# Design of Next Generation Renewable Fuels

Mark Romanczyk[1], Jorge Ramirez Velasco[3], **Petr Vozka[2]**, Lan Xu,[1] Katherine Wehde[1] , Brent Modereger[1],
Rodney Trice[3], Gozdem Kilaz[2], Hilkka Kenttämaa[1]
[1]Department of Chemistry, [2]School of Engineering Technology, and [3]Department of Materials Engineering, Purdue University

PURDUE UNIVERSITY Discovery Park
NEPTUNE CENTER FOR POWER AND ENERGY RESEARCH

**Goal:** Establish a databank of conventional and alternative aviation fuel constituents to be utilized in developing correlations between chemical composition, engine performance, and material performance.
Our goal is to serve Navy's mission to utilize resilient energy while training and educating midshipmen and US military personnel.

## Introduction:

Aviation fuels are vastly complex mixtures, including many different types of hydrocarbons, additives, and impurities. As chemical group concentrations cannot be used to sufficiently explain fuel properties, our research focuses on correlations between the exact chemical composition of a fuel and its properties as well as performance. One such example is the impact of specific aromatic compounds on the swelling of o-ring seals and their tensile strength. Similarly, a detailed investigation of fuel impurities is necessary for implementing safe aircraft operational limits.

## Methods:

- Two-dimensional gas chromatography coupled with high resolution time-of-flight mass spectrometry (GCxGC/TOF MS): identification of aromatic compounds in CHCJ and Jet A/HEFA
- Two-dimensional gas chromatography with flame ionization detector: quantification of fuel components
- Nikon optometer: measurement of the thickness of o-rings
- Formulation of synthetic fuel impurities model
- Ablation rig: high temperature test of gas turbines coatings

## Conclusions:

As the aromatic compound's molar volume and molar mass decrease, their propensity to swell o-ring seals increases. O-ring seal volume is not a static property; it changes depending on what compounds it is exposed to. Different fuels can cause very different extents of swelling.

With increasing temperature of the gas turbine, fuel impurities melt and infiltrate coatings. Consecutively, upon solidification these impurities crack, nucleate and propagate between the infiltrated and non-infiltrated regions; ultimately causing coating delamination.

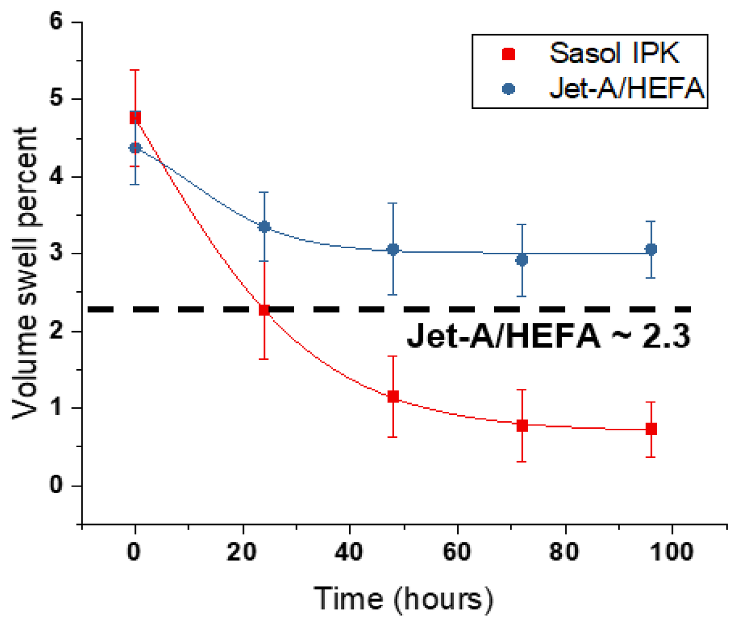
## Future plans:

Develop semi-quantitative relationships for the volume swelling of o-ring seals immersed in mixtures containing different aromatic dopants.

