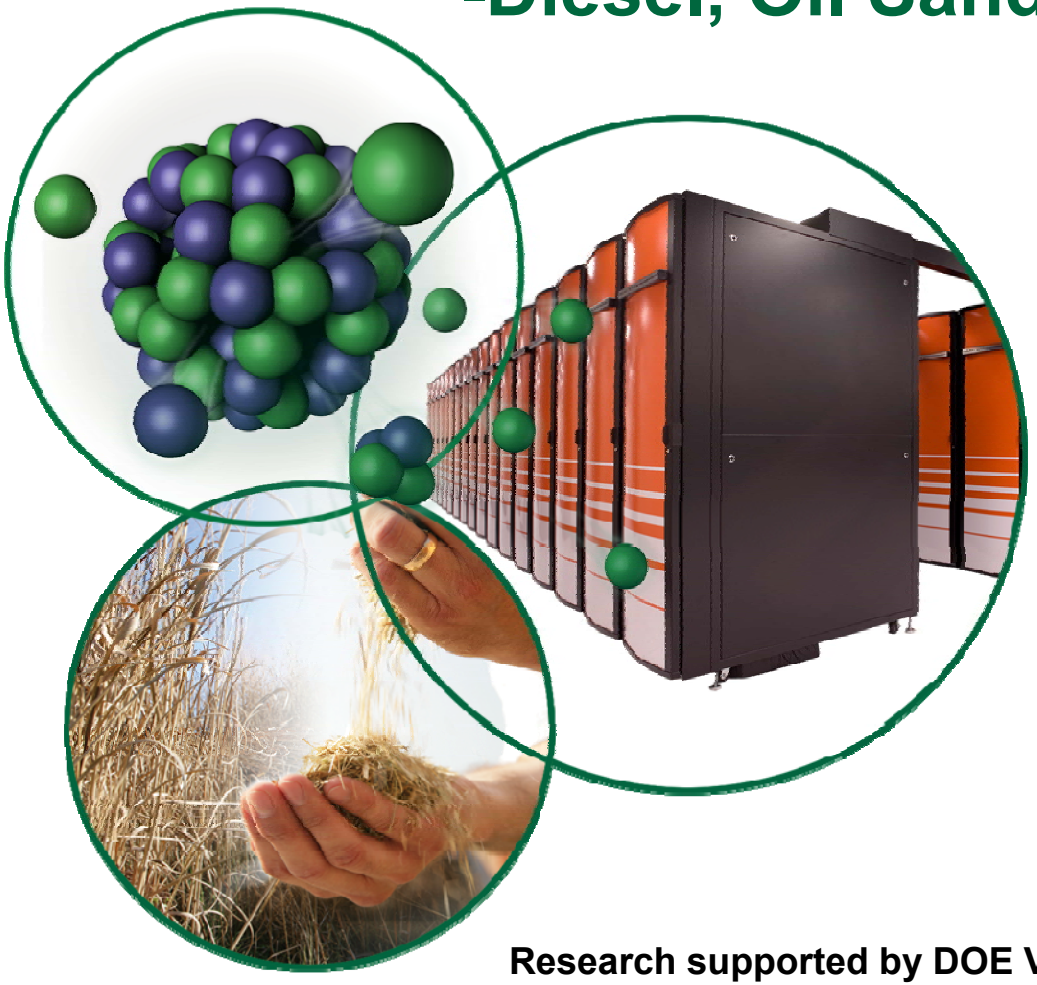
New Results for HCCI Diesel Engine Fuels
-Diesel, Oil Sands, Bio-Diesel-



Bruce Bunting

Scott Eaton

Jim Szybist

Diesel Crosscut

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Outline of presentation

- Background
- Fuels / blends
  - Diesel, oil sands derived, bio-diesel
- Engine used for research
- Typical experimental plan
- Analysis
- Results
- Conclusions
- Future work
- Acknowledgements

