High Performance Fuels

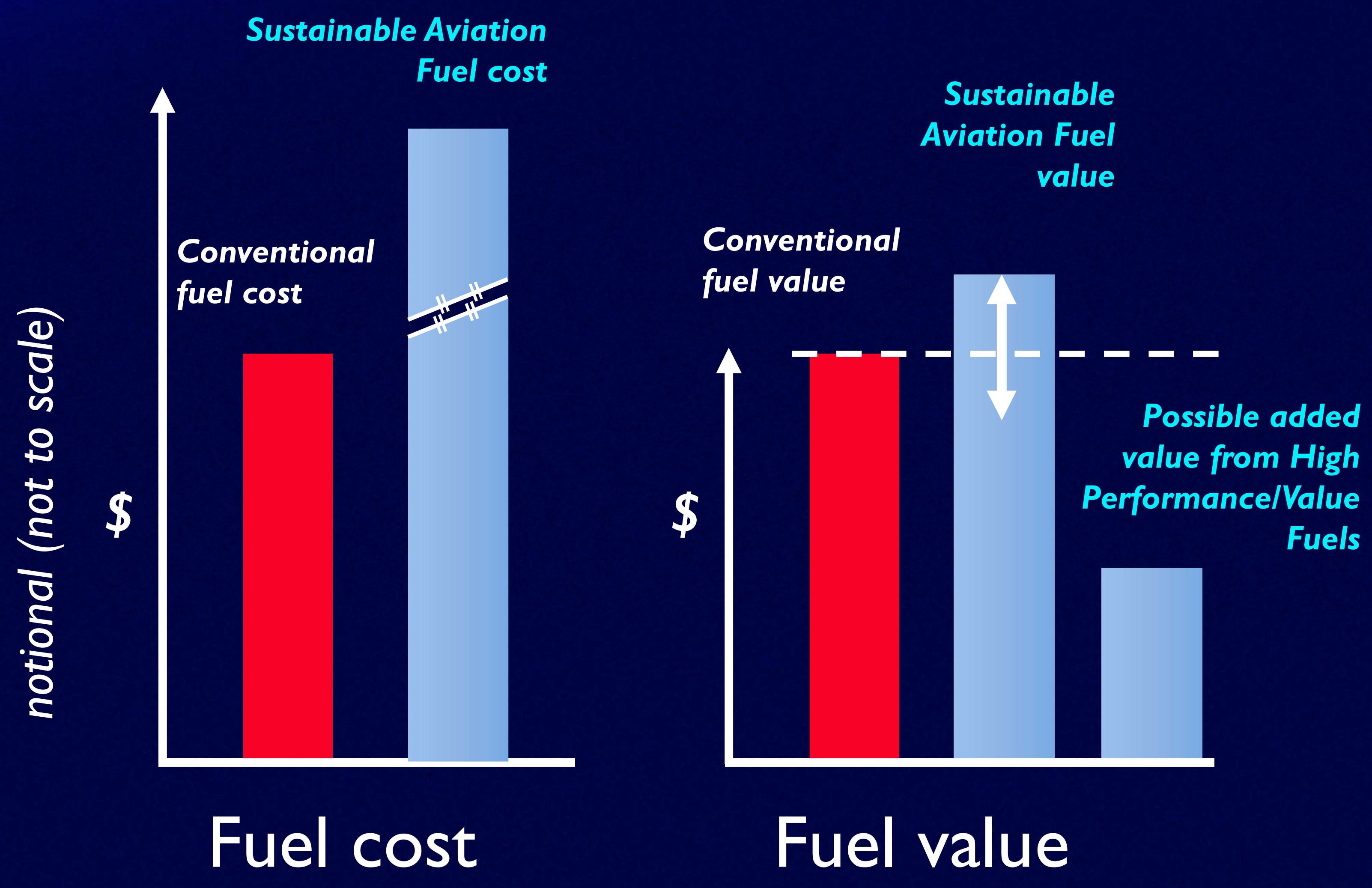
From Molecule Selection to Mission Benefits

Joshua Heyne (jheyne1@udayton.edu) | 26 November 2019

SAF Benefits Beyond CO_2 Reduction | JETSCREEN Workshop | Brussels, Belgium

University *of* Dayton
HEAT Lab

The Problem: *Cost Discrepancy – Value Uncertainty*



Project aims:

- Quantify value of high performance jet fuel (HPF)
- Determine structure-activity relationship for high energy content
- Define molecule classes that can be derived from renewable resources
- Understand cost-benefit relationship

Alternative fuels are more expensive, can we maximize monetized benefits to minimize the cost discrepancy?

"every dollar a barrel increase in oil prices result in $425 million dollars in airline expenses"

Davidson et al., 2016

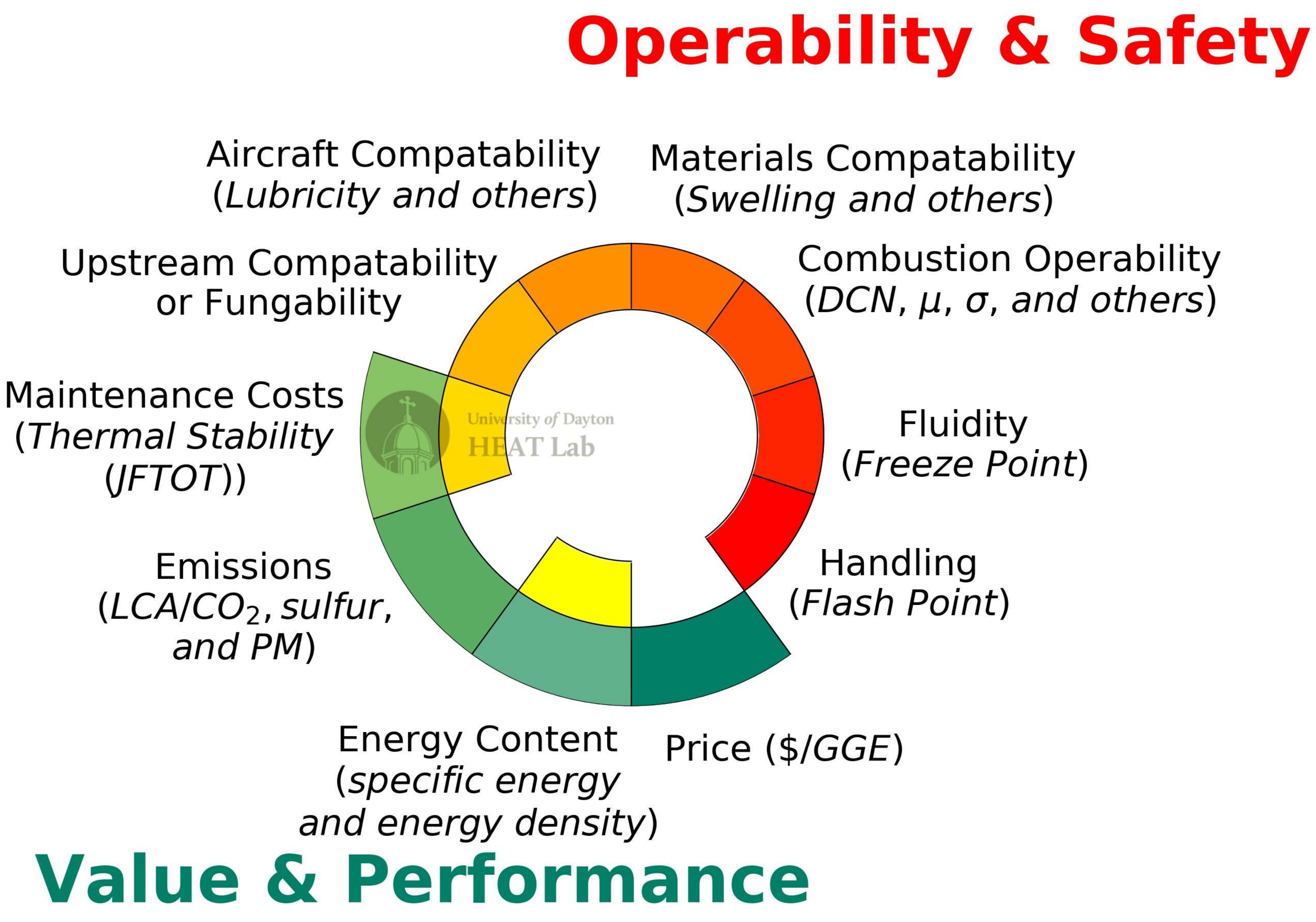
Value Addition

Operability & Safety Maintained

Four Value & Performance Properties to Optimize:

1. Specific Energy, MJ/kg
2. Energy Density, MJ/L
3. Thermal Stability
4. Emissions

Many Operability & Safety properties to maintain.