Expand on a detailed chemical group classification of fuel constituents, such as defining subgroups of mono-, di-, and tricycloparaffins. Similarly, distinguish between alkylbenzenes, naphthalenes, and cycloparaffins (indans and tetralins).

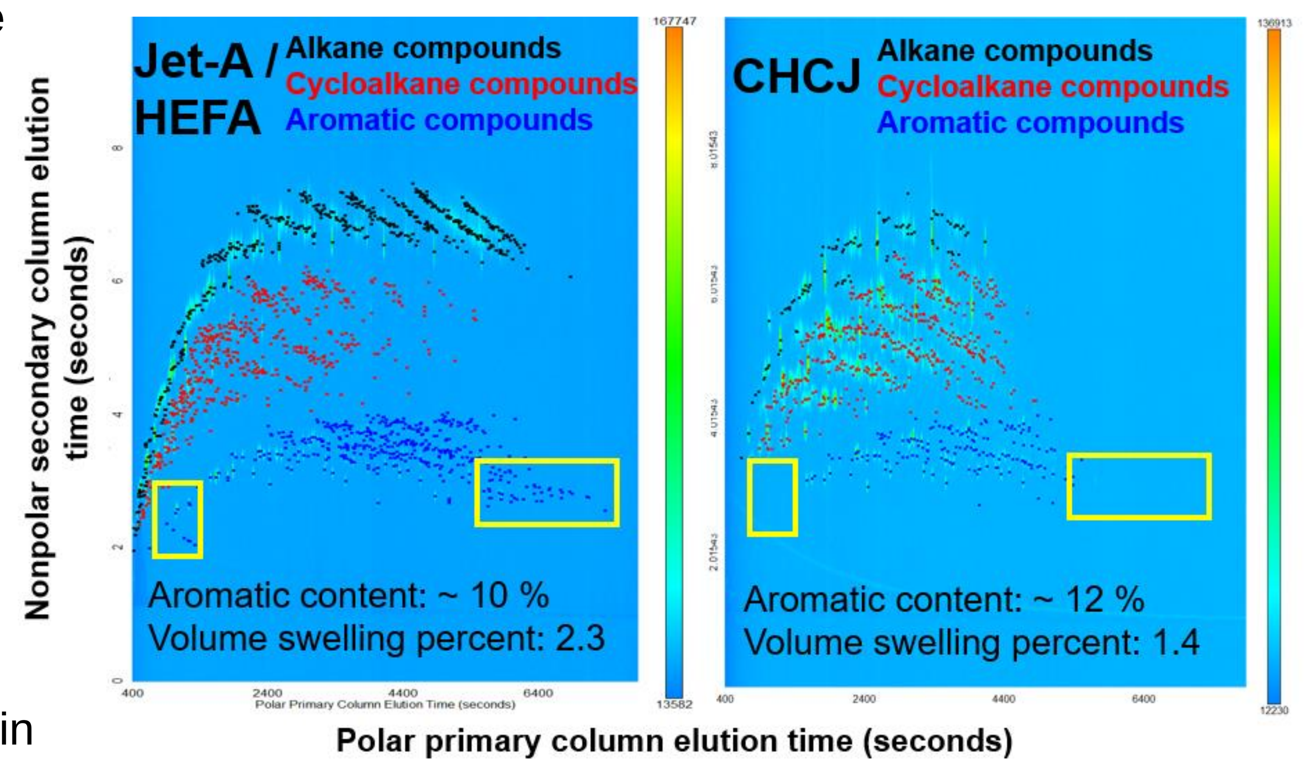
Identify the thermomechanical and thermochemical mechanisms that obliterate gas turbines coatings.