Background

- Advanced combustion engines (HCCI, LTC, PCCI, etc.) hold potential of improved fuel economy and reduced emissions
- Advanced combustion engines are more sensitive to fuel chemistry than conventional diesel engines since ignition is controlled by kinetics to a greater degree
- Data is needed to determine:
  - Ability to use and interchange fuels in advanced combustion engines
  - If new fuels might offer performance advantages
  - If new laboratory based fuel measurements are required to control fuel performance
  - If on-board fuel or engine based measurements can result in more optimum engine control over a range of fuels

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Our approach

- Use a wide range of fully formulated fuels and surrogate blends to study effects of fuel properties and chemistry on HCCI engines
  - Performance and emissions
  - Diesel range, gasoline range, bio-derived fuels
  - Focus on fuel efficiency
- Use simple HCCI-type engines
  - Fewer variables to map
  - Only small fuel quantities required
  - Separation of LT and HT chemistry
  - Same processes occur in 'real' engines
    - But, more mixed up in time and space
- Statistical analysis and on-going mining of previous data sets as we learn new things

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Multiple fuel matrices and programs

- Diesel fuel blends (Cummins + BP, 10 fuels & baseline)
  - ≈ 35, 45, and 55 cetane
  - Boiling point distributions span from above to below #2 and #1
  - Aromatics varied in meeting other properties, ranged 18 to 53 percent
  - Cetane improver (ethyl hexyl nitrate) in 3 fuels
- Oil sands derived (Shell Canada and NCUT, 17 fuels & intermediates)
  - 34 to 60 cetane
  - 196 to 336°C T50
  - 15 to 38% aromatics
  - 41 to 63% cyclo-paraffins
- Biodiesels (Cummins + BP, 5 fuels & baseline)
  - B20 blends in ULSD
  - Mixed methyl esters derived from palm, coconut, soy, rape, mustard
  - Cetane, boiling point, % unsaturates, and % oxygen are main variables

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Fuel notes

- BP diesels
  - Mono-aromatics used to lower cetane
  - Poly-aromatics used to raise boiling points
  - Cetane improver used to broaden matrix
- Oil sands derived
  - Mono-aromatics are major variable affecting cetane
  - Cetane also increases with boiling points
  - No special cyclo-paraffin related effects found
- Biodiesels
  - B20 blends
  - All provided worse fuel economy
  - Specific chemistries affected performance and control

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HCCI engine used for experiments

- Fully premixed, un-throttled, no EGR, dilute combustion, ignition initiated kinetically near top of compression stroke
- Advantages
  - Potential for more efficient combustion
  - Low NOx, low smoke
  - Simple platform for fuels research
    - Uses only small amount of fuel
    - Only 2 engine control parameters, intake temperature and fuel rate (recently added A/F ratio)
    - Can be represented with single and multi-zone combustion models
- Same chemistry processes occur in low NOx LTC or PCCI engines, but more mixed up in time and space

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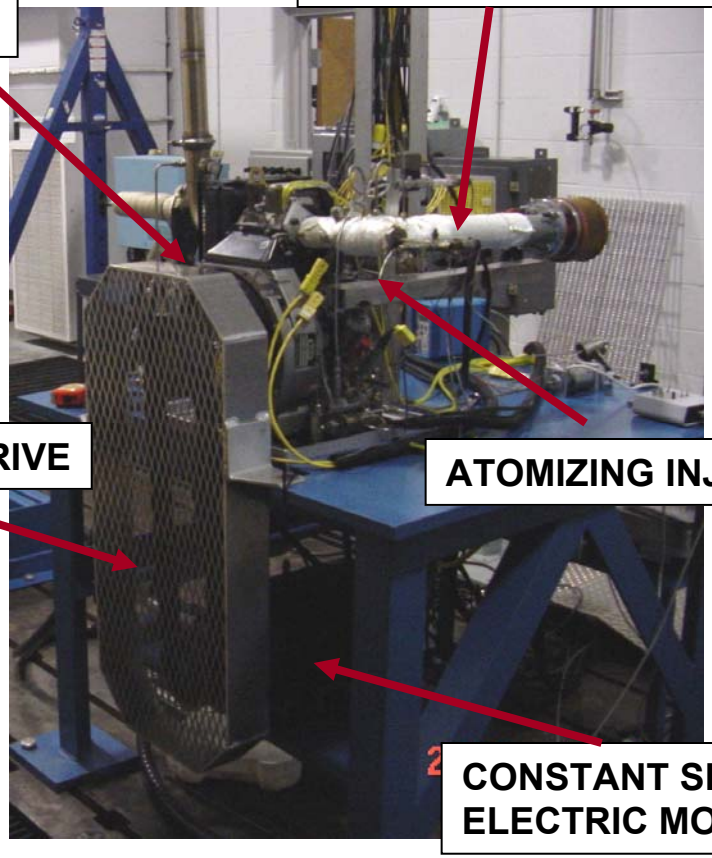
ORNL HCCI research engine
derived from Hatz single cylinder diesel engine

