Application of big data analytics to fuel property datasets

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This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 723525

Data for the JETSCREEN Objectives

- Development of a f**uel screening and optimization platform/framework** incorporating the distributed design tools and generic experiments
- Provide technical data to explore risks and benefits of **near drop-in fuels**
- Development of advanced and **reliable design tools capturing accurately fuel-related effects** on airframe and aero-engine, delivered with low cost small scale experimental and model-based testing
- All require fuel technical data
- Develop and populate searchable database for:
  - Beyond specification physical and fit for purpose properties of fuels
  - Utilize existing public domain data in addition to outputs of JETSCREEN program
- Collaboration with the University of Illinois – ASCENT Alternative Fuel Test Database Team

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Existing data storage methods…

Issues	**Uncoordinated** fuel data storage systems	• Coordinate fuel data archiving
	Analysis needs time	• Facilitate standardized analysis in common format
	Uninformed fuel processing/logistics systems	• Track fuel supply information
Needs	Increased research **data dissemination**	• Link upstream (feedstock, processing) and downstream (testing, emissions) data
	Fuel blending **system impact**	• Determine critical safety roadmap

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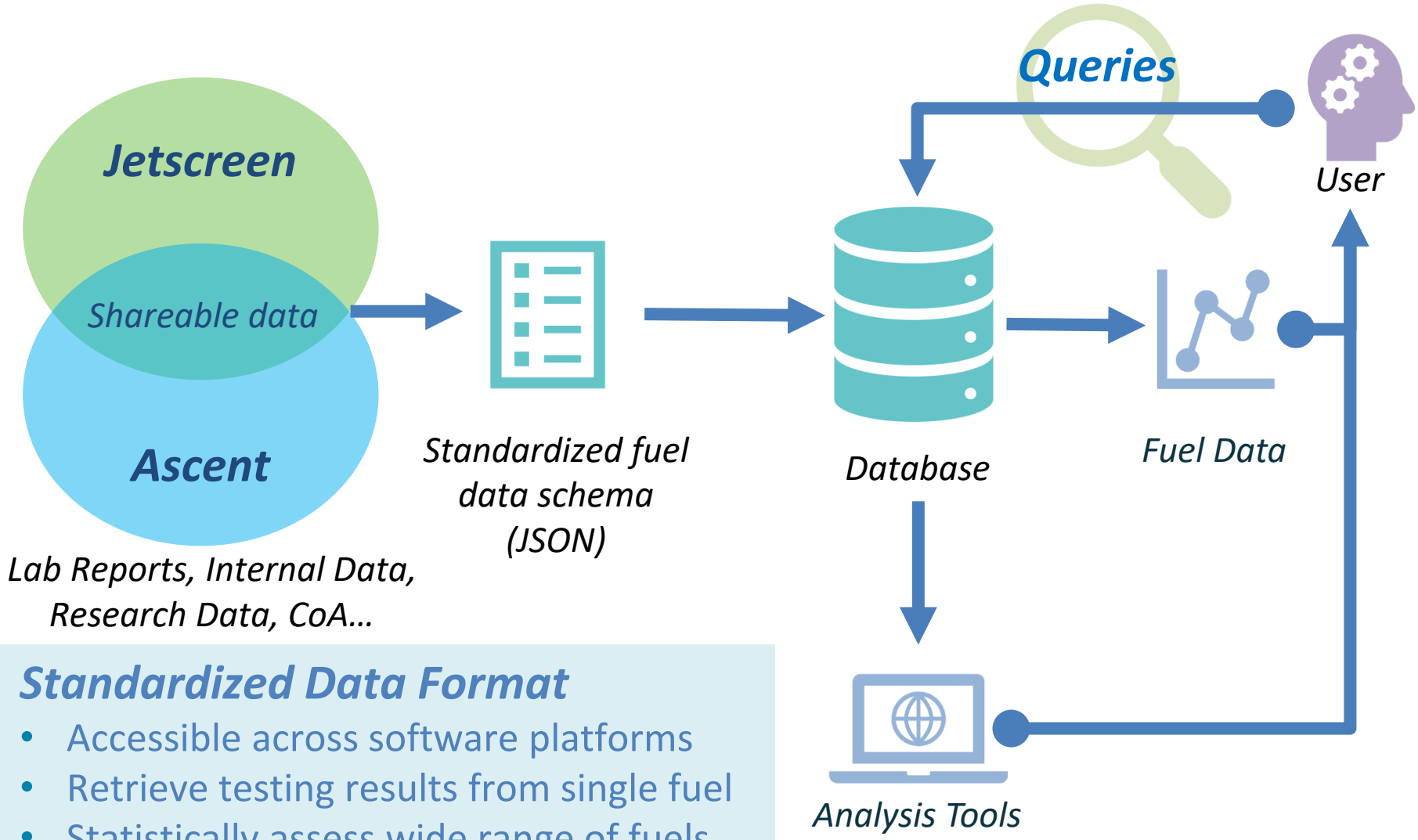
Database