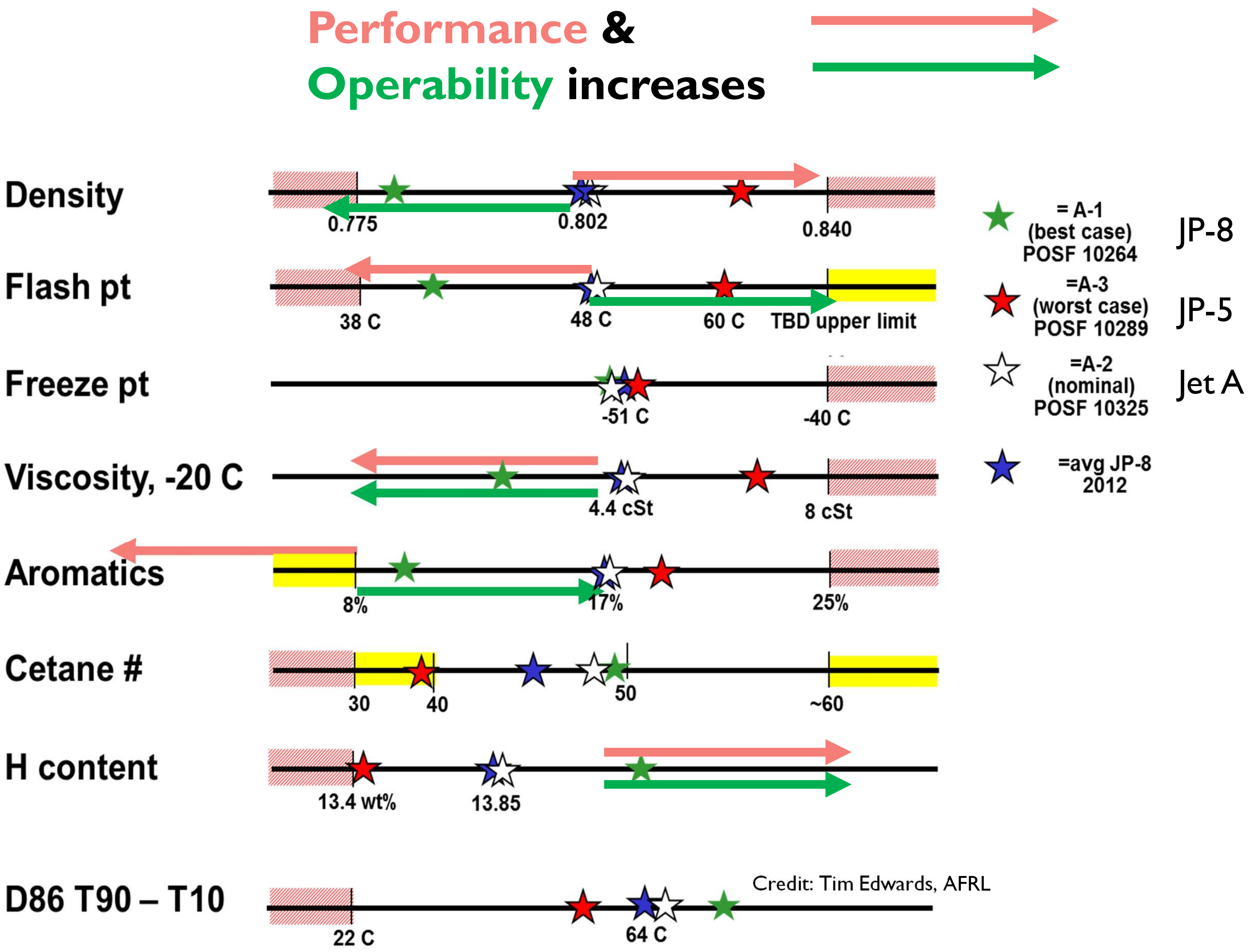


Conventional Fuel:

Operability Properties

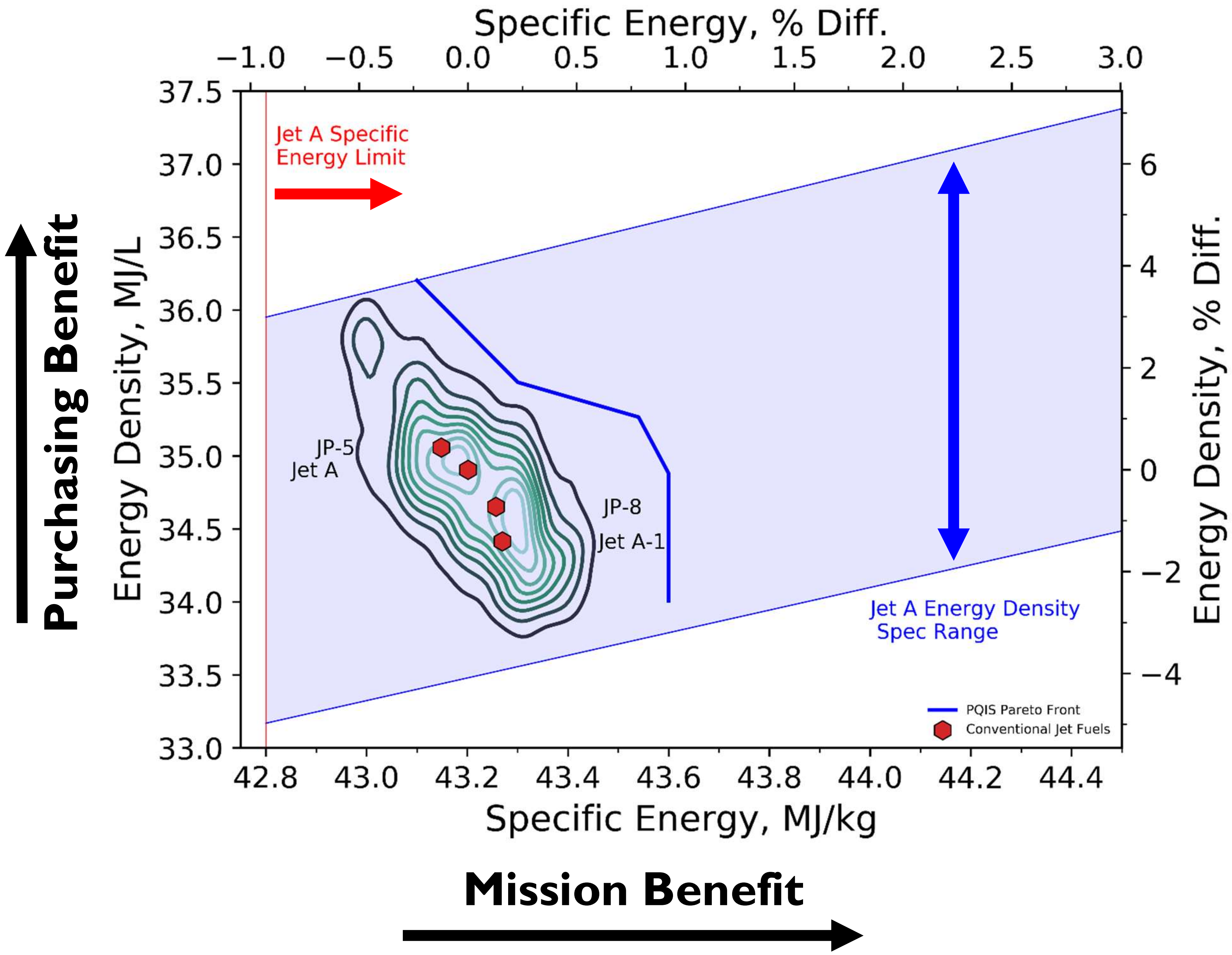
Operability properties enable increased:

- combustion stability with increased propensity to hold a flame and ignite
- safer handling
- lower freeze point



Credit: Tim Edwards, AFRL

Conventional Fuel: *Performance Properties*



Performance Metrics of Interest:

- Specific Energy
- Energy Density

Jet Fuel Specifications:

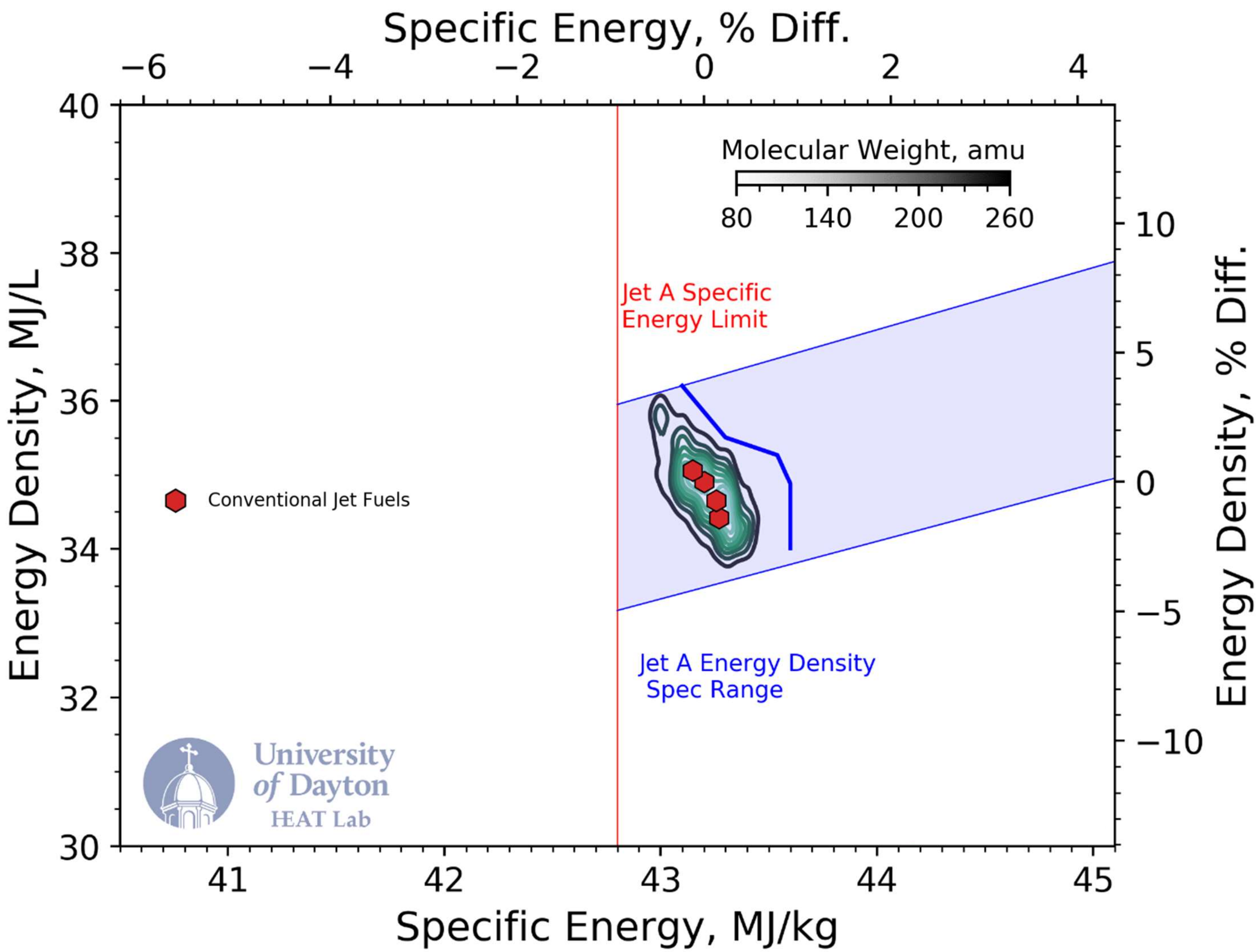
- Specific Energy
  42.8 MJ/kg
- Density
  0.775-0.84 gm/mL

