ASCENT Project 065a

Fuel Testing Approaches for Rapid Jet Fuel Prescreening

University of Dayton

PI: Joshua Heyne

PM: Anna Oldani

Cost Share Partner: VUV Analytics and DLR Germany

Objective:

To develop early-stage low volume evaluations of novel Sustainable Aviation Fuel (SAF) candidates via ASTM property tests and internal predictions

Project Benefits:

Rapid feedback to novel fuel producers on the blend ratios, compatibility, and combustor operability impacts of SAF candidates

Research Approach:

Evaluation methodologies are developed around a two-tiered prescreening

Tier α focuses on predictions; Tier β focuses on measurements

Tier	Measured Property	Predicted Property	Vol. (mL)	No. tested
α	GCxGC	LHV, Density, Surface tension, Freeze point, Viscosity, DCN, Flash point	1	58
	Distillation			
β	Density	LHV	10	38
	Viscosity			
	Surface ten.			
	Freeze point			
	Flash point			
	DCN		140	8

Major Accomplishments (to date):

Facilitated the process development of a volatile fatty acid pathway (PNAS paper)

Tools developed in P65a have been used to evaluate **58 SAF candidate samples** from approximately 8 labs and 12 pathways

Publications: 3

Invited talks: 8

Future Work / Schedule:

Development of additional Tier α methods

May ’21 – Method completion on simple mixtures

August ’21 – Complex fuel method development

August ’21 – Property prediction updates

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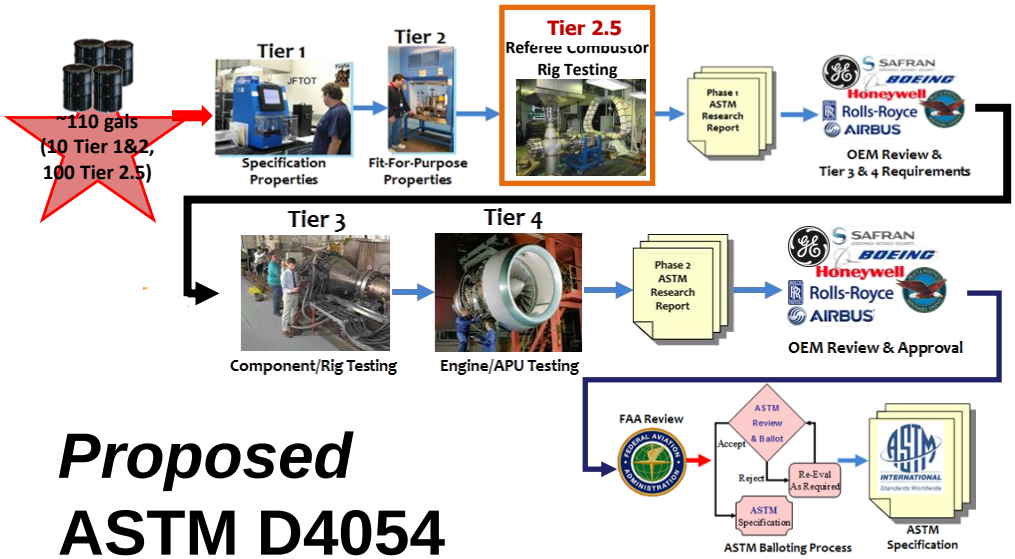
Introduction

Background and Motivation

- Bulk properties accounted for the vast majority of combustor operability variance in the NJFCP
- ASTM D4054 is volume intensive
- Measure or predict these properties (and others) ahead of the ASTM evaluation and qualification process



Proposed
ASTM D4054

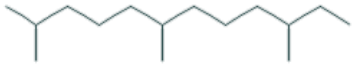
Volumes needed for various testing Tiers

Tier	$\mathcal{O}$(gal)	
α	~10^{-6}	***P65a prescreening***
β	~10^{-1}	
γ	~10	***P65b prescreening***
1 & 2	~10^{2}	
2.5	~10^{2}	***Referee Rig***
3 & 4	~10^{3}	

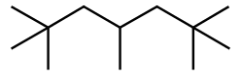
Motivation for approach

- SAF candidates can be selective structural and stereochemical isomers, e.g. Annex A3 and A5 (iso-butanol feedstock)
  - Statistical interpolation from experience without dedicated uncertainty quantification will yield misrepresented predictions
  - Isomers can significantly impact the DCN, freeze point, and viscosity

