Comparison of Derived Cetane Number and Indicated Cetane Number for Jet Fuels and Correlation with Lean Blowout

Jon Luecke[1], Ian Mylrea,[2] Josh Heyne,[3] and Bob McCormick[1]

[1]National Renewable Energy Laboratory

[2]Stanhope-Seta

[3]Washington State University

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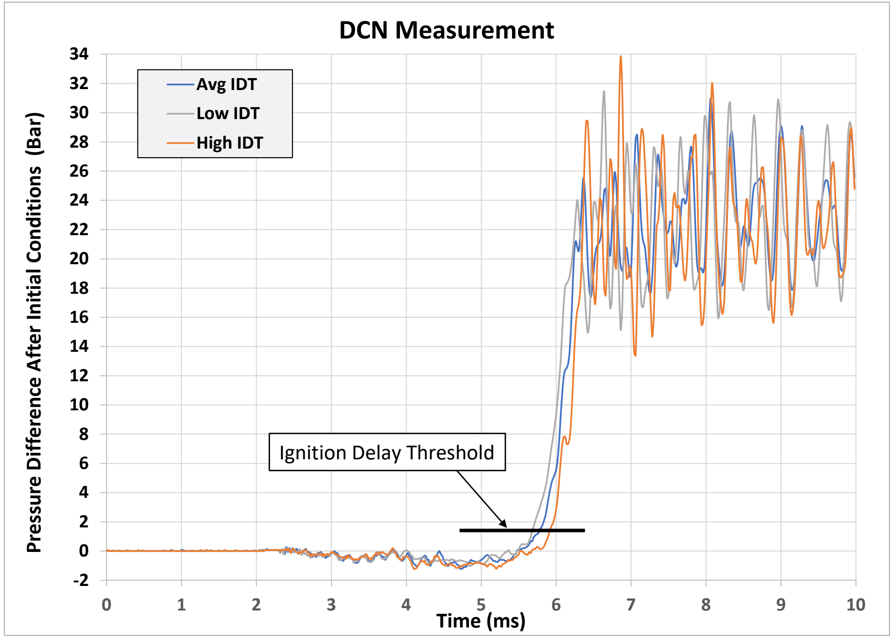
Introduction

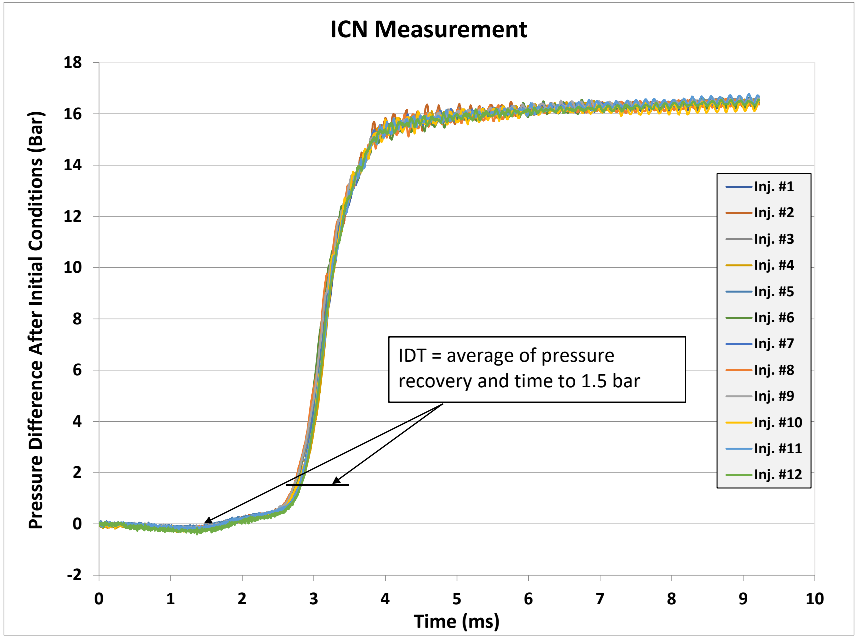
- DCN (derived cetane number) is inversely correlated under some conditions to Ø for lean blowout
  - Range of 35 to 60 specified in ASTM D4054 guidelines (Table A4.1)
  - DCN is a correlative method for measuring cetane number using a constant volume chamber (ASTM D6890)
  - 21.4 bar, 545°C start of injection conditions
- *Objective: Demonstrate equivalence of DCN (ASTM D6890) and ICN (ASTM D8183) for measuring reactivity of jet fuels*
  - ICN is indicated cetane number – also measured in a constant volume chamber
  - 17.5 bar, 580°C start of injection conditions
- Motivated by advantages of ICN for low technology readiness level biofuels research:
  - Only requires 40 mL vs 60 to 100 mL for DCN (key advantage for USDOE)
    - Even 25 mL can be used by modifying the method (appropriate for screening very early-stage samples)
  - Prototype fuels can cost thousands of dollars or more per mL to produce