→ Specific Energy x Density = <u>Energy Density Limits</u>

SEED Plot

Conventional Fuels:

- Fuels commonly used for commercial aviation



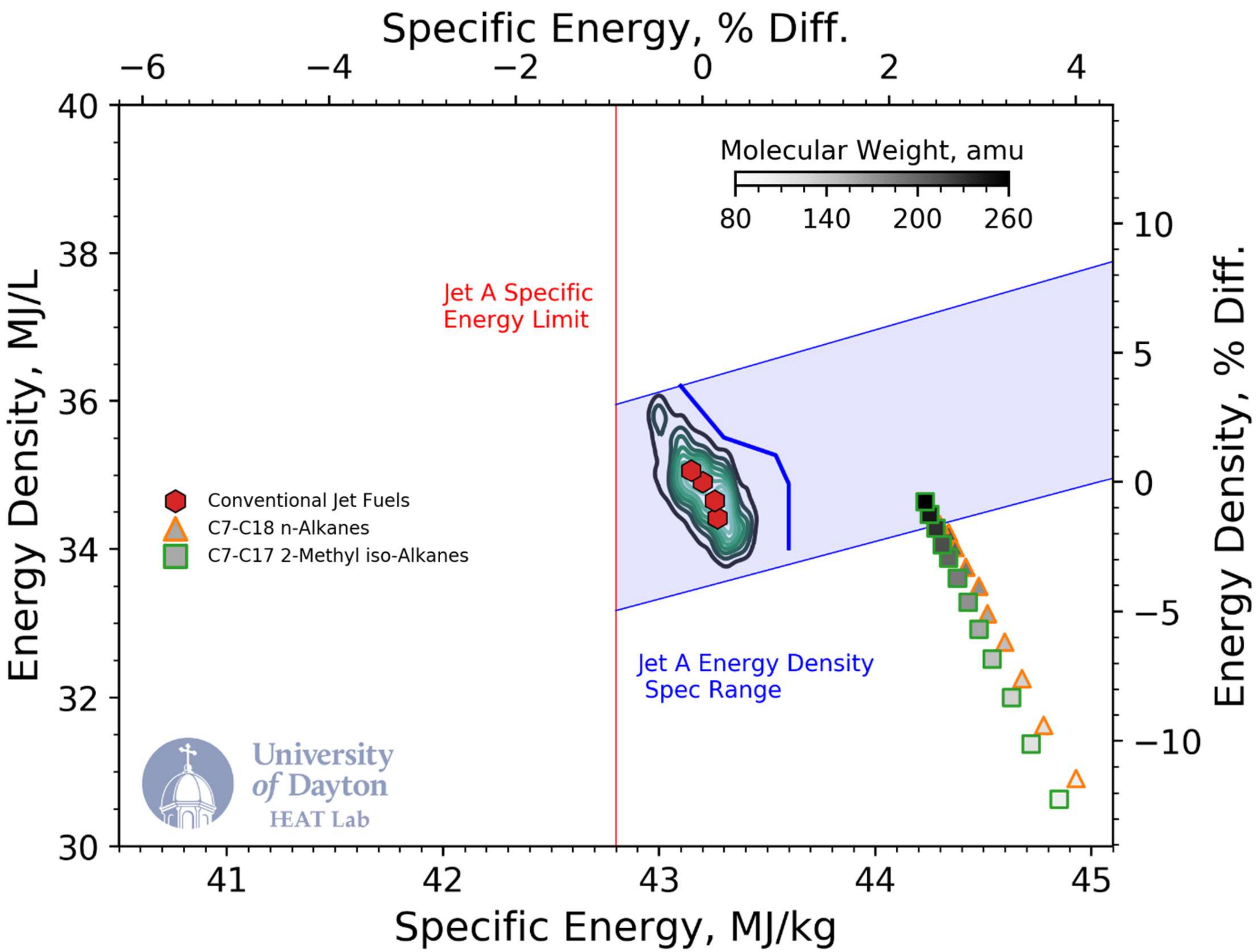
Jet-A is the primary fuel used by US commercial airlines.

SEED Plot

Conventional Fuels:

n- and iso-alkanes:

- High SE, low density
- Majority of AJF consist of n- and iso-alkanes



n- and iso-alkanes have low densities and require blending to be used.

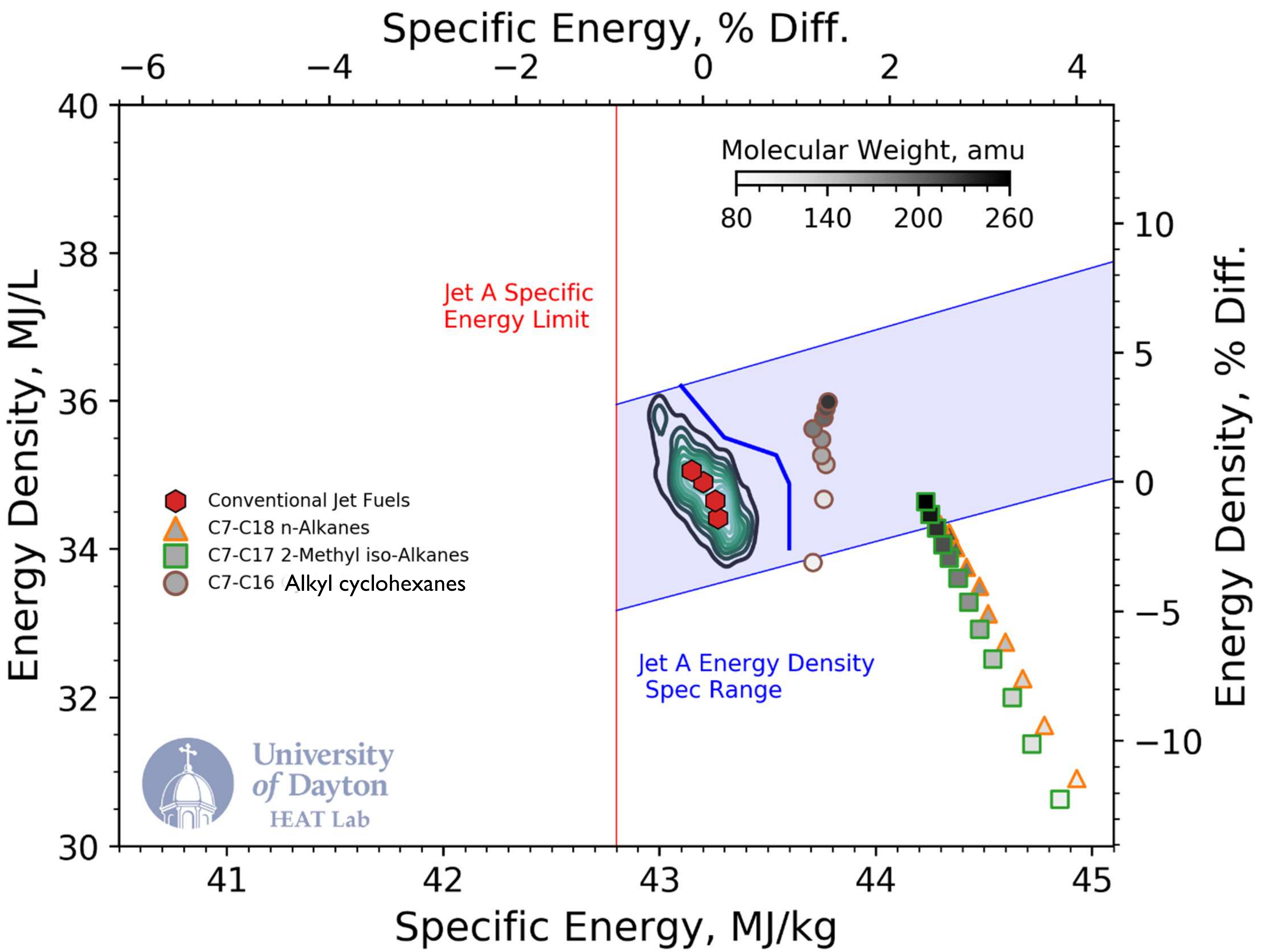
SEED Plot

Conventional Fuels:

n-and iso-alkanes:

Alkyl cyclohexanes:

- High SE and ED
  Potentially drop-in ready
- O-ring swelling properties



Monocycloalkanes are the only molecular group that is potentially drop-in ready.