https://github.com/JETSCREEN-h2020/FuelDatabase/wiki/JETSCREEN-Schema-philosophy

JETSCREEN



Standardized Data Format

- Accessible across software platforms
- Retrieve testing results from single fuel
- Statistically assess wide range of fuels

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Unify Disparate Data

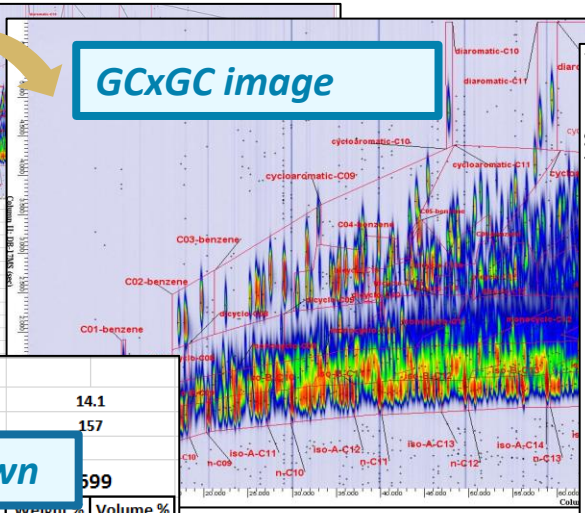
GCxGC Summary

neat injection	Hydrogen content (weight %)	14.1
analyzed: 01-08-14	Average Molecular Wt (g/mole)	157
JP-8		

POSF-5699

	Weight %	Volume %
Aromatics		
Alkylbenzenes		
benzene (C06)	<0.01	<0.01
toluene (C07)	0.08	0.07
C2-benzene (C08)	0.63	0.57
C3-benzene (C09)	3.21	2.91
C4-benzene (C10)	3.91	3.56
C5-benzene (C11)	2.63	2.38
C6-benzene (C12)	1.80	1.64
C7-benzene (C13)	1.08	0.98
C8-benzene (C14)	0.63	0.58
C9-benzene (C15)	0.22	0.20
C10+-benzene (C16+)	0.06	0.06
Total Alkylben	14.25	12.89
Dia...(naphthalenes, Biph..., etc.)		
...atic-C10	0.07	0.06
...atic-C11	.27	0.21
...omatic-C12	.40	0.32
diaromatic-C13	.16	0.13