### Temporal studies measuring reduction of o-ring seal volume



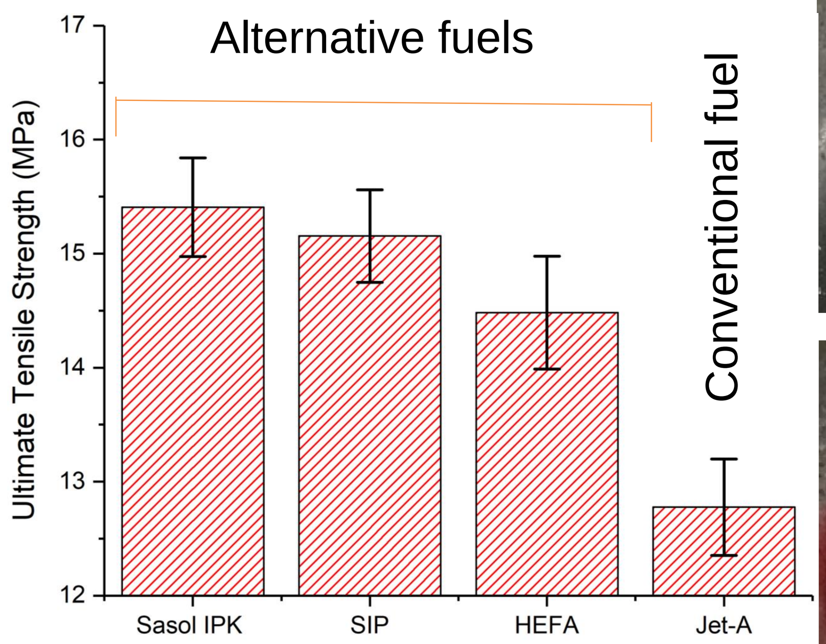

After o-ring seals had been immersed in Jet-A, they were immersed in Sasol IPK or a 50:50 mixture of Jet A and HEFA. The volume of the o-ring seals decreased. Hence, replacing Jet-A with an alternative fuel with less aromatic content may affect o-ring seals' volume and potentially contribute to leaks in fuel circulation systems and fuel tanks.