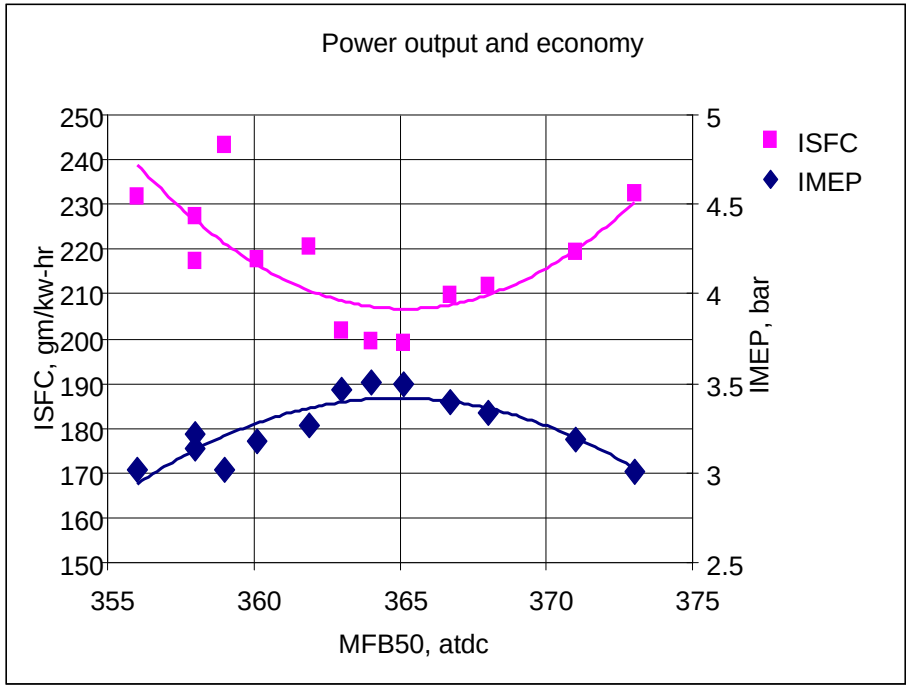


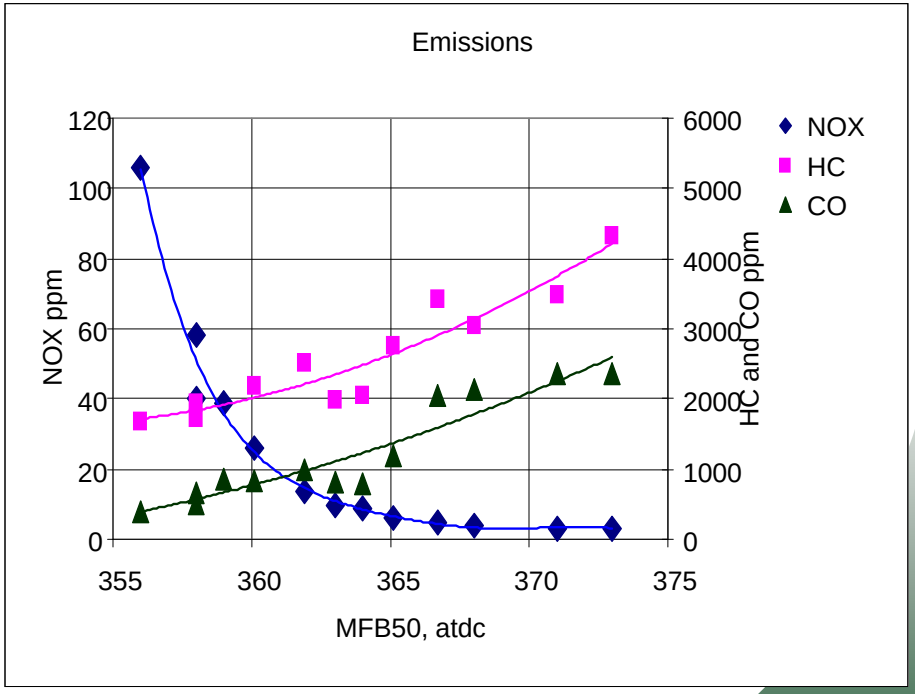
MODIFIED PISTON WITH SPHERICAL COMBUSTION BOWL