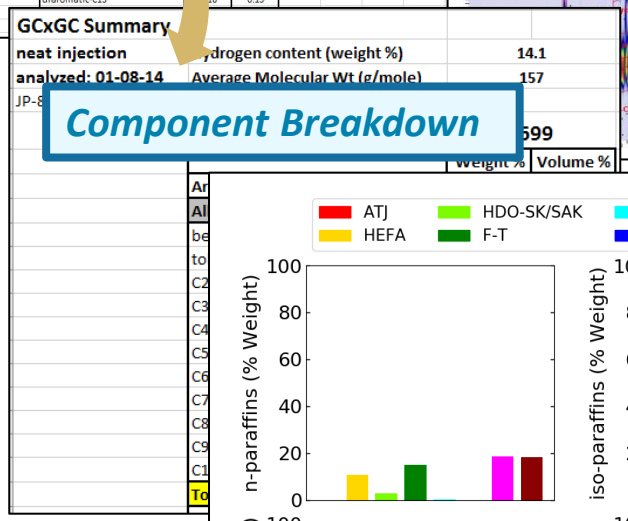
GCxGC image

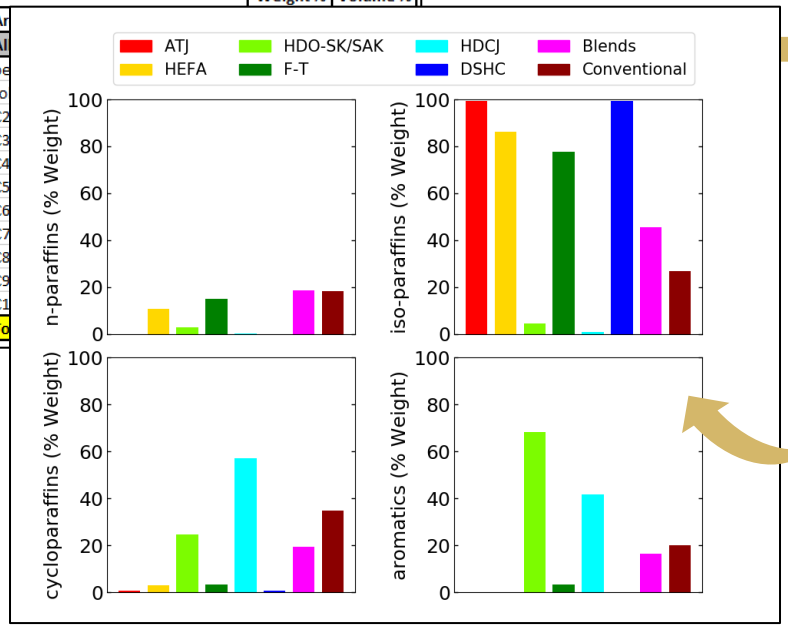


JSON Schema


```
{
    "header":{
        "origin":"NuStar Refining, LLC",
        "description":"New batch of JP-8 for use in T-63 an
S-12, remainder put into drum (13 total).\n\nCRATCAF A-1 \"
testing",
        "tags":[
            "10264",
            "JP-8",
            "NuStar Refining, LLC",
            "combustion \"rules and tools\" program"
        ],
        "fuel_type":"JP-8",
        "name":"10264",
        "date_received":"2013-04-03 00:00:00",
        "quantity":"7161.0 gallon(s)"
    },
    "property":{
        "micro_distillation_residue":[
            {
                "time_stamp":"2016/08/03 15:15:00",
                "unit":"%",
                "maximum_value":1.5,
                "value":1.3,
                "test_method":"D 7345"
            }
        ],
        "density":[
            {
                "temperature_value":"15",
                "maximum_value":0.84,
                "value":0.78,
                "temperature_unit":"C",
                "test_method":"D 4052",
                "time_stamp":"2013/04/16 14:11:00",
                "unit":"kg/L",
                "minimum_value":0.775
            }
        ],
```


Component Breakdown





Enables enhanced fuel comparison capabilities

Enabler for Screening & Safety

Develop screening guides to assess new fuels

- **Accelerate approval** through early-stage pre-screening
- **Assist fuel producers** with access to AJF property data

Coordinate fuel data with global aviation data

- **Track flight & aircraft system issues** with fuel supply data
- Investigate fuel-related system or component failures

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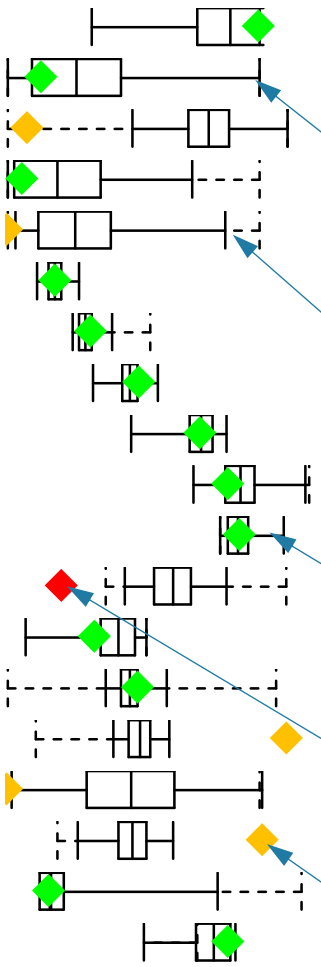
Enhanced fuel screening

Fuel specification	Min	Max	Fuel Sample	Whisker Chart
Colour			30	
Acidity (mg KOH/g)	0	0.015	0.002	
Aromatics IP 156 (%vol)	0	25	1.8	
Sulphur (%mass)	0	0.3	0.018	
Mercaptan (%mass)	0	0.003	0	
IBP (degC)			148.8	
10% (degC)		205	169.8	
50% (degC)			198.7	
90% (degC)			235.1	
FBP (degC)		300	251.9	
Flash point (degC)	38		41.5	
Density @15degC (kg/m3)	775	840	759.6	
Freezing point (degC)		-47	-59	
Viscosity @-20degC (cSt)	0	8	3.885	
Smoke point (mm)	5		50	
Naphthalenes (%vol) if SP > 25mm		3	0	
Specific Energy (MJ/kg)	42.8		44.023	
Existent Gum (mg/100 ml)		7	1	
MSEP	85		99	