### Total ion current chromatograms

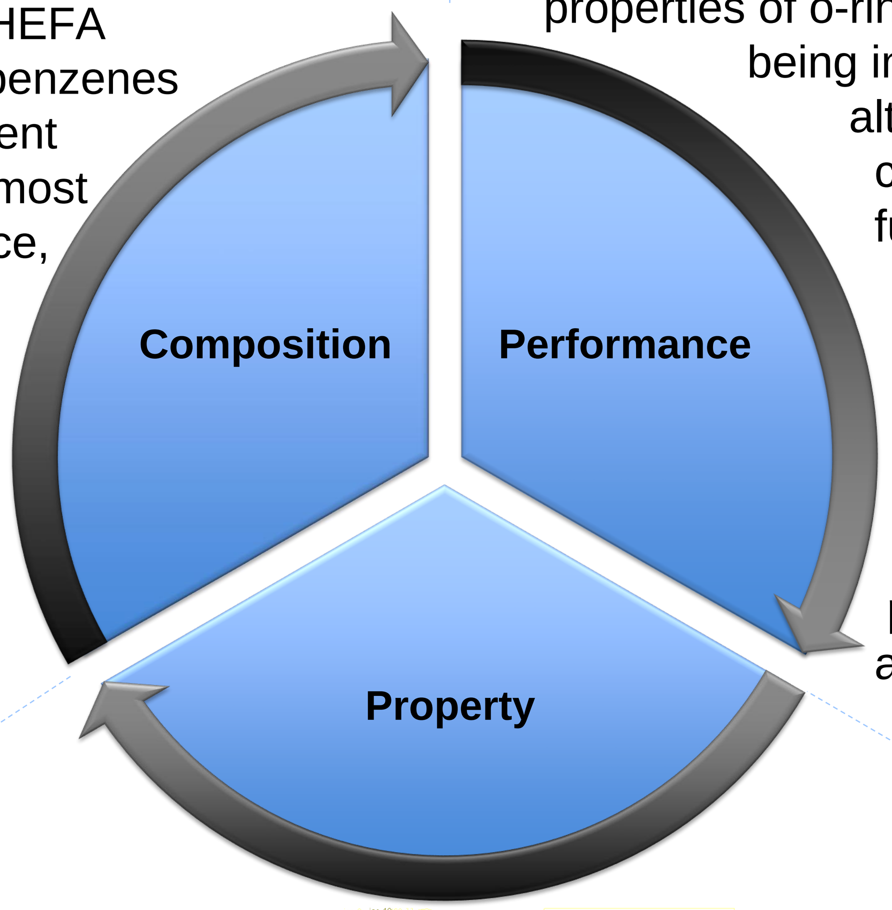



The chemical composition of Jet A / HEFA differs from CHCJ. Importantly, alkylbenzenes with a molar mass of 106 Da are absent in CHCJ. These are the compounds most efficient in swelling o-ring seals. Hence, CHCJ may not swell o-rings sufficiently to prevent fuel leaks.

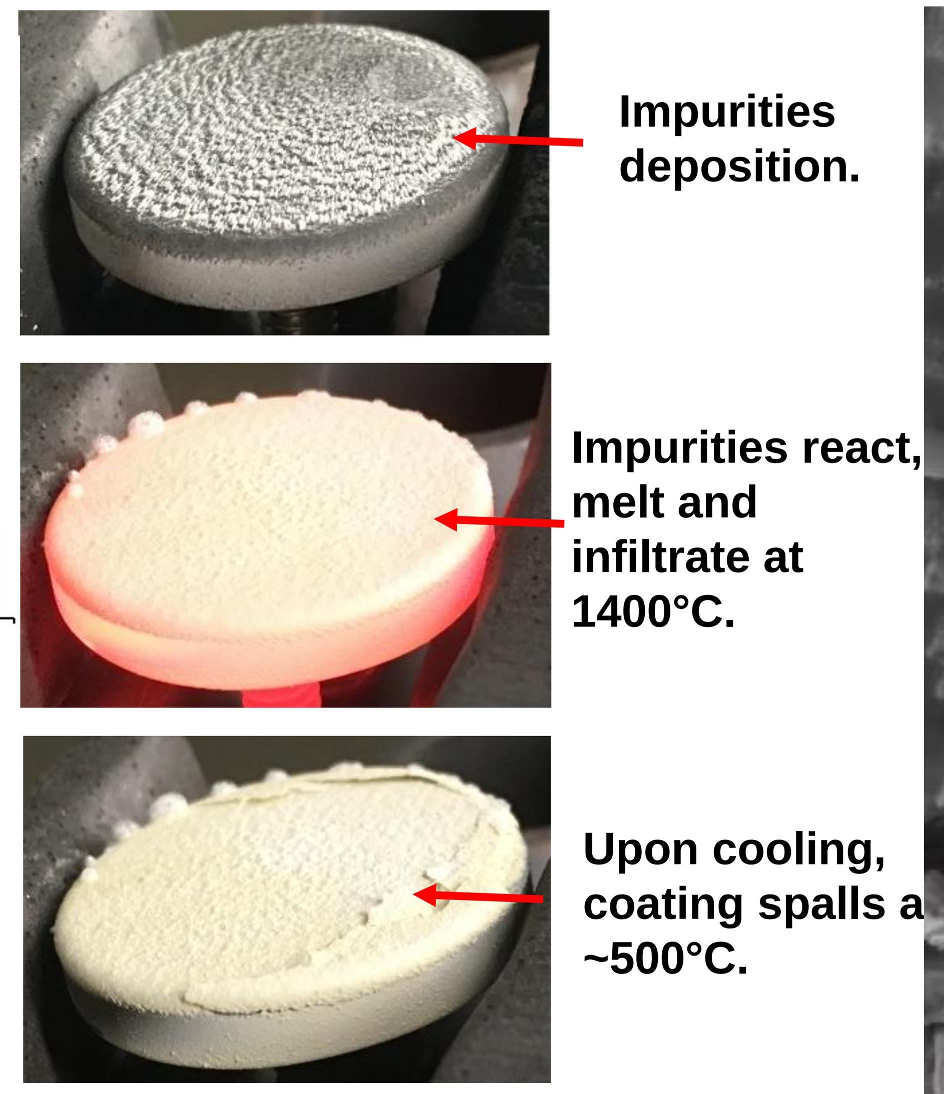
### O-rings tensile strength study.