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SEED Plot

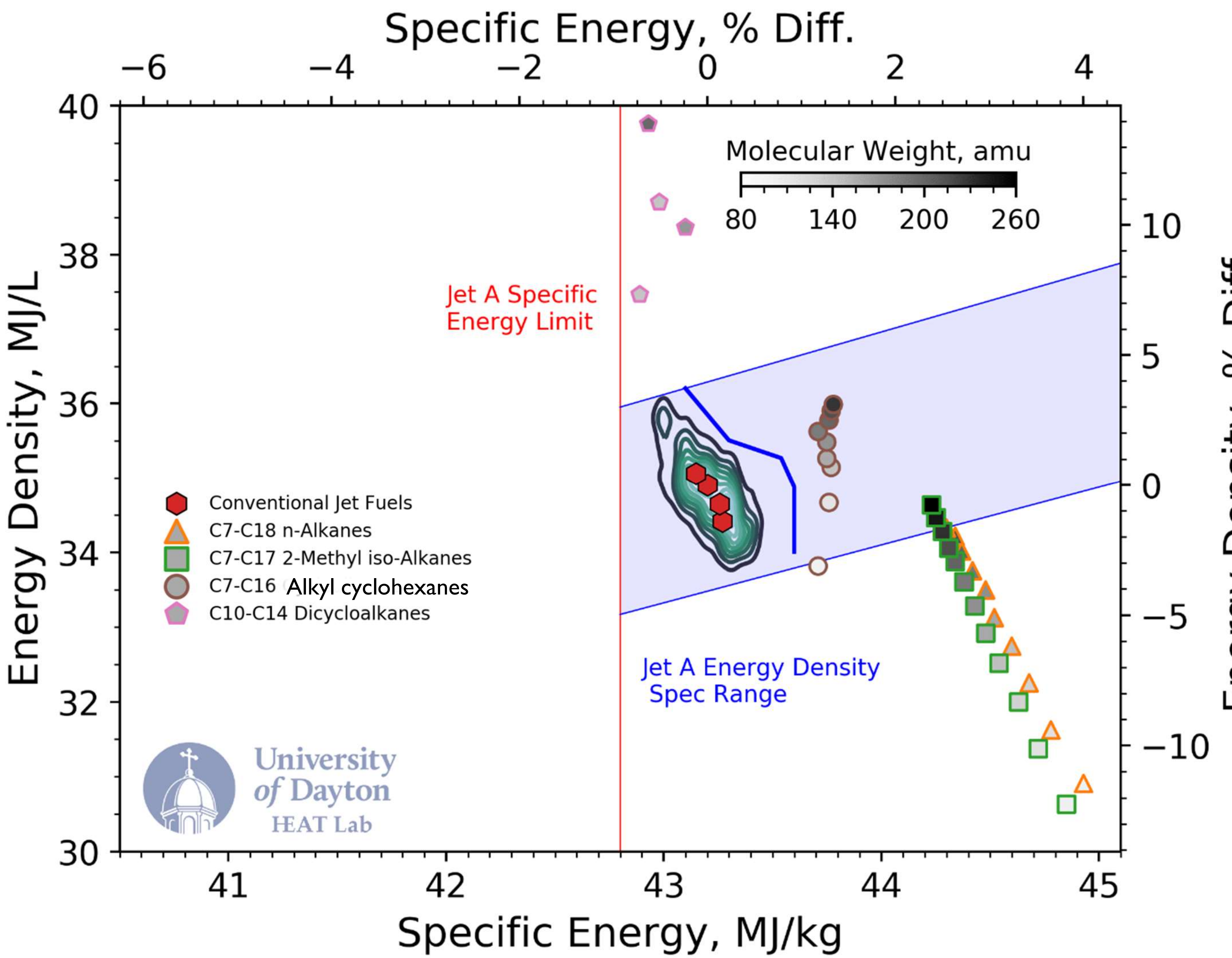
Conventional Fuels:

n- and iso-alkanes:

Alkyl cyclohexanes:

Dicycloalkanes:

- High ED
- O-ring swelling



Blends of 30% cycloalkanes with SPK swell within Jet A range.

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SEED Plot

Conventional Fuels

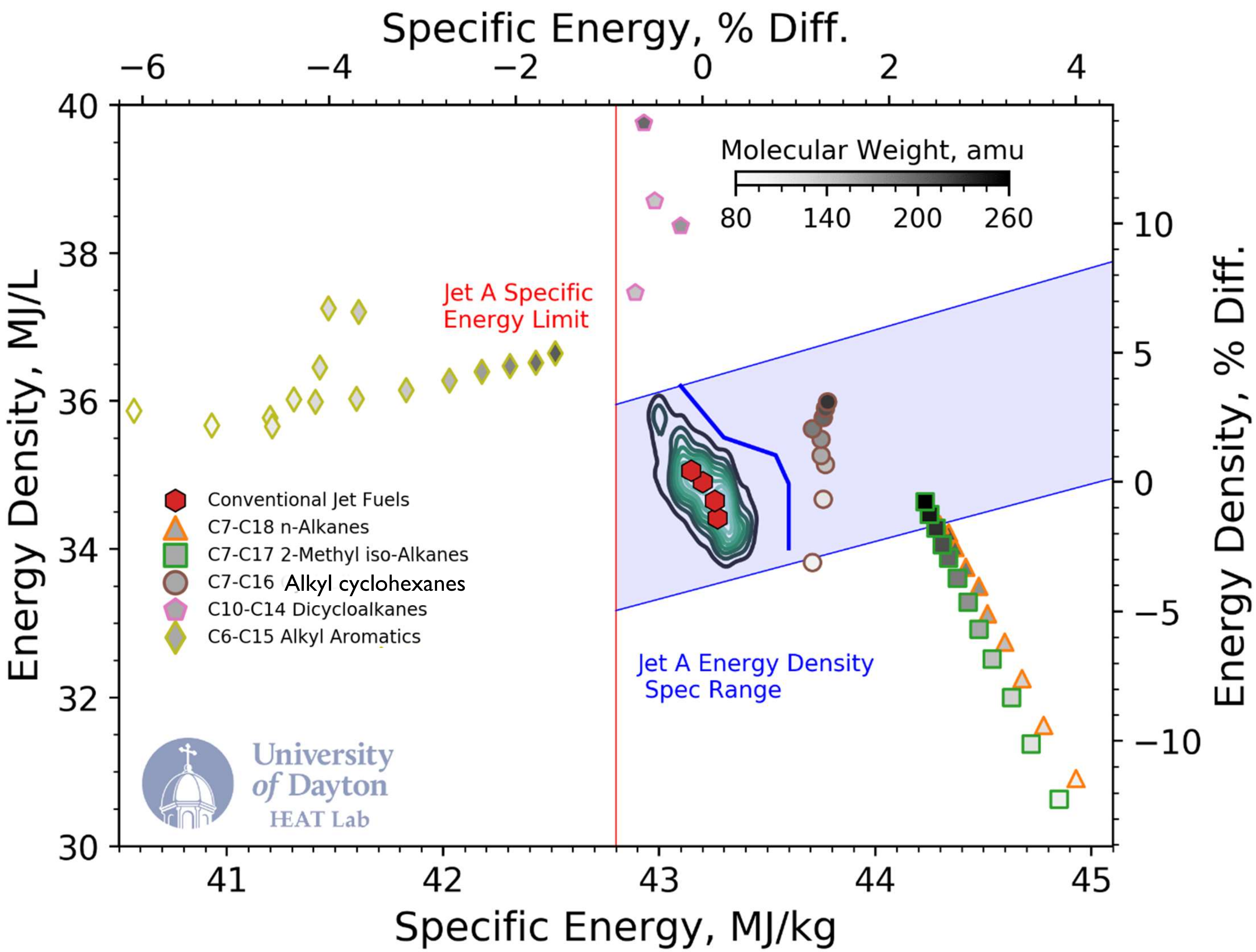
n- and iso-alkanes

Alkyl cyclohexanes:

Dicycloalkanes

Aromatics:

- Low SE
- Produce soot



Aromatics currently have an 8% minimum blending limit.

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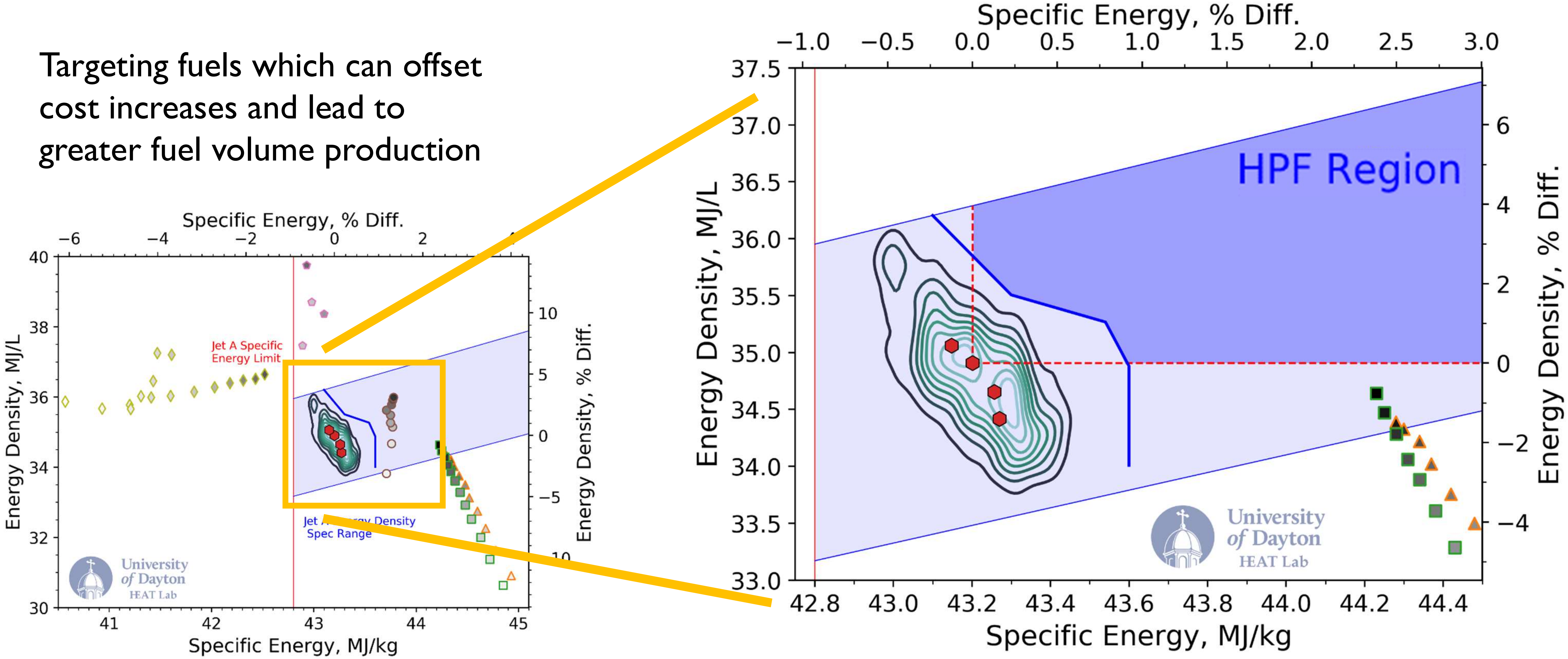
HPF *Energy Density & Specific Energy*