Engine displacement	517 cc
Bore	9.7 cm
Stroke	7.0 cm
Fuel injection	Port atomization
Intake air temperature	30 to 400 deg.C
Compression ratio	10.5

HCCI engine behavior

- **A fuel produces ISFC and combustion trade-offs as a function of combustion phasing**
- **A collection of fuel and engine characteristics determines where optimum performance occurs**
- **The fuel story also depends on the engine story**





Typical experimental plan (oil sands derived)

- Run 17 fuels in HCCI engine, mapping performance across multiple loads (fuel rates) and combustion timings (intake temperatures)
  - 1800 rpm
  - 6 to 11 gm/min fuel rate
  - 1.4 to 3.0 bar IMEP
  - 130 to 300° C IMT
  - 352 to 378° CA MFB50 (TDC = 360)
- 240 data points total
  - 3 fuel rates per fuel
  - ≈4 timings per fuel rate (2 to 6)
- Measure performance, emissions, and combustion characteristics
- Correlate results to fuel properties

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Analysis plan

- Use statistical models, based on principal components analysis (PCA)
  - Independent variables are resolved into eigenvectors, co-linearity in the variables does not cloud picture
  - Each eigenvector represents a relationship in the data, resulting from feedstock, processing, or control choices
  - Eigenvector models can maintain all the variables; do not force either-or choices among variables
- Use model to study response effects of engine and fuel variables
  - PCA model represents independent variable space, and is used in regression analysis against selected dependent variables
- Use model to 're-run' experiments with specific restraints or targets such as constant IMEP, intake temperature, or MFB50 and/or emission or performance restraints

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PCA model in simulator format

INPUTS

FuelFlow	IntakeT	n Para	iso Para	mono Para	poly Para	Mono Arom	Poly Arom	Olefins
9.0	205	4.3	7.8	12.7	35.2	29.7	9.0	1.3
7.9	215	7.8	9.9	18.9	31.1	25.9	5.4	1.1
7.9	222	2.9	12.3	31.4	23.8	24.1	3.3	2.2
8.3	195	5.1	10.8	23.6	26.9	26.9	4.9	1.8
8.2	170	7.0	14.6	24.0	31.2	18.7	3.6	1.0
8.2	205	6.8	11.3	21.5	34.1	24.7	0.8	0.8
10.2	110	7.7	16.2	24.8	35.9	10.6	4.7	0.1
8.2	210	7.0	11.6	19.4	29.8	29.8	1.8	0.7
8.1	200	5.3	12.5	18.0	34.5	22.5	4.9	2.3
8.0	195	5.8	14.1	23.9	32.5	18.7	3.8	1.2
8.1	215	10.1	11.9	18.8	28.9	27.2	1.6	1.5
9.1	195	4.6	8.7	12.7	37.6	26.1	9.9	0.3
9.1	120	20.3	17.4	19.0	22.4	17.9	1.8	1.2
8.4	205	6.3	11.0	14.9	32.9	27.4	5.2	2.3
8.4	165	2.9	18.5	23.9	29.4	21.0	3.3	0.9
7.8	235	5.5	18.2	33.4	12.7	27.3	0.8	2.1
9.9	120	2.1	18.1	24.8	37.7	11.4	5.4	0.5