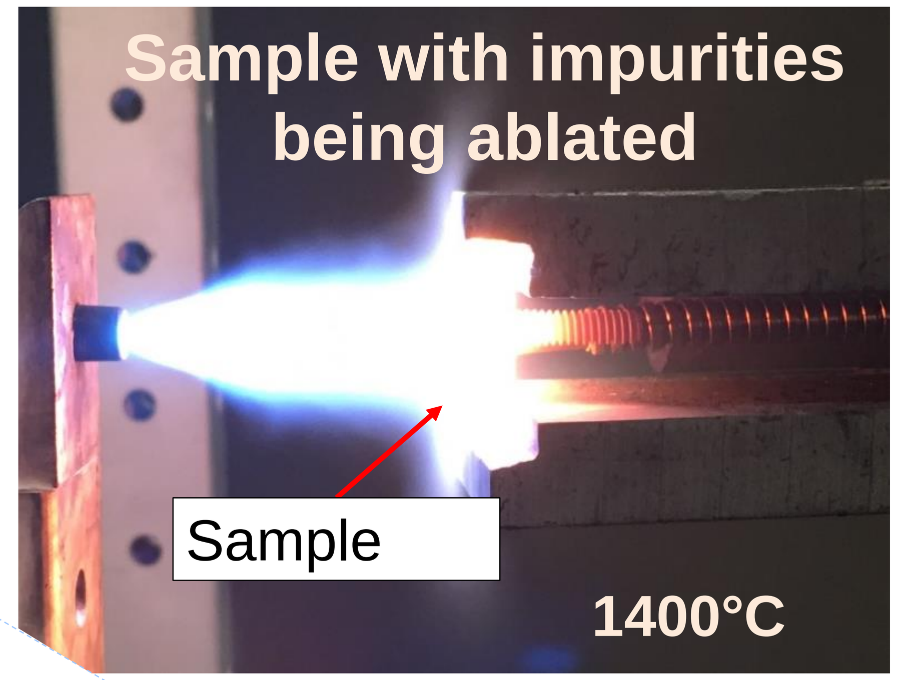


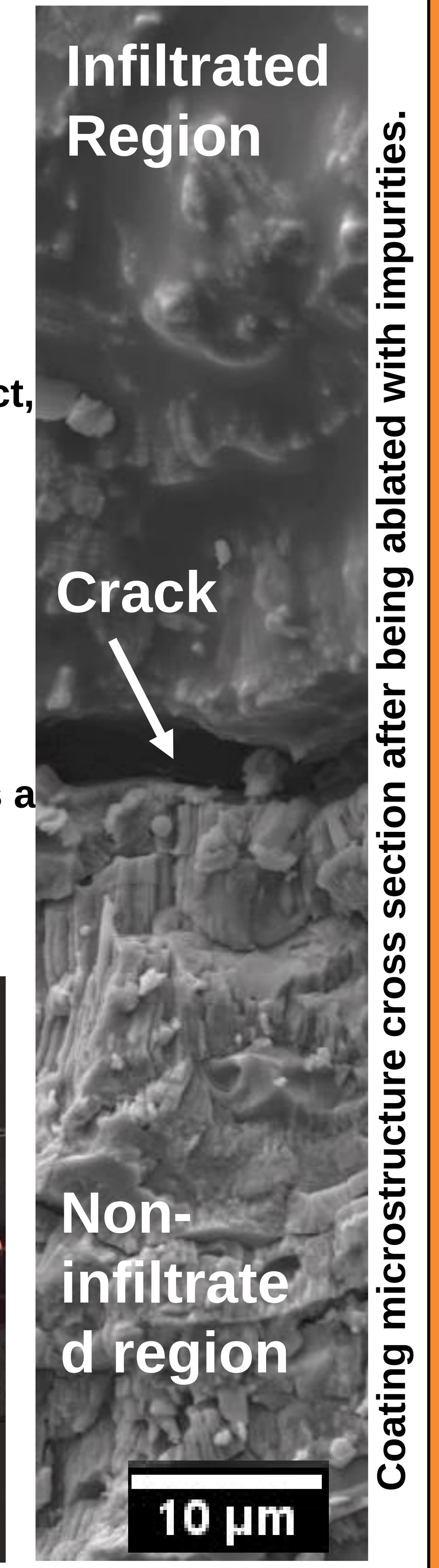

Comparison of the mechanical properties of o-ring seals after being immersed in alternative and conventional fuels revealed significant differences. To achieve the same performance, a detailed study of possible dopants and their effects is necessary.