Ignition Delay in Constant Volume Combustion Chambers

- DCN and ICN are based on ignition delay in constant volume combustion chambers
- Chamber initially filled with air at specified T and P
- Fuel is injected at time=0
- High speed pressure transducer monitors pressure increase as combustion starts
- Based on an experiment specific definition of ignition delay, the ignition delay time is extracted from the pressure vs time data
- Ignition delay is correlated with cetane number
  - Comparing results for fuels in CVCC and Cooperative Fuels Research (CFR) engine (for DCN), *or*
  - Comparing to a calibration curve based on primary reference fuels for CN measurement (for ICN)
    - CN=100 defined by n-hexadecane
    - CN=0 defined by 1-methylnaphthalene
    - Mixture CN defined by vol% n-hexadecane

Data Comparisons for DCN/ICN Conditions: 50% HEFA-SPK in NJFCP A-2

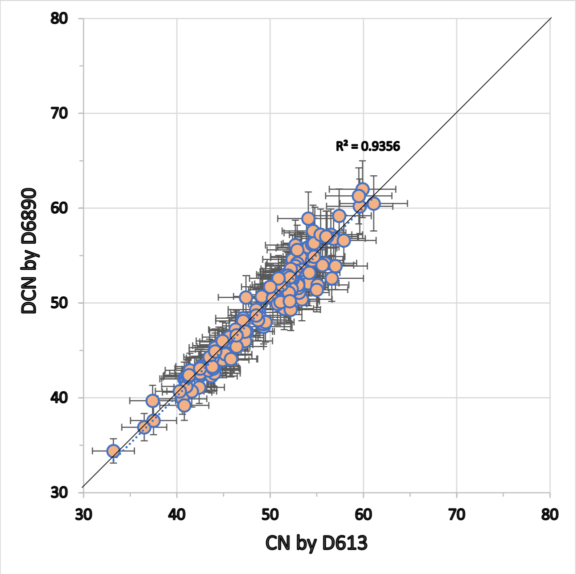




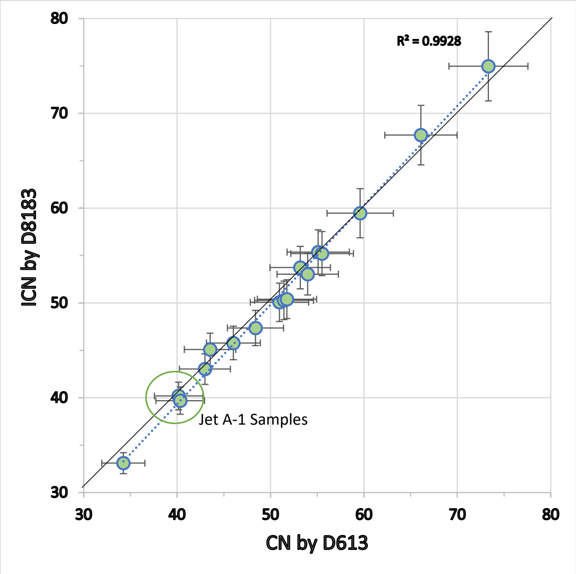
- Ignition delay definition differences between methods
  - DCN uses a single point definition while ICN uses the average of two points
- Less noisy pressure trace with AFIDA should allow more accurate measurement of low CN values (< 30)

HEFA-SPK – Hydrogenated esters and fatty acids – synthetic paraffinic kerosene
NJFCP – National Jet Fuel Combustion Program

Comparison of DCN and ICN to CFR Engine CN



Research Report RR: D02-1700 / IP 498 2009 Research Report "An evaluation of data, from the 2002 round robin, the ASTM NEG programme, and the Energy Institute correlation scheme, to calculate a revised Precision Statement for ASTM D6890 and IP 498/EN 15195 and a bias statement for D6890