Engine variables

Fuel variables

In this case, engine variables were adjusted to achieve constant power and constant phasing

Engine response

OUTPUTS

IMEP	ISFC	NOx	CO	HC	LTHRPct	COVPct	AFR	MFB	Smoke	FB1090	dPdCA
2.5	282	0.55	40	240	0.4	4.7	30.7	365	2.87	5.6	5.4
2.5	249	0.53	25	125	0.4	6.2	35.5	365	0.03	5.6	5.9
2.5	249	0.61	21	116	0.2	3.5	34.5	365	0.02	5.2	6.5
2.5	256	0.37	27	77	0.5	5.1	34.7	365	0.15	5.7	5.7
2.5	257	0.24	46	156	2.4	4.7	36.9	365	0.16	8.4	4.9
2.5	255	0.68	24	121	0.4	5.3	34.4	365	0.02	5.9	6.4
2.5	290	0.01	246	10481	26.6	4.7	33.7	365	10.00	6.4	2.1
2.5	253	0.69	22	116	0.4	5.9	34.1	365	0.01	5.8	6.2
2.5	257	0.17	34	108	0.7	4.4	35.2	365	0.38	5.5	5.6
2.5	251	0.12	37	109	1.1	4.7	35.7	365	0.10	5.5	5.6
2.5	251	0.56	23	78	0.4	5.4	34.0	365	0.02	6.0	6.5
2.5	282	0.20	61	1040	1.9	5.4	30.9	365	1.55	6.1	5.0
2.5	277	0.02	141	593	14.4	5.6	36.8	365	0.83	11.0	1.7
2.5	263	0.47	30	94	0.4	4.8	33.9	365	0.24	5.8	6.3
2.5	256	0.12	40	148	2.4	3.7	36.4	365	0.08	6.5	5.6
2.5	246	0.65	21	39	0.4	5.3	34.6	365	0.01	5.4	6.7
2.5	299	0.00	421	3358	33.3	2.3	33.2	365	10.00	5.5	1.9

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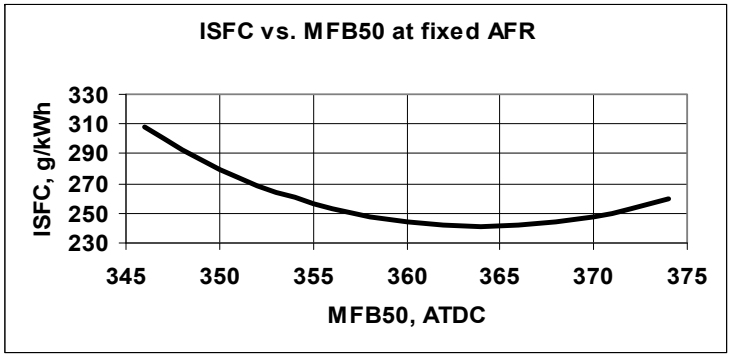
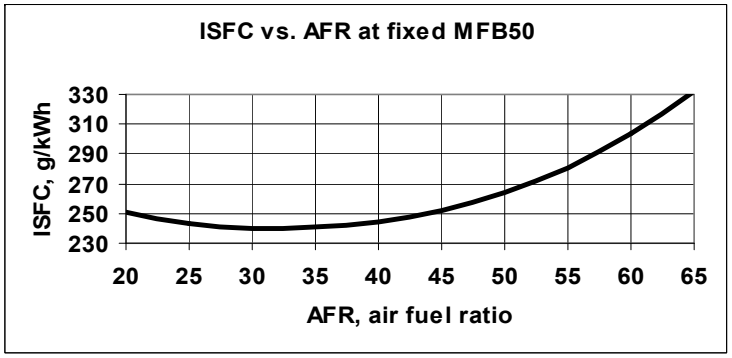
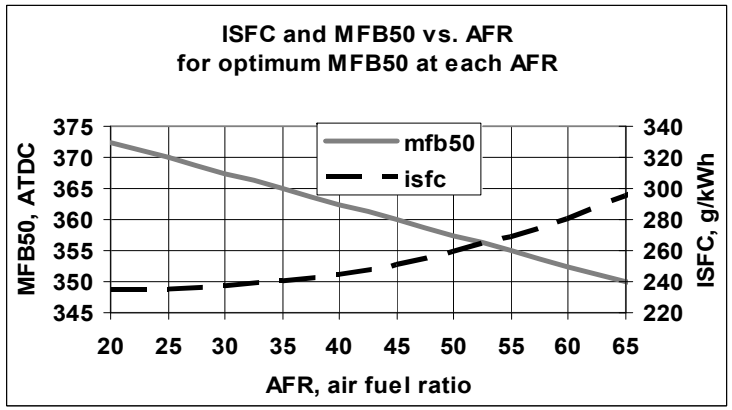
Diesel fuel blends at mid-point fuel properties, showing response characteristics of engine