### Effect of alternative fuel impurities on gas turbine coatings.

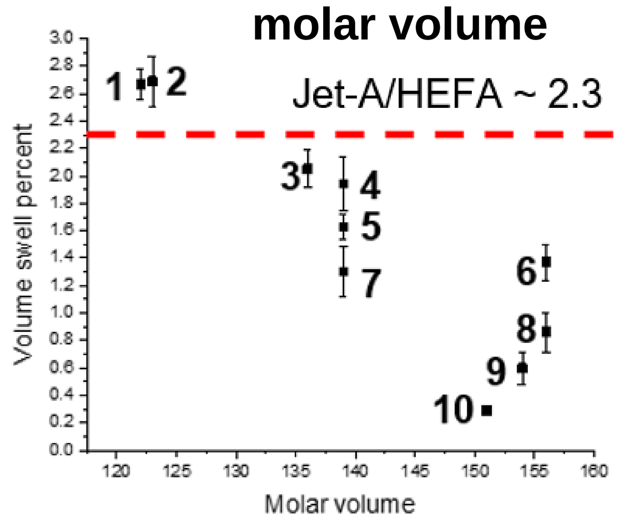


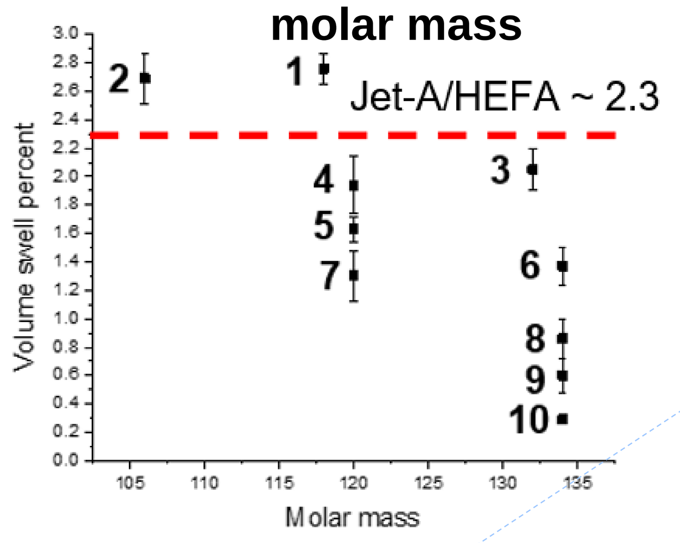




Impurities react and infiltrate as a CMAS-like compound, and upon cooling, they form horizontal cracks that cause delamination to nucleate and propagate between infiltrated and non-infiltrated regions.