A new fuel, some properties within spec, but outside experience:

Solid lines represent distribution of the conventional fuels in the database

Dashed lines represent the limits of the specification

Properties within specification, and within range of fuels already in use

Properties outside of specification

Properties outside of norm, but within specification

Survey data from EI - The Quality of Aviation Fuel Available in the Untied Kingdom Annual Survey 2014

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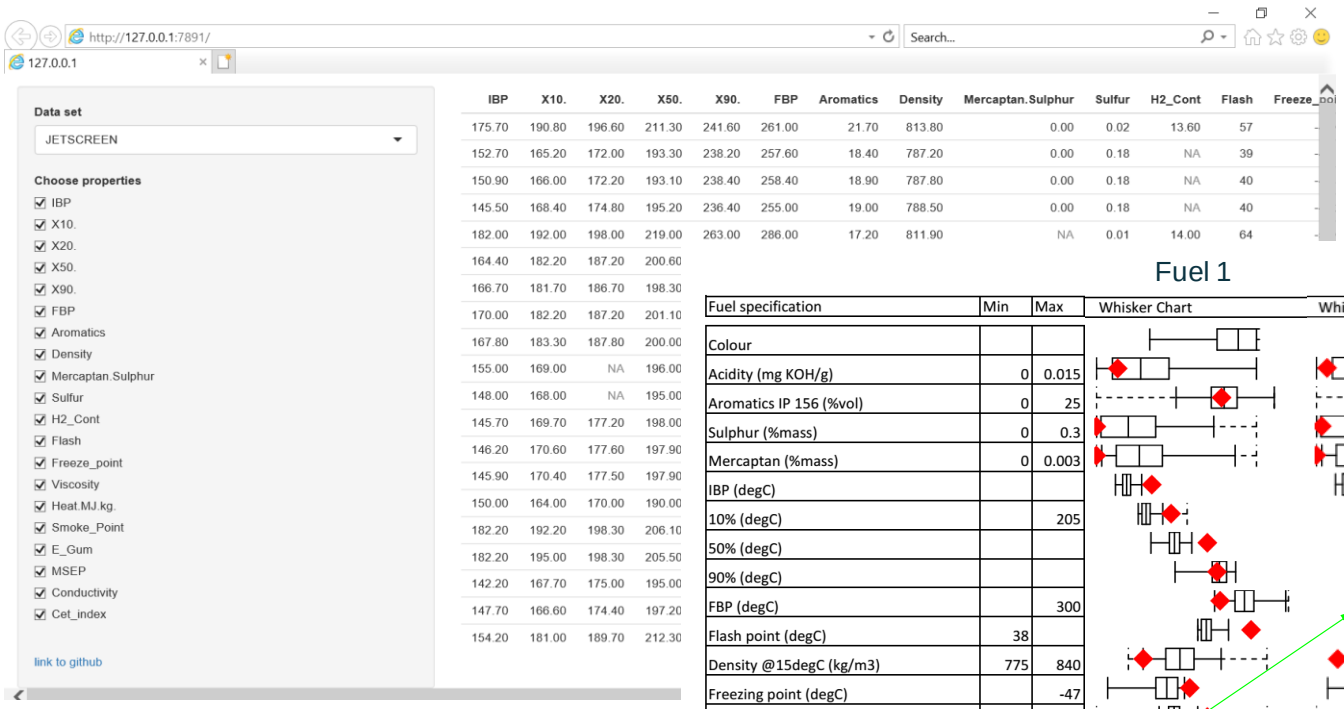
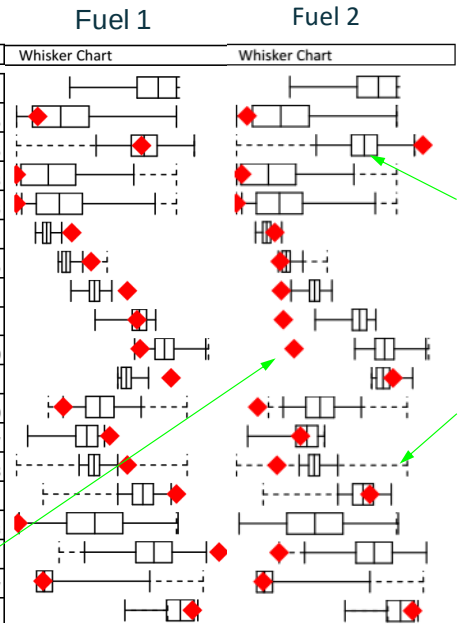
Online Access JETSCREEN data