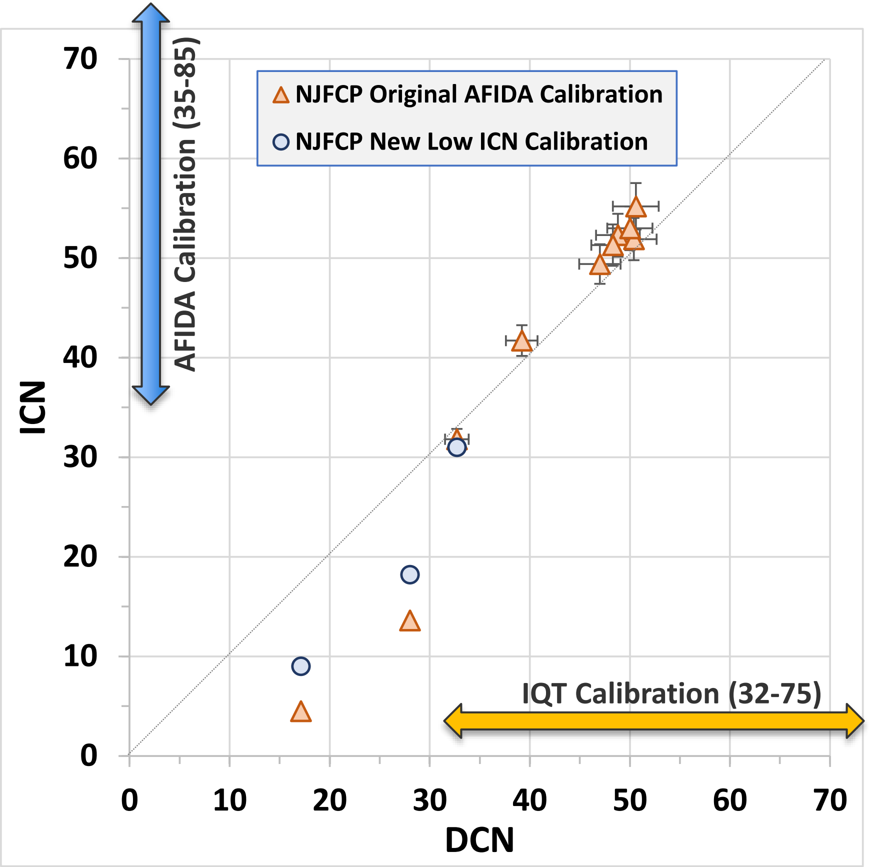


Research Report IP 617 "Determination of indicated cetane number (ICN) of fuels using a constant volume combustion chamber - primary reference fuels calibration (PRFC) method"

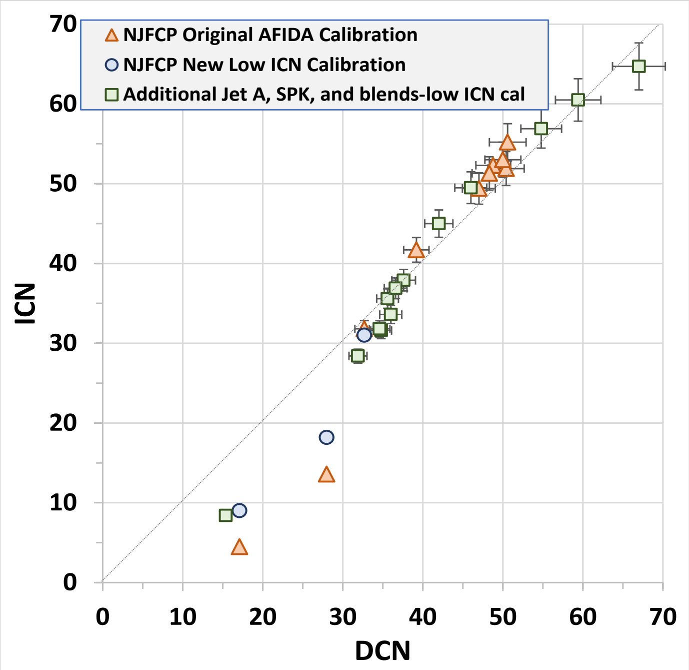
- Both methods are well correlated with referee method ASTM D613 (CFR engine CN) for CN > 32 (DCN) or 34 (ICN)
- Synthetic jet fuel constrained to DCN of 35 to 60
- Error bars are +/- R from method precision statements