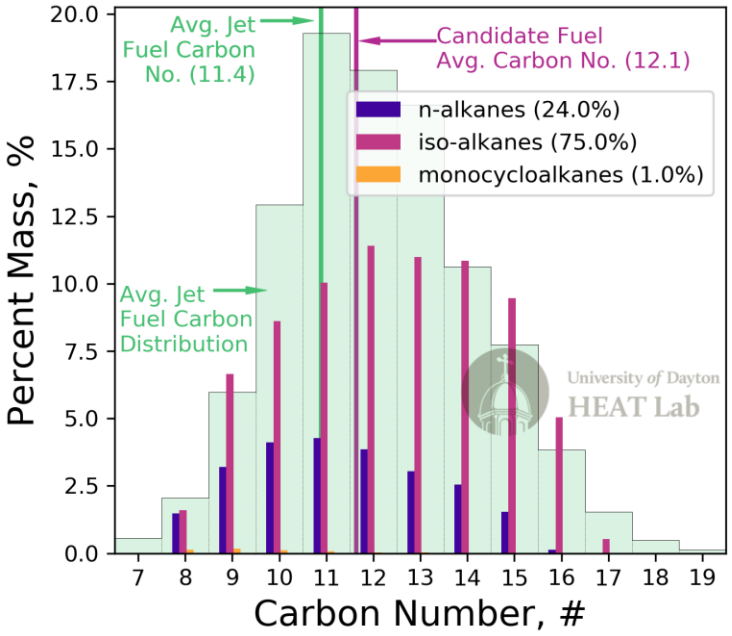
Farnesane (A3)

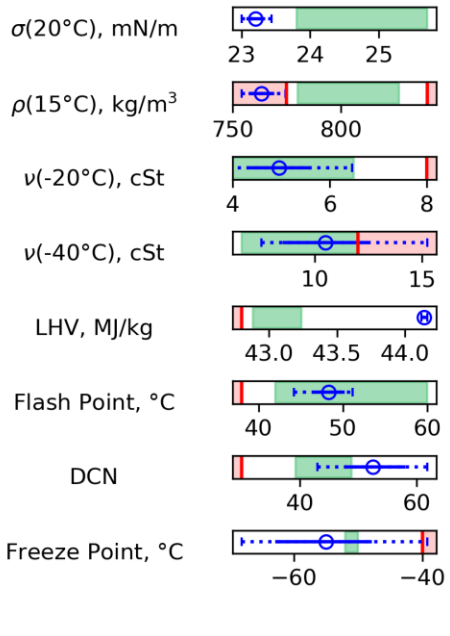


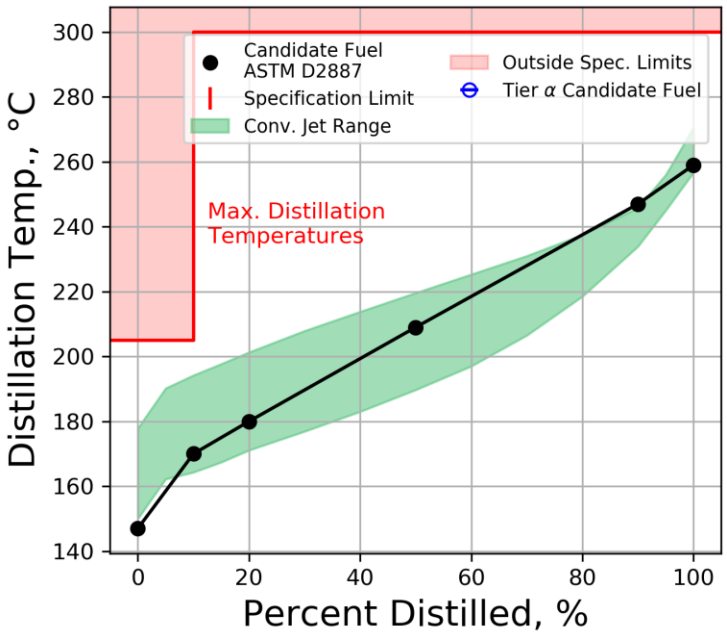
iso-Dodecane (A5)



- Typical methods for property predictions from minimal material are either separations or diagnostic limited, diagnostic limited (GCxGC-FID below)