Targeting fuels which can offset cost increases and lead to greater fuel volume production



Four Scenarios Explored

Scenario	Molecule Set	Constraint	Color
1	Optimization of Conventional Fuel Molecules	Aromatics [8-25%v]	
2	Optimization of Conventional Fuel Molecules	Aromatics, relaxed	
3	Scenario 1 + Novel Cycloalkanes	Aromatics [8-25%v]	
4	Scenario 2 + Novel Cycloalkanes	Aromatics, relaxed	

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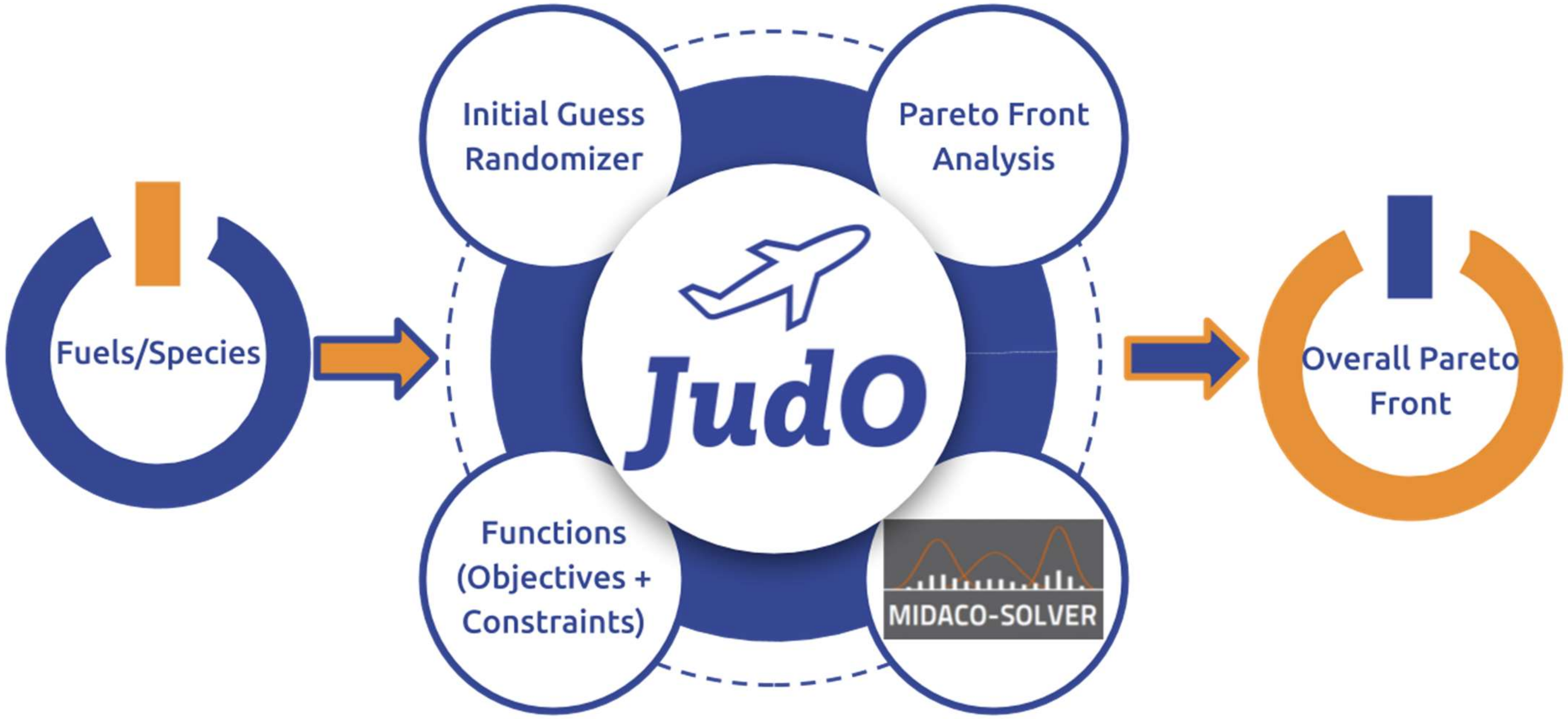
Optimization

Drop-in "on spec" Pareto front for SAFs

- Blending rules were used to create JudO (Jet Fuel Blend Optimizer)
  - Predicted the limitations and estimations for all approved SAFs
- Repoted fuels meet:
  - Flash point,
  - Freeze point,
  - Viscosity,
  - Density,
  - Heat of Combustion, and
  - Distillation curve.

JudO (Jet Fuel Blend Optimizer)



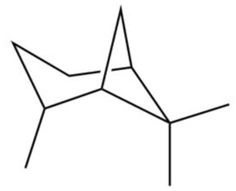
Molecules with known synthetic biopathways:
Novel cycloalkanes and hydrogenated cyclic monoterpenes

Sandia National Laboratories
Anthe George

Understanding structure-property SEED trends to guide molecule selection, *not estimate the property of every molecule possible*

Structural features evaluated

- Cyclic alkane size
- Length & location of methyl appendage on cyclohexanes
- Multicyclic systems,

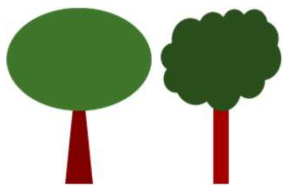
Molecule **{source molecule}** / biosynthesis reference		**formula**	**Density, gm/mL**	**Specific energy, MJ/kg**	**Energy density, MJ/L**
sabinane **{sabinene}** / Cao, et al. 2018, Appl Microbiol Biotechnol (2018)		$C_{10}H_{18}$	0.81	42.8	34.5
p-menthane **{Limonene}** / Jongedijk, et al. 2016, Appl Microbiol Biotechnol (2018)		$C_{10}H_{20}$	0.80	44.3	35.6
pinane **{α-pinene}** / Sarria, et al., ACS Synth. Biol. (2014)		$C_{10}H_{18}$	0.85	44.3	37.8
cis-carane **{3-carene}** / Reiling et al., Biotechnology and Bioengineering (2004)		$C_{10}H_{18}$	0.86	45.0	38.7
Jet-A specification			0.775-0.84	≥42.8	33.2