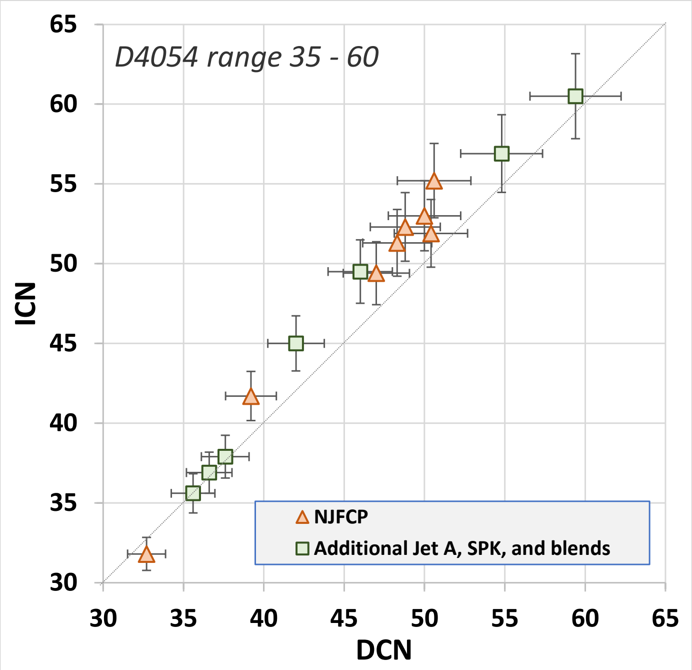
Jet Fuel ICN / DCN Comparisons – NJFCP Fuels Only

- Excellent agreement within method calibration ranges
  - DCN from NJFCP
  - ICN measured by NREL
  - Error bars are R from method precision statements
- ICN produces lower values relative to DCN outside of calibration range (low end)
- AFIDA low ICN calibration by NREL using primary reference fuels
- Not as straightforward to expand range for DCN (need D613 data)
- NJFCP fuels courtesy of Ed Corporan and Paul Wrzesinski, AFRL



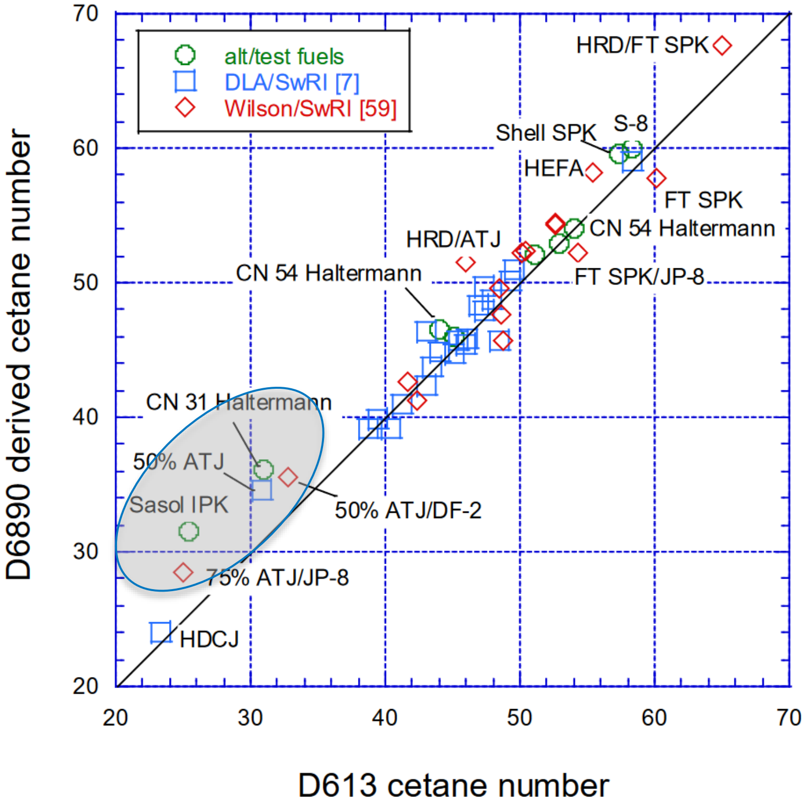
Jet Fuel ICN / DCN Comparisons – All Fuels