IBP	X10.	X20.	X50.	X90.	FBP	Aromatics	Density	Mercaptan.Sulphur	Sulfur	H2_Cont	Flash	Freeze_poi
175.70	190.80	196.60	211.30	241.60	261.00	21.70	813.80	0.00	0.02	13.60	57	-
152.70	165.20	172.00	193.30	238.20	257.60	18.40	787.20	0.00	0.18	NA	39	-
150.90	166.00	172.20	193.10	238.40	258.40	18.90	787.80	0.00	0.18	NA	40	-
145.50	168.40	174.80	195.20	236.40	255.00	19.00	788.50	0.00	0.18	NA	40	-
182.00	192.00	198.00	219.00	263.00	286.00	17.20	811.90	NA	0.01	14.00	64	-
164.40	182.20	187.20	200.60									
166.70	181.70	186.70	198.30									
170.00	182.20	187.20	201.10									
167.80	183.30	187.80	200.00									
155.00	169.00	NA	196.00									
148.00	168.00	NA	195.00									
145.70	169.70	177.20	198.00									
146.20	170.60	177.60	197.90									
145.90	170.40	177.50	197.90									
150.00	164.00	170.00	190.00									
182.20	192.20	198.30	206.10									
182.20	195.00	198.30	205.50									
142.20	167.70	175.00	195.00									
147.70	166.60	174.40	197.20									
154.20	181.00	189.70	212.30									

Fuel specification	Min	Max
Colour		
Acidity (mg KOH/g)	0	0.015
Aromatics IP 156 (%vol)	0	25
Sulphur (%mass)	0	0.3
Mercaptan (%mass)	0	0.003
IBP (degC)		
10% (degC)		205
50% (degC)		
90% (degC)		
FBP (degC)		300
Flash point (degC)	38	
Density @15degC (kg/m3)	775	840
Freezing point (degC)		-47
Viscosity @-20degC (cSt)	0	8
Smoke point (mm)	5	
Naphthalenes (%vol) if SP > 25mm		3
Specific Energy (MJ/kg)	42.8	
Existent Gum (mg/100 ml)		7
MSEP	85	



Solid lines represent distribution of the conventional fuels in the UK, 2014

Dashed lines represent the limit of the specification

Inside the specification, but outside of experience

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SimFuel Platform (DLR)

JETSCREEN

SimFuel Platform

simulation and assessment platform for alternative fuels

upload a file with detailed composition for assessment

Drag and Drop or Select Files

Select property or composition:

density

Select the models for property computation

- Discrete Components Model
- Continuous Thermodynamic Model
- Machine Learning

computed value:

812.2162170461379

Select reference fuels for comparison:

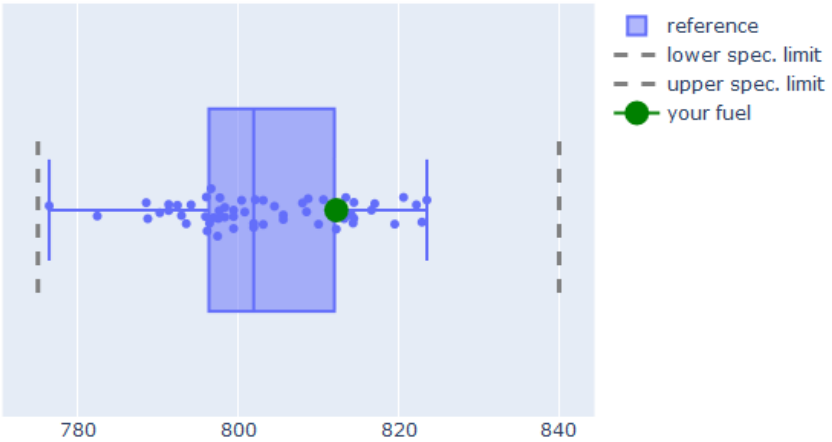
CRC world survey

Load a composition file and press show

SHOW

press calculate to calc droplet properties with SPRAYSIM

CALC.



data:

CRC002_POSF4110_JETA_mass.csv

OEM need for data – preliminary survey results

"[…] Fuel properties are useful as a baseline on which to compare new synthetic fuels that are being developed today. These datasets become our "experience" […]."

"for example, what is the range of distillation profiles for jetA/A1 throughout the world?
What is the range of viscosities at a specific temperature?
Is fluorocarbon compatible with Jet A?
What is the hydrocarbon distribution of a specific fuel?"