Scenario 4: *Jet A molecules + Novel Cycloalkanes*

Conventional Fuel Molecules

+

Novel Cycloalkanes



+

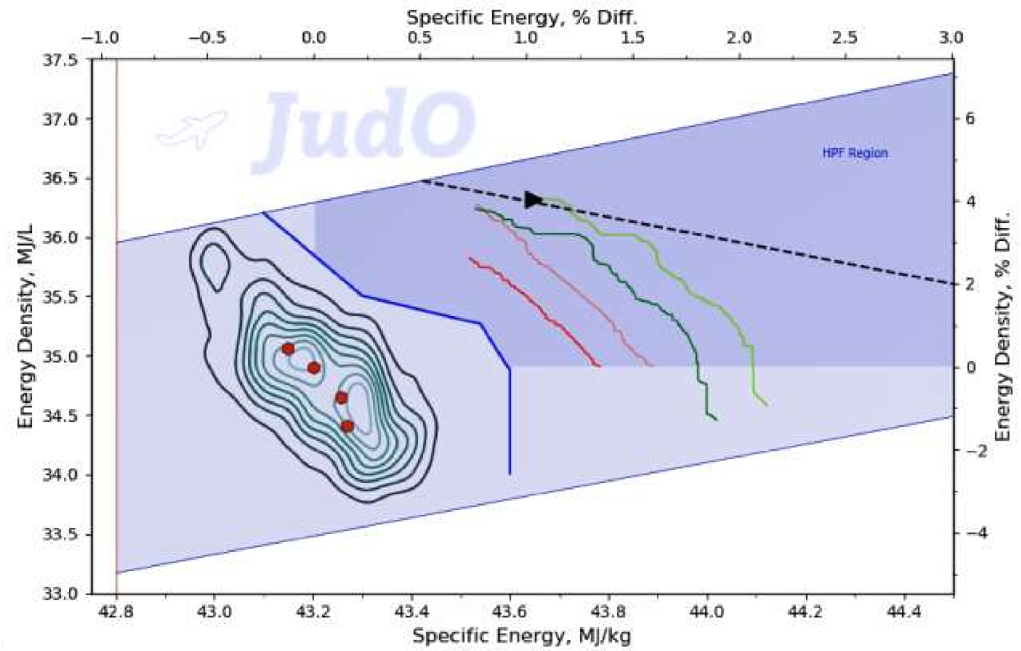
Drop-in Operability Limits

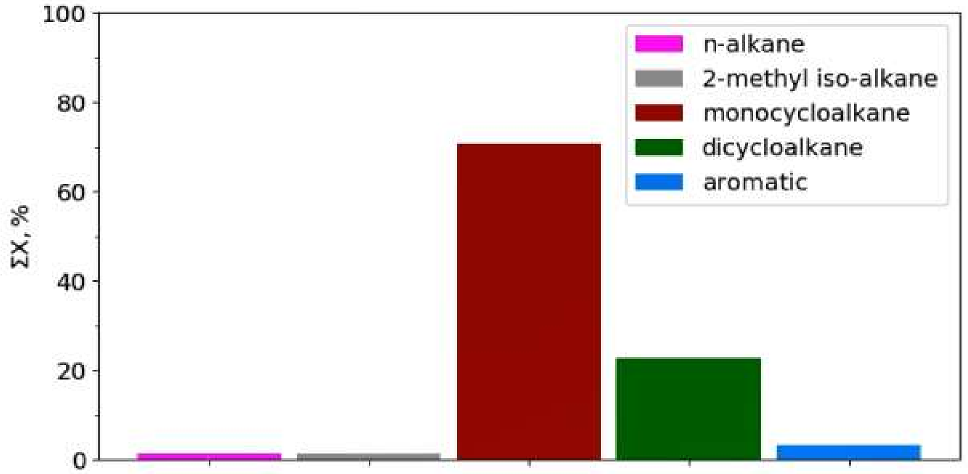
+

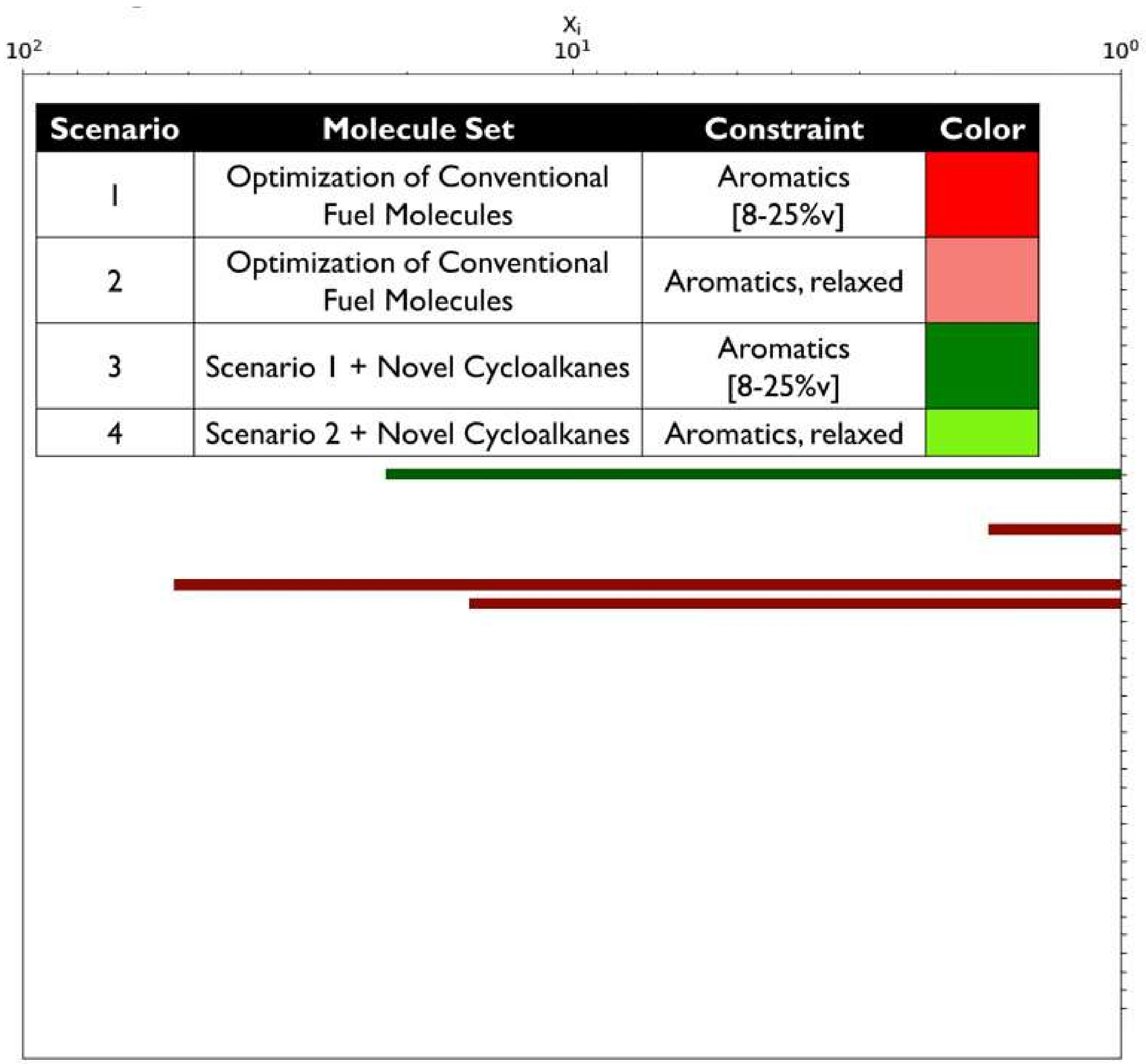
NO Aromatic Constraints

Drop-in Blending & Optimization

JudO







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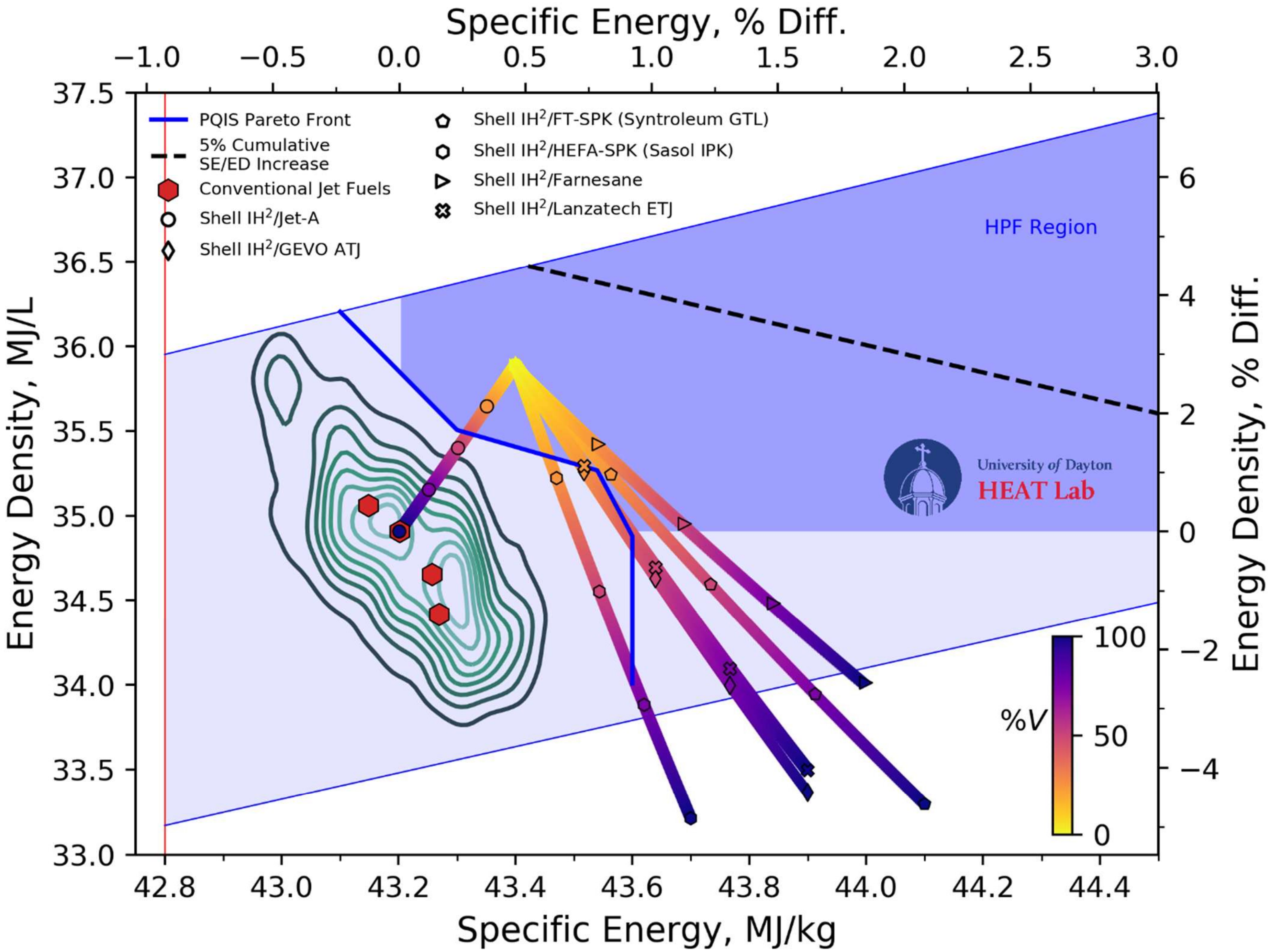
Near Term HPF

Shell IH^2 with Currently Approved Alt. Fuels



Currently approved alt. fuels and one undergoing the process can exceed Jet A performance

Preliminary energy content blend results does not reflect other potential blend/property issues, e.g. viscosity.