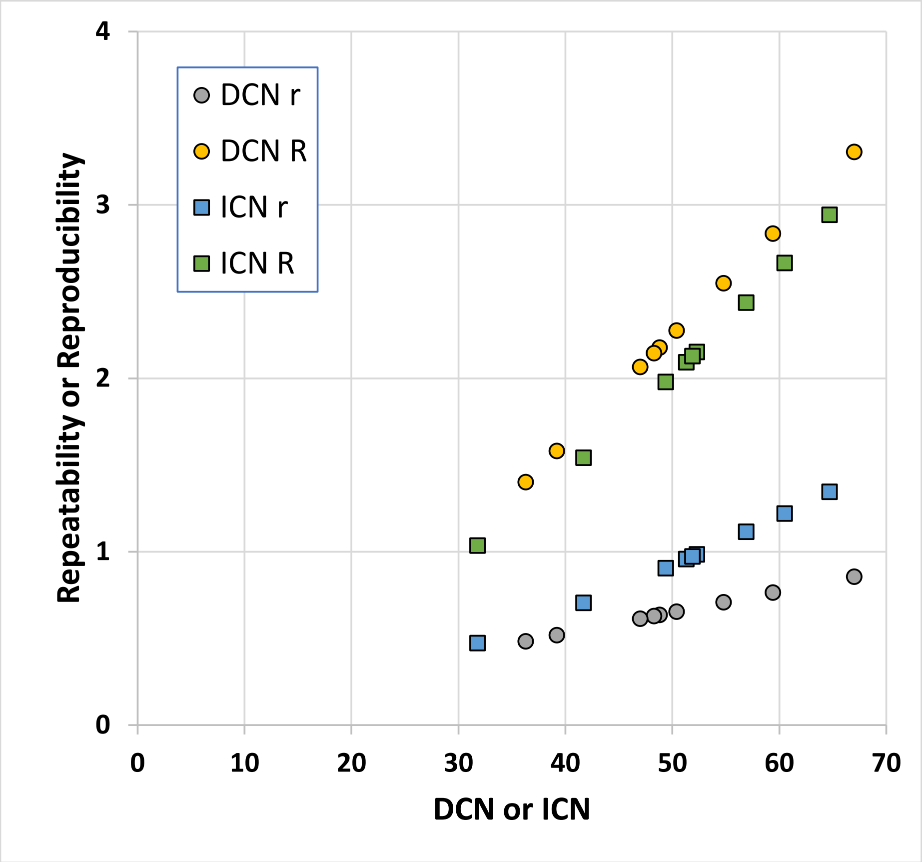
- Additional samples prepared by NREL
  - Commercial Jet A and blends with isobutanol ATJ-SPK (Gevo)
  - Results for HEFA-SPK anf 50% also included
- DCN and ICN measured at NREL
- Excellent agreement between methods for D4054 required range of 35 to 60

DCN Tends to Overpredict CN for Values Below 35



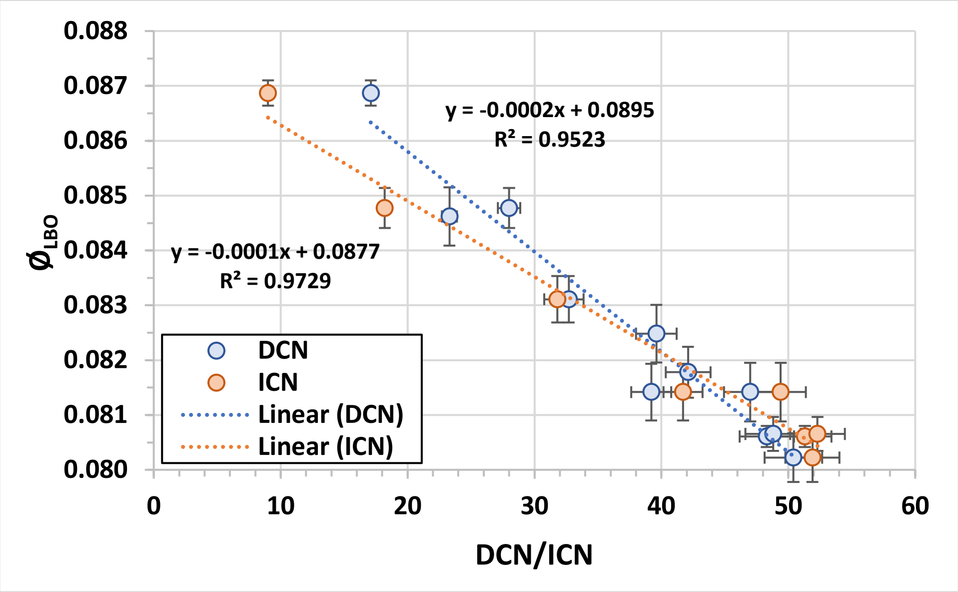
Edwards, J.T. "Jet Fuel Properties" AFRL-RQ-WP-TR-2020-0017, January 2020. https://apps.dtic.mil/sti/tr/pdf/AD1093317.pdf