### Volume swell percent vs molar volume

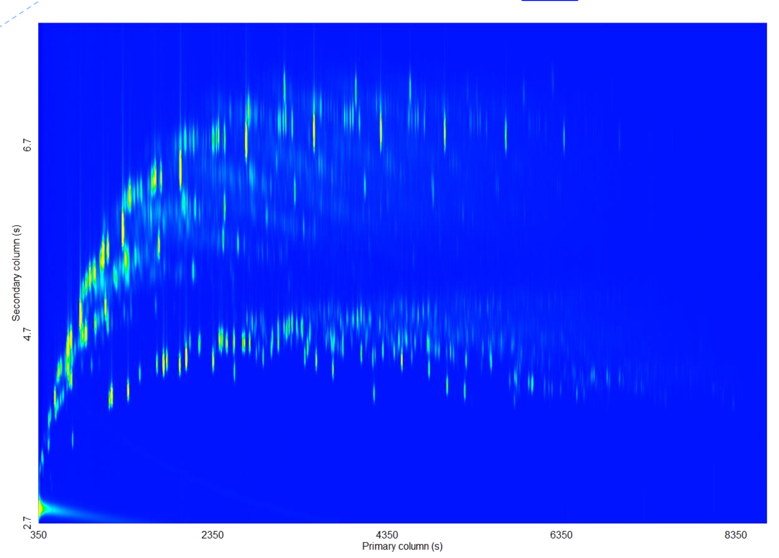



### Volume swell percent vs molar mass

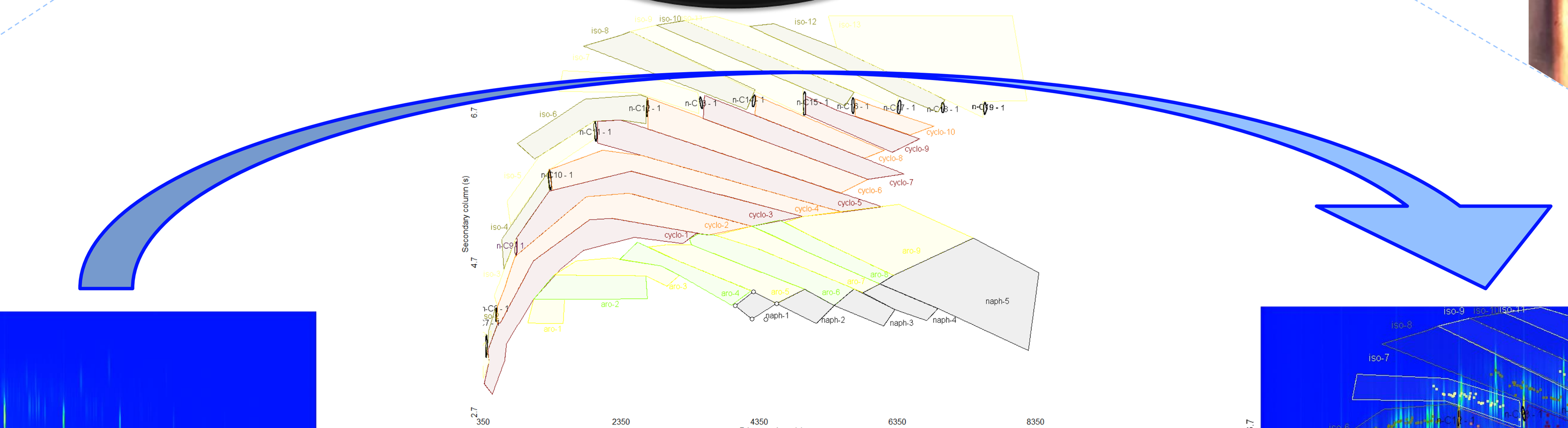



(1) Indane, (2) ethylbenzene, (3) tetralin,
(4) n-propylbenzene, (5) isopropylbenzene,
(6) n-butylbenzene, (7) 1,3,5-trimethylbenzene,
(8) *sec*-butylbenzene, (9) *tert*-butylbenzene,
(10) 1,2,4,5-tetramethylbenzene

Generally, when the molar volume and molar mass of aromatic compounds increase, their ability to swell o-ring seals decreases.