High Performance Fuel Usage Scenarios and Results

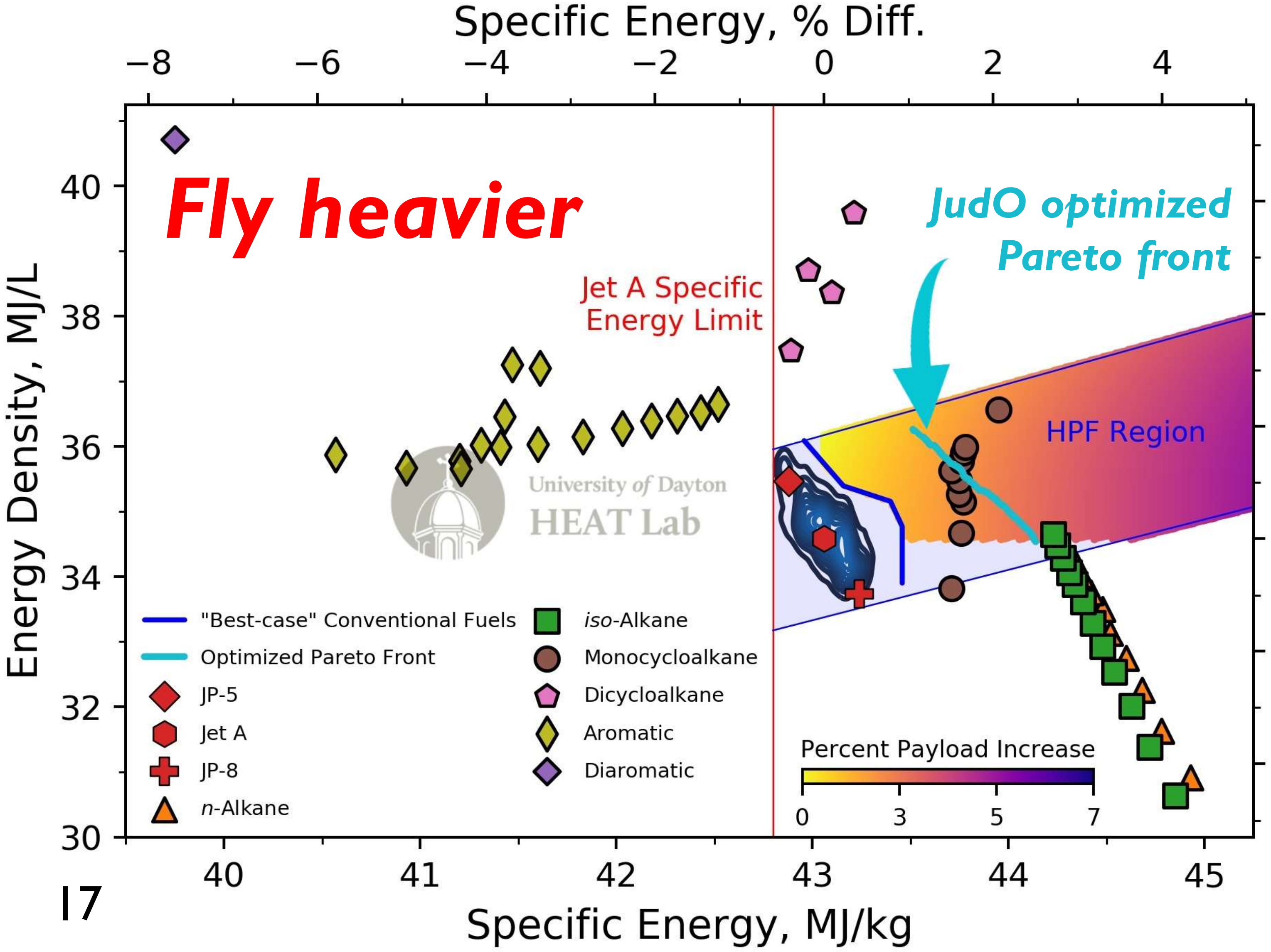
Fly heavier or save fuel

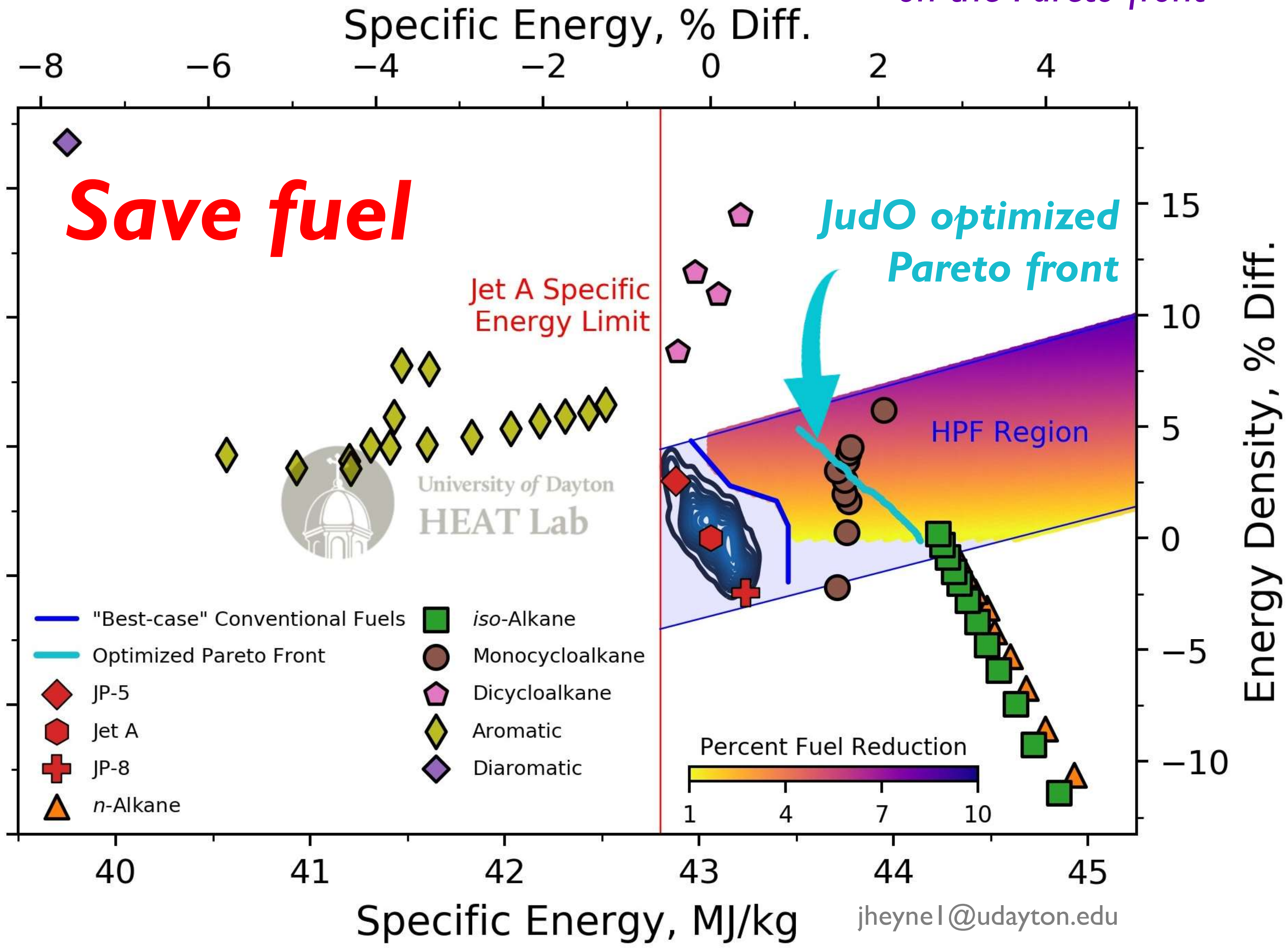
Michele Kirby, Russel Denney

Georgia Tech Aerospace Systems Design Laboratory

	Payload Increase, % / kg	Fuel Burn Reduction, % / L
Min	0.5 / 49	0.0 / 0.5
Median	1.7 / 113	2.0 / 162
Max	2.2 / 147	4.4 / 357

***Payload Increases** and **Fuel Burn Reduction** for a 787-8 as a function energetic properties on the Pareto front*





Potential Performance Budget *Gas Turbine Centric*

Fuel Consumption:

2. Energy Density, MJ/L ~4.4%
3. Thermal Stability
   - Sensible energy recovery 1-3%
   - Other efficiency gains ?%

TOTAL <2-5%

CO_2 Emission:

4. SAF *varies by feedstock and pathway*

Payload:

1. Specific Energy, MJ/kg 2%

Other Emissions:

4. PM via Removal of Aromatics ~90%
4. SO2 via Removal of Sulfur

Metrics are hard to monetize:

- Thermal stability for market transformation is
- Range increases are hard to monetize (vs. payload and fuel savings)

ACKNOWLEDGMENTS

DOE-BETO

Technical Lead: Mark Shmorhun, Zia Haq, *Mohan Gupta

*Now at FAA

QUESTIONS?

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Aircraft Performance Analysis

- **Three different aircraft/engine combinations were modeled using NPSS (Numerical Propulsion System Simulation)[1] and FLOPS (Flight Optimization System)[2]**
- **Given thrust and specific fuel consumption data from NPSS, the mission is flown stage-by-stage using FLOPS**
  - **Allows for the generation of payload-range diagrams**

1. Jones, S.M., "Steady-State Modeling of Gas Turbine Engines Using the Numerical Propulsion System Simulation Code", 2010.
2. McCullers, L.A., "Aircraft Configuration Optimization Including Optimized Flight Profiles", 1984.