Comparing Precision of DCN and ICN



ICN and DCN Comparison to Referee Rig Lean Blowout Results

- Referee rig data courtesy of Scott Stouffer and Zach West – UDRI
- Low ICN calibration was used
- Error bars are ASTM method R for ICN and DCN, +/- 95% conf for $Ø_{LBO}$
- For ICN or DCN > 30, $Ø_{LBO}$ prediction is the same
- Slopes are different, but this apparently is not significant for CN > 30



LBO – Lean blowout

Summary

- ICN provides equivalent measurement to DCN for jet fuels and synthetic blend components in the relevant range
  - And more conservative values below 35
- ICN or DCN > 30, $Ø_{LBO}$ prediction is the same (referee rig)
- A significantly smaller volume of fuel is required for ICN vs DCN
  - Advantage to early-stage synthetic aviation fuel producers
- Proposing to ballot addition of D8183 to D4054
- For example, modify D4054 Table A4.1:

COMBUSTION			
Derived Cetane Number **OR**	Max Min	60 35	D6890
Indicated Cetane Number	**Max** **Min**	**60** **35**	**D8183 or IP617**

Thank you

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robert.mccormick@nrel.gov

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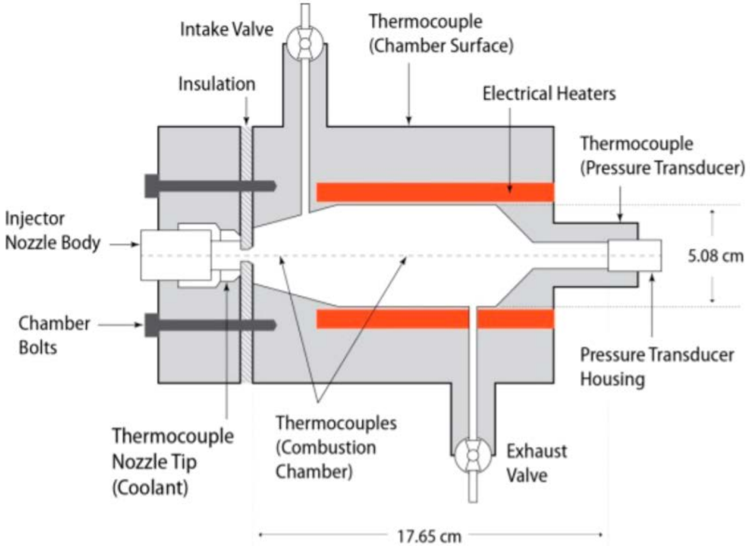
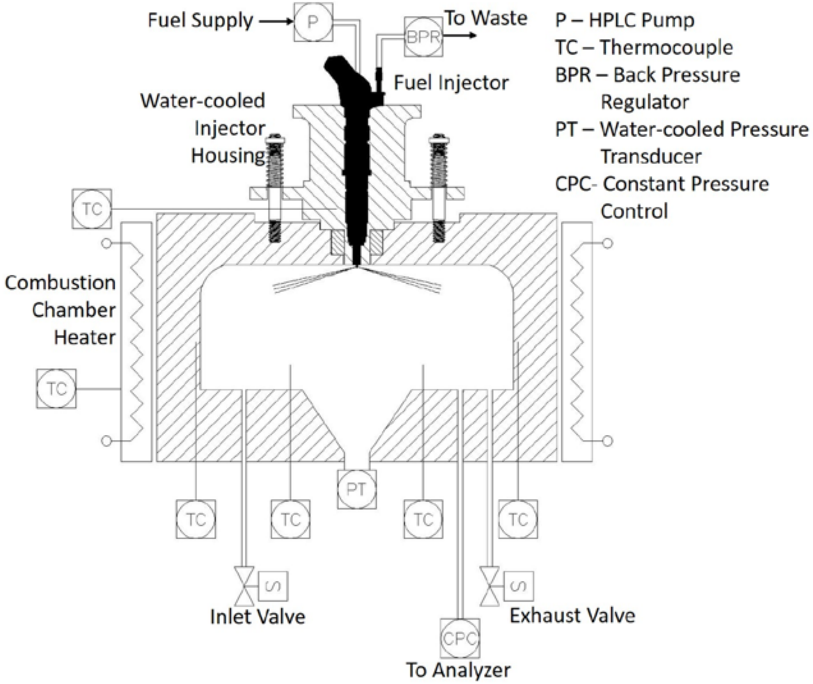
IQT (DCN) Experimental Details