Jet A chromatogram obtained using GCxGC FID



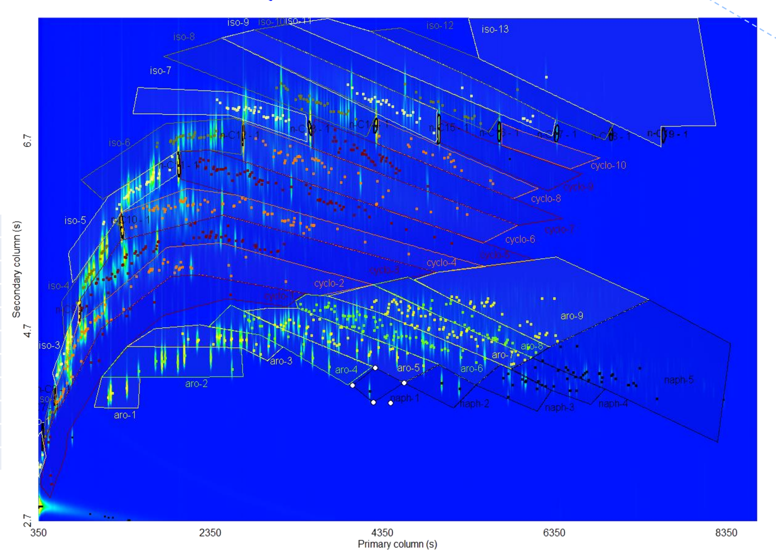
Quantitative results for Jet A sample:

| n-alkanes | wt. % |
|---|---|
| n-C7 | 0.01 |
| n-C8 | 0.73 |
| n-C9 | 4.54 |
| n-C10 | 4.94 |
| n-C11 | 3.46 |
| n-C12 | 2.49 |
| n-C13 | 1.94 |
| n-C14 | 1.36 |
| n-C15 | 0.83 |
| n-C16 | 0.38 |
| n-C17 | 0.13 |
| n-C18 | 0.02 |
| **total n-alkanes** | **20.81** |

| iso-alkanes | wt. % |
|---|---|
| iso-C7- | 0.20 |
| iso-C8 | 0.42 |
| iso-C9 | 4.27 |
| iso-C10 | 6.65 |
| iso-C11 | 4.99 |
| iso-C12 | 3.09 |
| iso-C13 | 2.90 |
| iso-C14 | 2.35 |
| iso-C15 | 1.24 |
| iso-C16 | 0.76 |
| iso-C17 | 0.17 |
| iso-C18 | 0.06 |
| iso-C19+ | 0.03 |
| **total iso-alkanes** | **27.11** |

| cycloalkanes | wt. % |
|---|---|
| cyclo-C7 | 0.36 |
| cyclo-C8 | 6.42 |
| cyclo-C9 | 6.52 |
| cyclo-C10 | 5.57 |
| cyclo-C11 | 3.63 |
| cyclo-C12 | 2.64 |
| cyclo-C13 | 1.44 |
| cyclo-C14 | 0.46 |
| cyclo-C15 | 0.00 |
| cyclo-C16 | 0.00 |
| cyclo-C17 | 0.02 |
| **total cycloalkanes** | **27.07** |

| aromatics | wt. % |
|---|---|
| arom-C8 | 1.91 |
| arom-C9 | 4.80 |
| arom-C10 | 3.63 |
| arom-C11 | 2.18 |
| arom-C12 | 4.59 |
| arom-C13 | 3.90 |
| arom-C14 | 2.23 |
| arom-C15 | 0.87 |
| arom-C16 | 0.58 |
| **total aromatics** | **24.69** |



Once the compound classification had been completed, quantitative analysis was performed using standards.