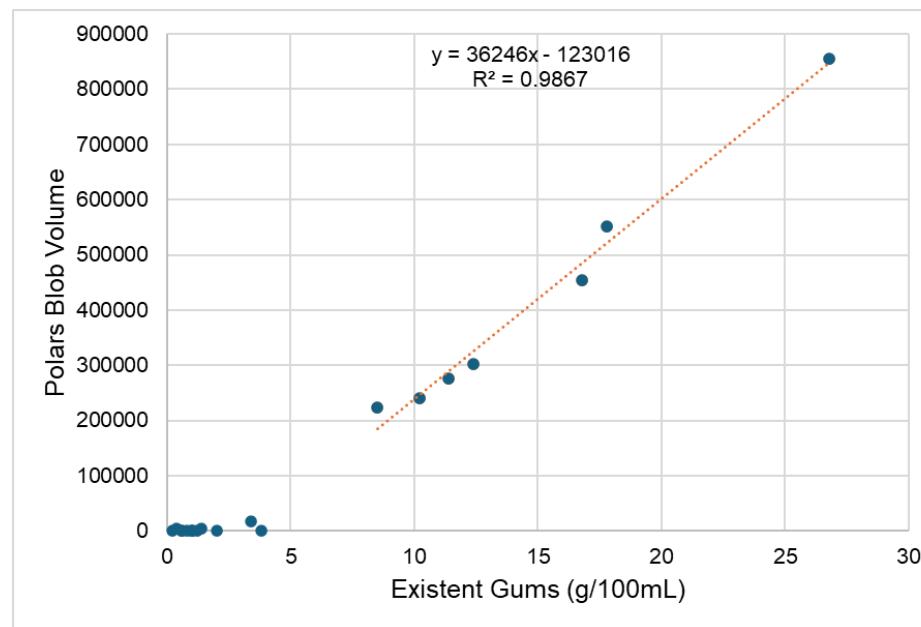
**Example 1:** Aircraft sample contains high existent gum content, sample collected in a readily available container (glass mason jar)

## Extractable Polars Analysis



Sample 1  
Gums <1mg/100mL

Sample 2  
Gums >20mg/100mL



**Gum content due to incompatibility with mason jar lid's gasket material**

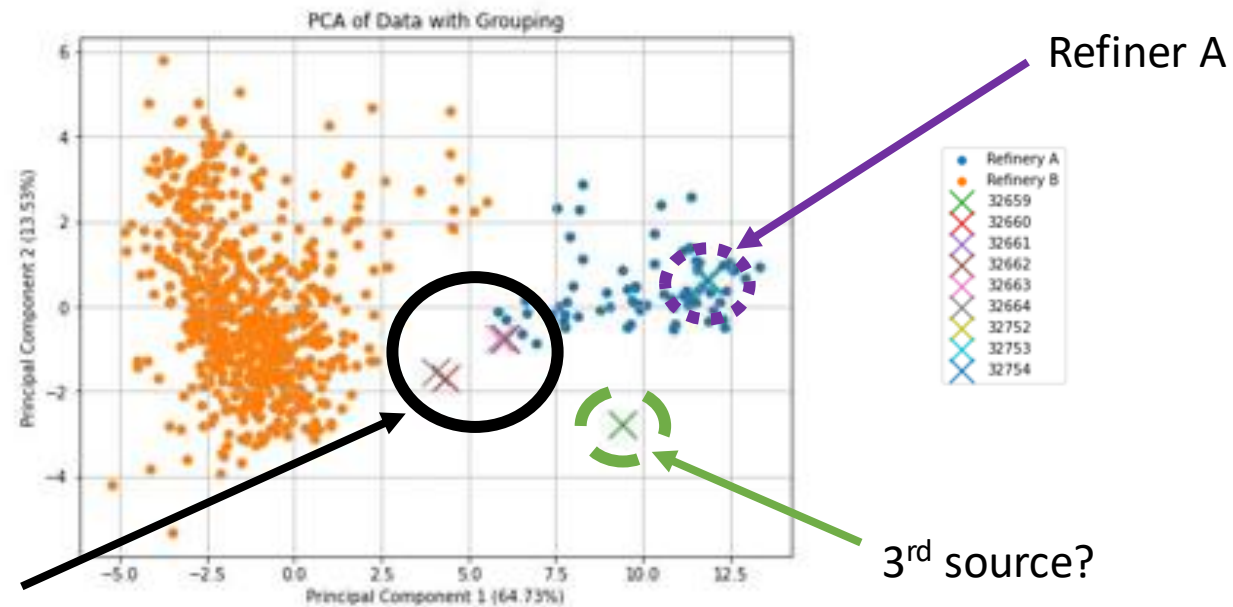
# What's Wrong with the Fuel?



**Example 2:** Subset of aircraft at a site experience an engine issue

## Challenge:

- Bulk properties don't provide enough granularity to separate source of fuels
- Regional sampling + classification techniques provide additional information on source of fuels



Mixture of Refiner A and B

3<sup>rd</sup> source?

# Summary



**Compositional Analysis:** Standardized high-throughput analytical methods enable a more robust and "first-order" understanding of fuel quality beyond traditional specification testing

**Practical Applications:** Accessibility enables compositional data to be used for Quality Assurance, Quality Surveillance, and Investigations

**NFACT:** Scalable, Python-based platform

**Predictive Modeling:** Artificial intelligence creates new opportunities to address old challenges