"it would be useful to comment on data and see comments from others"

"Data traceability is important for me in that I must have sound reference sources to make decisions that will likely impact the operation, safety and durability of gas turbine engines and the certification of these engines."

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Enabler for Engineering & Science

JETSCREEN

Statistical analysis / feature detection for aircraft-related fuel properties

- Facilitate design of aircraft components impacted by fuel properties

Development & validation of statistical & physical-based models

- Streamline approval, reduce early stage testing
- Enhance development & production of alternative fuels

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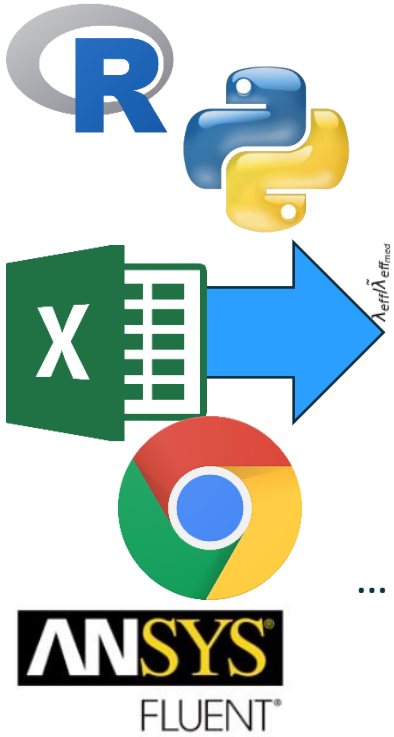
.json files as a flexible storage solution


```
            "test_method": "IP 564",
            "Particles": "less than 30microns",
            "unit": "counts/ml",
            "value": 2.9,
            "iso_code": 9
            }
        ]
    },
    "property": {
        "saybolt_color": [
            {
                "test_method": "D156",
                "unit": "rating",
                "value": 26
            }
        ],
        "acidity_total": [
            {
                "test_method": "D3242",
                "unit": "mg KOH/g",
                "value": 0.004
            }
        ],
        "distillation": [
            {
            "test_method": "D86",
            "volume_evaporated_unit": "%",
            "volume_evaporated_value": 0.0,
            "volume_evaporated_unit": "C",
            "value": 156.6
            },
            {
            "test_method": "D86",
```


Can be read by multiple software using conversion / interpretation script



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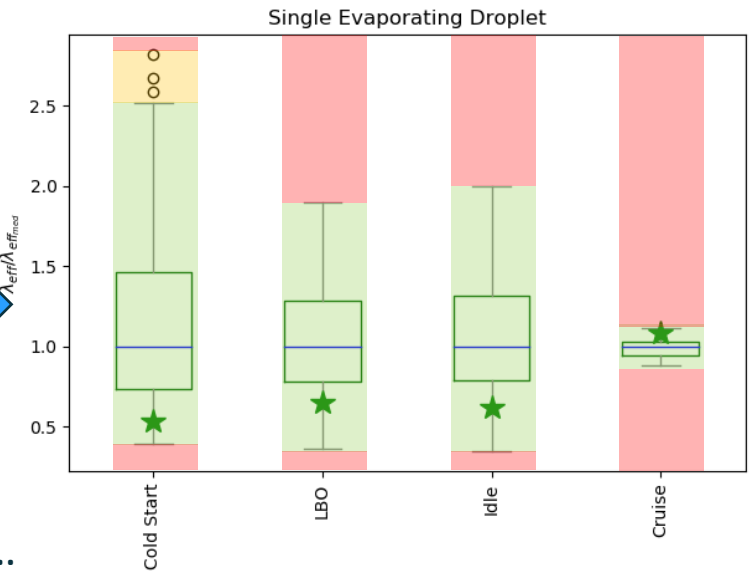