- Ignition Quality Tester (IQT) measures Derived Cetane Number (DCN)
- Approved alternative method for CN in D975 (diesel fuel specification) – ASTM D6890
- 20 min test (15 pre-injections + 32 recorded injections)
- Single-hole S-type-delayed (inward opening) pintle nozzle operating at 225 bar
- **100 mL** required for DCN
  - Calibration (and ILS) covers the range of 32-75
  - 21.4 bar, 545°C start of injection conditions
  - Temperature adjusted such that IDT results of n-heptane correlate with CFR-engine based ASTM D613 results
  - Ignition delay converted to DCN using empirical equation based on CFR engine data
  - Expanding calibration range requires CFR engine data



AFIDA (ICN) Experimental Details

- Advanced Fuel Ignition Delay Analyzer (AFIDA) measures Indicated Cetane Number (ICN)
- Approved alternative method for CN in D975 (diesel fuel specification) – ASTM D8183
- 10 min test (2 pre-injections + 12 recorded injections)
- Bosch production CRI3-18, 7 hole piezo-electric diesel injector operating at 1000 bar
- **40 mL** required for ICN
  - Calibration covers the range of 35-85
  - 17.5 bar, 580°C setpoint
  - Calibrated with binary blends of primary reference fuels (n-hexadecane/1-methylnaphthalene) – which define the cetane number scale
  - Ignition delay conversion to ICN by instrument specific PRF based calibration curve