Proposed Three Tiered Screening and Approval

Pre-Screening

mLs

Property Predictions & Blend Estimations

- GCxGC,
- IR absorption, and/or
- NMR

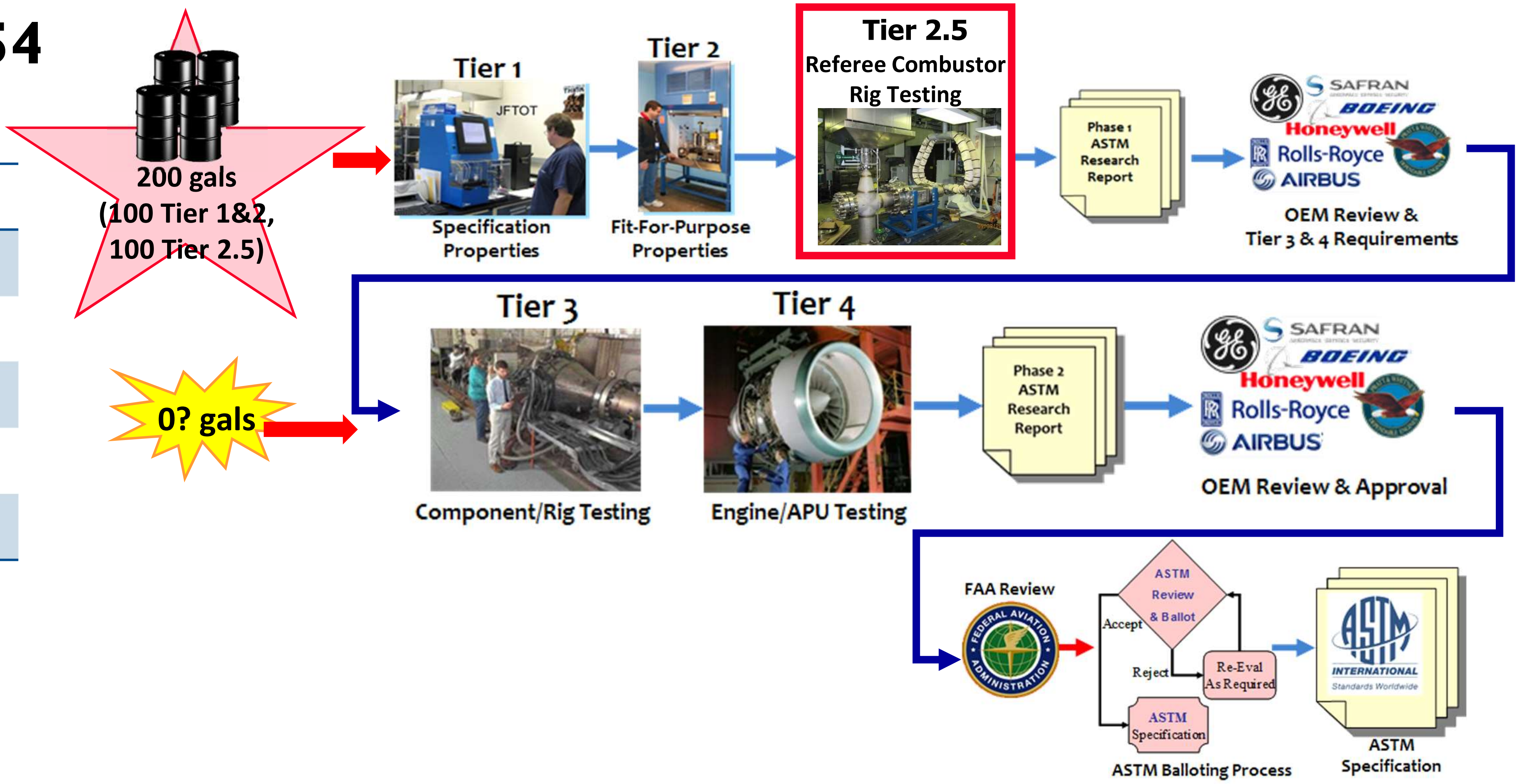
< 1 gal

Critical Properties & Blend Limits

- DCN
- Density
- Distillation Curve
- Viscosity
- Surface Tension

ASTM D4054

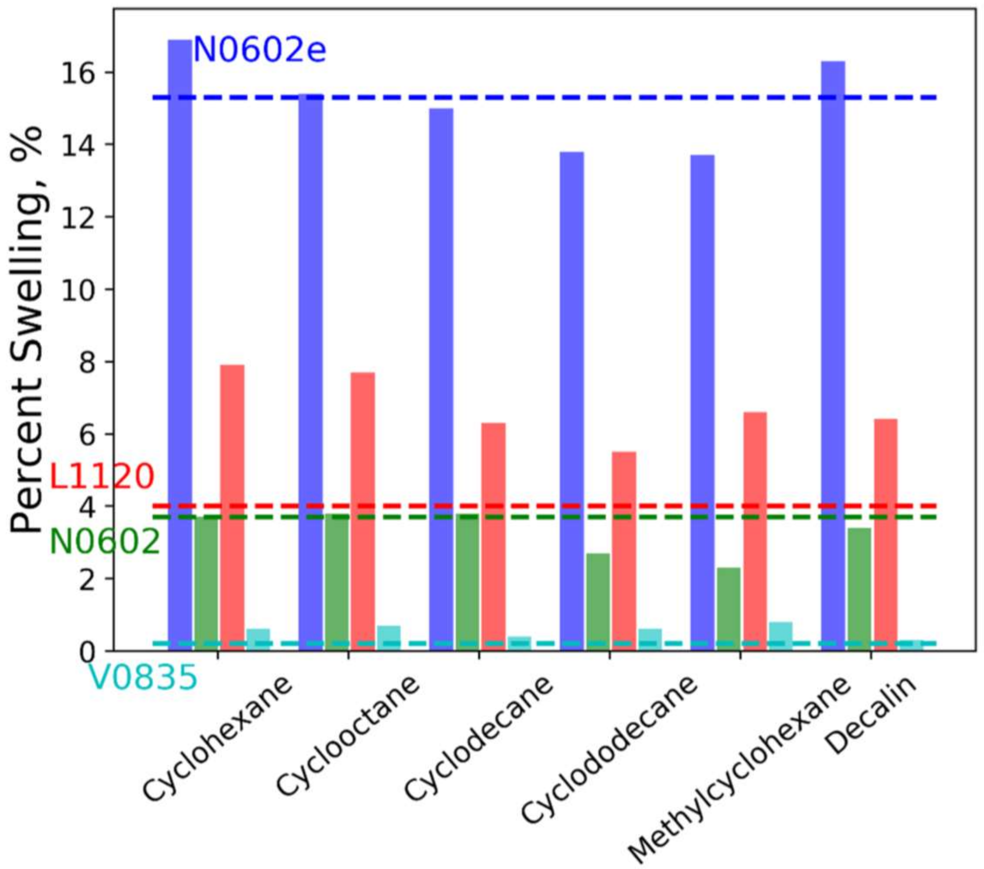
Tier	$\mathcal{O}$(gal)
α	~10^{-4}
'ZERO'	~10^{0}
1 & 2	~10^{2}
2.5	~10^{2}
3 & 4	~10^{3}

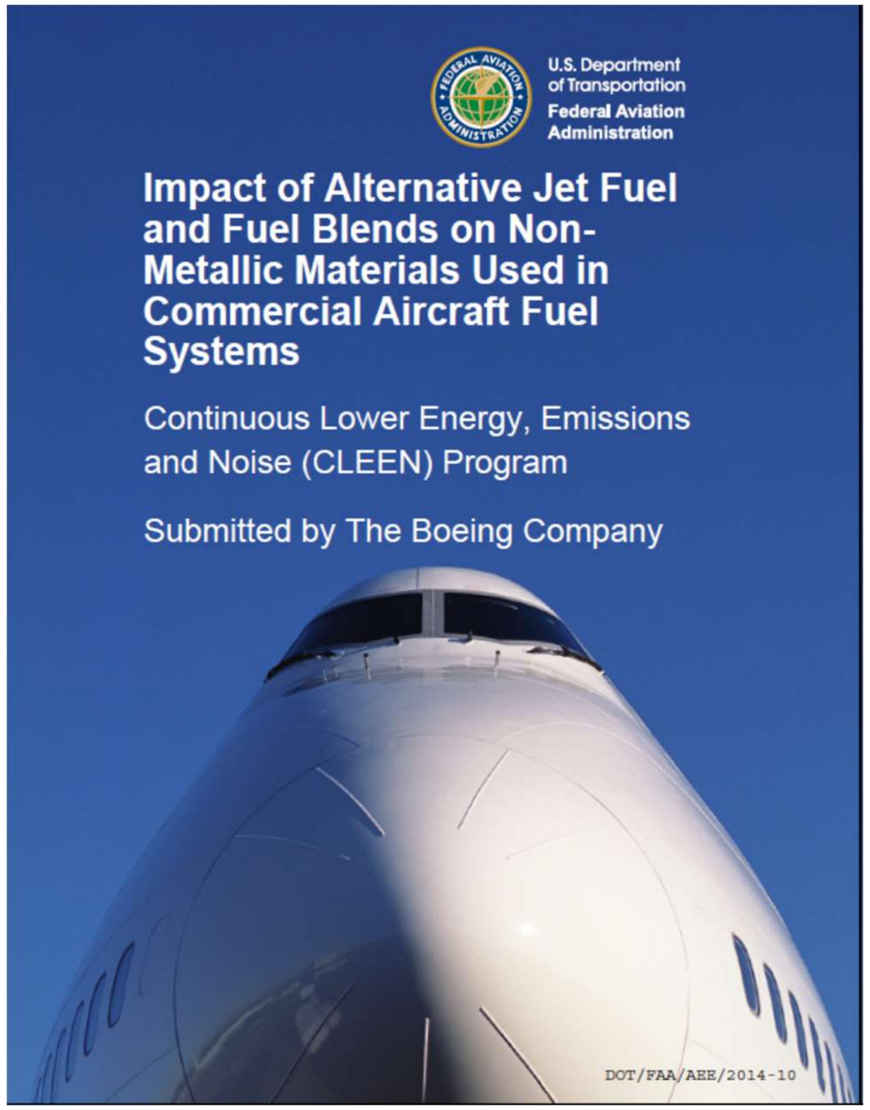


Emissions Reductions and Aromatic Removal

- Aromatics contribute to a significant fraction of emissions.
- Cyclic molecules can potentially replace aromatics for O-ring swelling
- Cycloalkanes in a 30% blend with an IPK swell within the Jet A range
  - ***JudO*** results suggest >50% composition of cycloalkanes

– – –
Lower swelling limit for Jet A





Authored by UDRI (John Graham) & Boeing