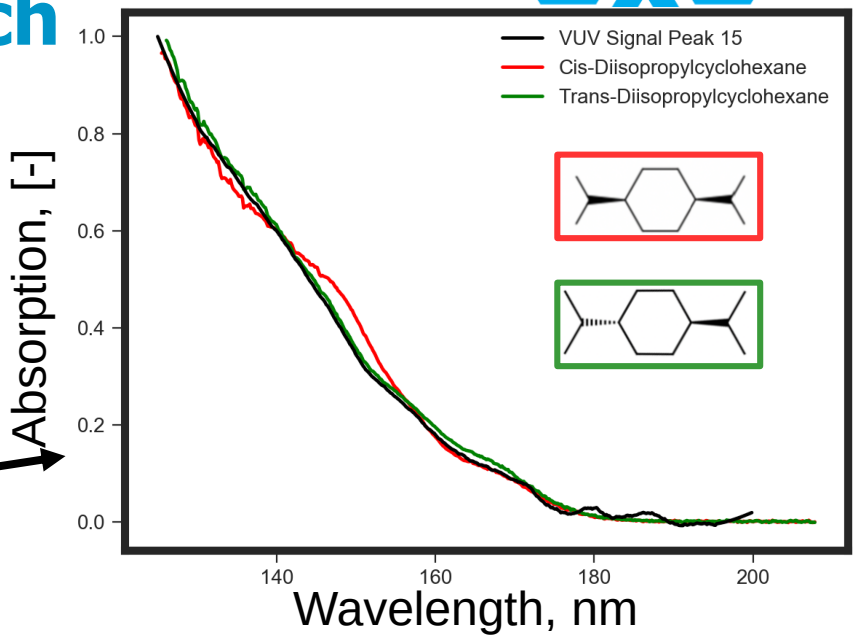


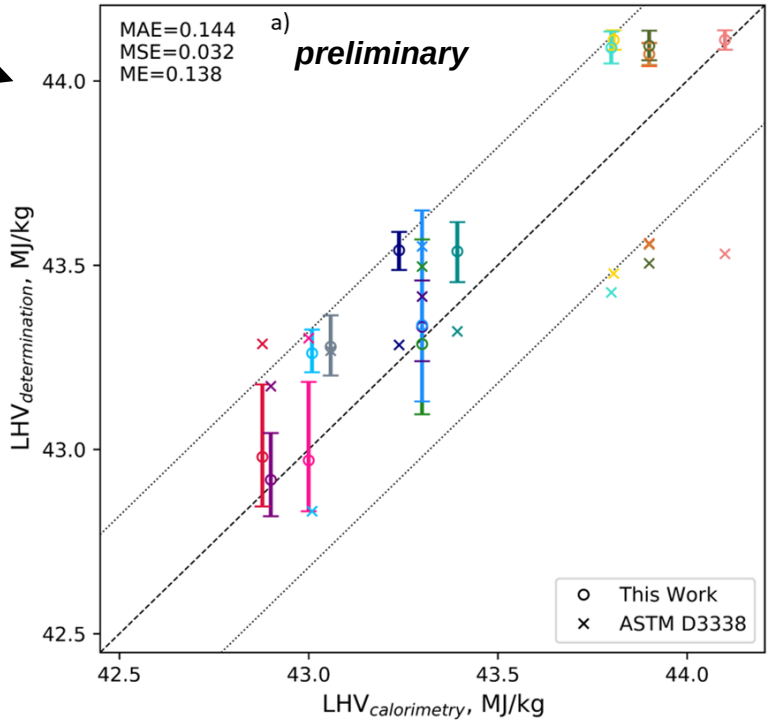




Tier α GCxGC-VUV approach

1. Multidimensional gas chromatography separation
2. Hydrocarbon type quantification
3. Analyte identification or estimation of each hydrocarbon type with vacuum ultraviolet (VUV) spectrum light
4. Property predictions with Monte Carlo uncertainty quantification
   - 3,000+ molecules in the database
   - Uncertainty considered
     1. Uncertainty of property data
     2. Analyte identification (or lack there of)
     3. Blending rules for a given property
     4. Experimental method repeatability
5. Producer feedback with sensitivity analysis on specific hydrocarbons to bring compositions within experience range

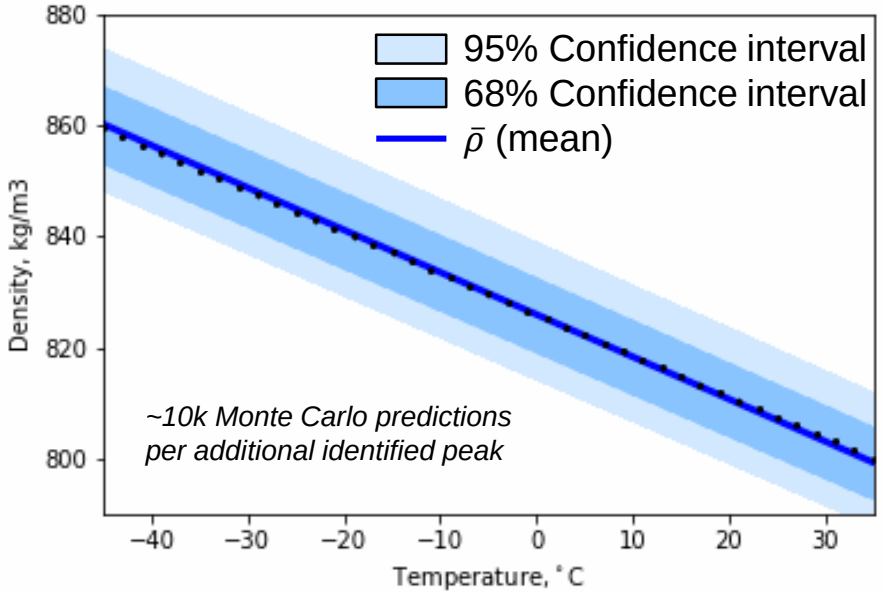




Tier α uncertainty minimization

property uncertainty is reduced with increased identification

- Initial predictions have significant error cancelation
- The density variance withing a hydrocarbon type and carbon number increases with carbon number, *identifying the heaviest molecules is important*
- Not all the carbon is identified, and the remaining carbon imparts uncertainty
- *Blend model uncertainty not included here*



iso-octane