To create tailored, reproducible output

Engine operational conditions

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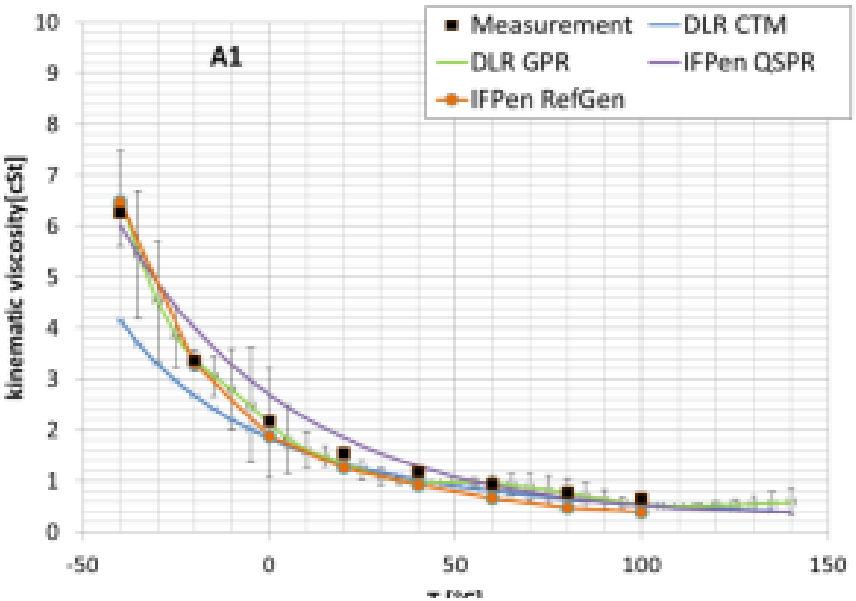
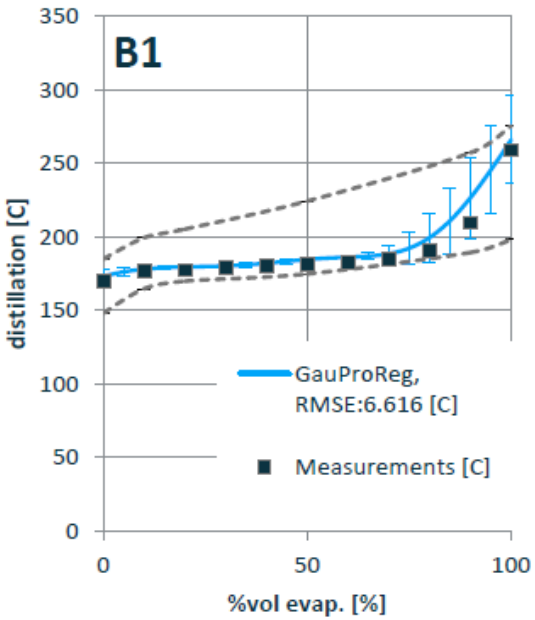
Chemistry – Property Analysis

- Building high fidelity models capable of predicting properties for given hydrocarbon “recipe”
  - Thermodynamic theory
  - Machine Learning
- Construction of lower fidelity models
  - Using experimental results from JETSCREEN fuels
- Providing datasets for the design of fuel flexible components





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agreement No 723525

Enabler for System Operations

JETSCREEN

Track properties of fuels in use: processing, supply chain, end use

- Improve quality control in fuel production & supply
- Connect blend and flight data

Increase data access for airports & airlines

- Demonstrate safe usage of AJFs with detailed supply info
- Build trust between producers, suppliers, & consumers

Expand operational data compilation & dissemination

- Increase system optimization across industry

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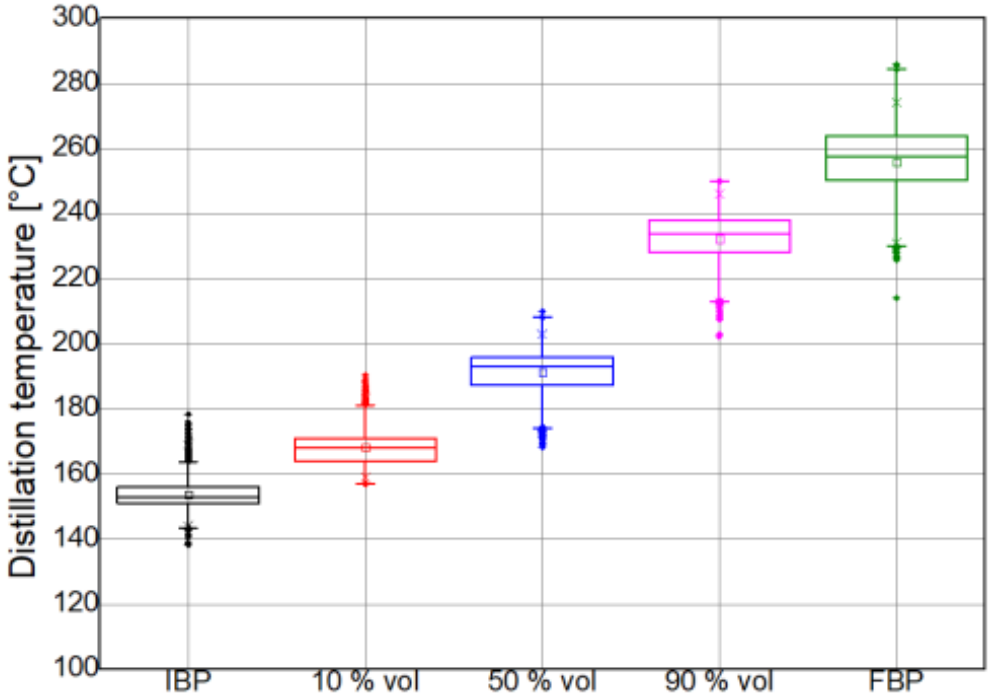
Enabler for Systems Operations