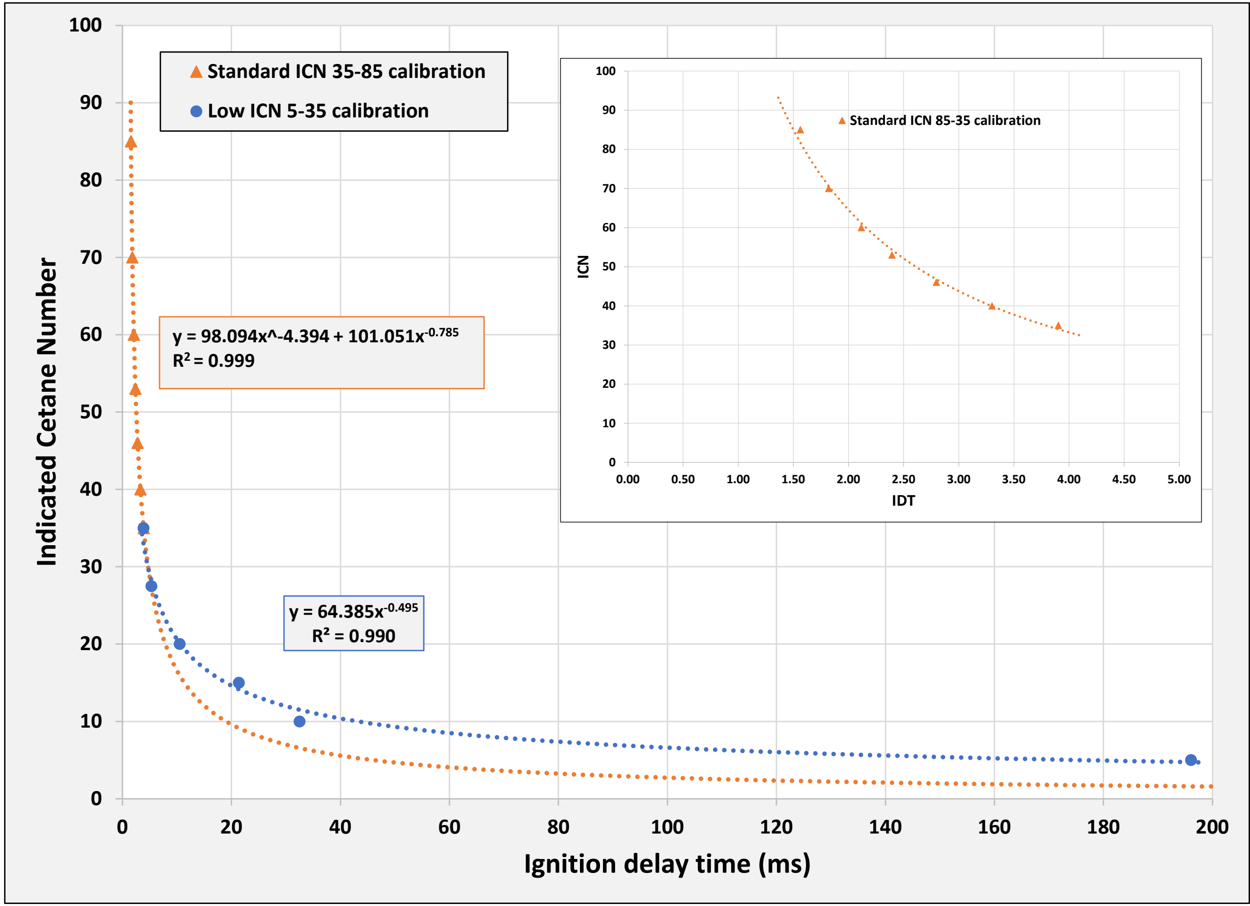
ICN/DCN Results

Values from low ICN calibration

	NJFCP ID	DCN Edwards	DCN NREL	ICN NREL	Description
NJFCP fuels	A-1 (10264)	48.8		52.3	JP-8
	A-2 (10325)	48.3		51.3	Jet A
	A-3 (10289)	39.2		41.7	JP-5
	C-1 (13718)	17.1		4.5 (9.0)	ATJ from Gevo
	C-2 (12223)	50.4		51.9	84% C14 iso-paraffins/16% 1,3,5 trimethyl benzene
	C-3 (12959)	47.0		49.4	64% A-3/36% Amyris farnesane
	C-4 (13217)	28.0		13.6 (18.2)	FT:ATJ Blend 60% Sasol IPK (FT-SPK)/40% C-1
	n-C12	75.0		77.3	n-dodecane
	S-1	50		53	59.3 n-C12, 18.4 i-C8, 22.2 1,3,5 TMB
	S-2	50.6		55.2	52.6 n-C16, 25.1 i-C8, 22.22 1,3,5 TMB
	50:50 A-2+C-1	32.7		31.8 (31.0)	
Additional fuels	Commercial HEFA-SPK		59.4	60.5	HEFA-SPK#1
	Commercial HEFA-SPK		67.0	64.7	HEFA-SPK#2
	Commercial ATJ-SPK		15.4	4.0 (8.4)	ATJ from Gevo (different lot)
	NREL Blend		54.8	56.9	50/50 blend of A-2/HEFA-SPK#1
	NREL Jet A (2023 #1)		46.0	49.5	
	2023 #1 + 50% Gevo		34.8	31.6	
	2023 #1 + 45% Gevo		36.0	33.6	
	2023 #1 + 35% Gevo		37.6	37.9	
	NREL Jet A 2023 #A		42	45	
	2023 #A + 50% Gevo		31.9	28.4	
	2023 #A + 40% Gevo		34.6	31.8	
	2023 #A + 30% Gevo		35.6	35.6	
	2023 #A + 25% Gevo		36.6	36.9	

AFIDA Easily Calibrated to Lower ICN Values

- AFIDA is easily calibrated by user to a wider CN range
- Primary reference standard calibration using purified n-hexadecane / 1-methlynaphthalene
- Standard calibration PRFs (85, 70, 60, 53, 46, 40, 35)
- Low calibration PRFs (35, 27.5, 20, 15, 10, 5)



Volumetric Blending CN for NREL Blends

- Calculate volumetric blending CN = $vol\%_{Jet\ A} * CN_{Jet\ A} + Vol\%_{Gevo} * CN_{Gevo}$
- Volumetric blending DCN agrees well with ICN for CN <35

	DCN	Vol Blend DCN	ICN
Gevo ATJ-SPK	15.4		8.4
NREL Jet A (2023 #1)	46		49.5
2023 #1 + 50% Gevo	34.8	30.7	31.6
2023 #1 + 45% Gevo	36	32.2	33.6
2023 #1 + 35% Gevo	37.6	35.3	37.9
NREL Jet A 2023 #A	42		45
2023 #A + 50% Gevo	31.9	28.7	28.4
2023 #A + 40% Gevo	34.6	31.4	31.8
2023 #A + 30% Gevo	35.6	34.0	35.6
2023 #A + 25% Gevo	36.6	35.4	36.9