- New direction for JETSCREEN fuels data, already well advanced through the ASCENT programme.
- Avoid using lowest quality or average fuel properties for design purposes
- Can we get benefits from moving the specification away from the lowest common denominator fuels?



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Other datasets / cross over

- May include CORSIA relevant emissions data
  - CORSIA CERT model doesn't have fuel type specification – however clearly impacts overall emission predictions
  - Tracking fuels within the system
  - Methods for receiving / storing data need to be developed
- May Include fuel production information (where publically available), LCA etc.
- We expect non-CO2 impacts to become increasingly important
  - Storage and information system already in place
- Survey to get your perspectives….
  - Report results at CRC (May 2020)

Survey

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Summary

- Developed approach and schema to prepare universal analysis tools for existing fuels data, will in part become publicly available through the JETSCREEN programme.
- Development of further predictive capability using fundamental models
- Contribute to accelerating screening process
- Provide the starting toolset required to optimise the fuel system and engines for a future of increasingly synthetic fuels

Schema

Survey

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JETSCREEN

JETSCREEN

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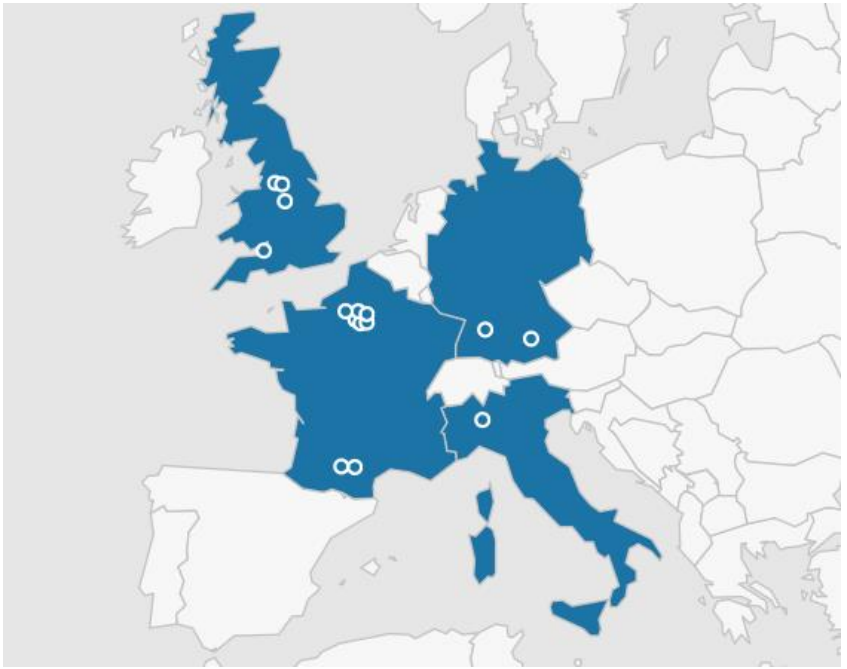

A project gathering **15 partners** from **5 European countries:**

DLR Deutsches Zentrum für Luft- und Raumfahrt German Aerospace Center

AIRBUS

ZODIAC AEROSPACE

SAFRAN

The University Of Sheffield.

ARTTIC INTERNATIONAL MANAGEMENT SERVICES

CERFACS

MTU Aero Engines

Manchester Metropolitan University

POLITECNICO MILANO 1863

Rolls-Royce

ifp Energies nouvelles

ONERA THE FRENCH AEROSPACE LAB

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Challenge to current approach

- High Costs of high standards
  - Credibility gap?
- Conventional Fuels are the lowest common denominator, whilst standard is so high for synthetic products
- Benefits beyond CO2
- Could / Should be included in assessment to create financial incentive for adoption

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