OPTIMUM ISFC AT ABOUT 365° MFB50

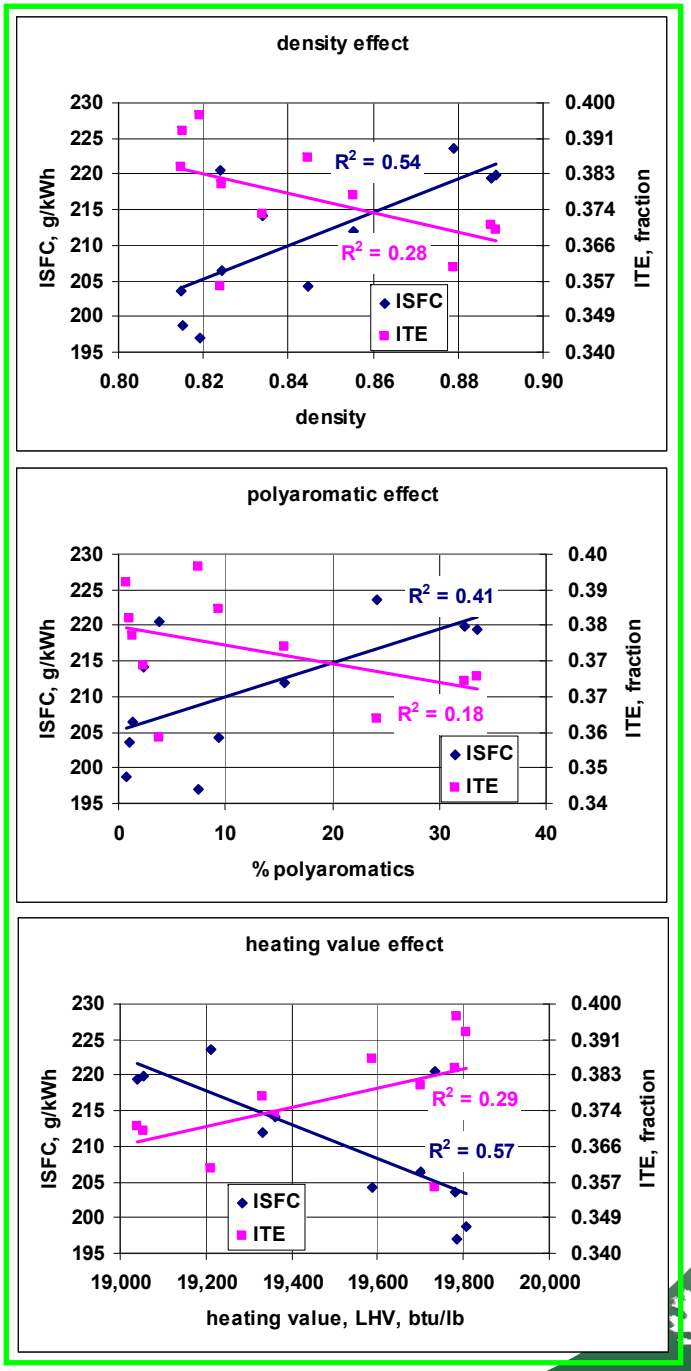
OPTIMUM AFR AT ABOUT 30

LOWER LOAD OPERATION (HIGHER AFR) REQUIRES MORE ADVANCED TIMING FOR BEST FUEL ECONOMY

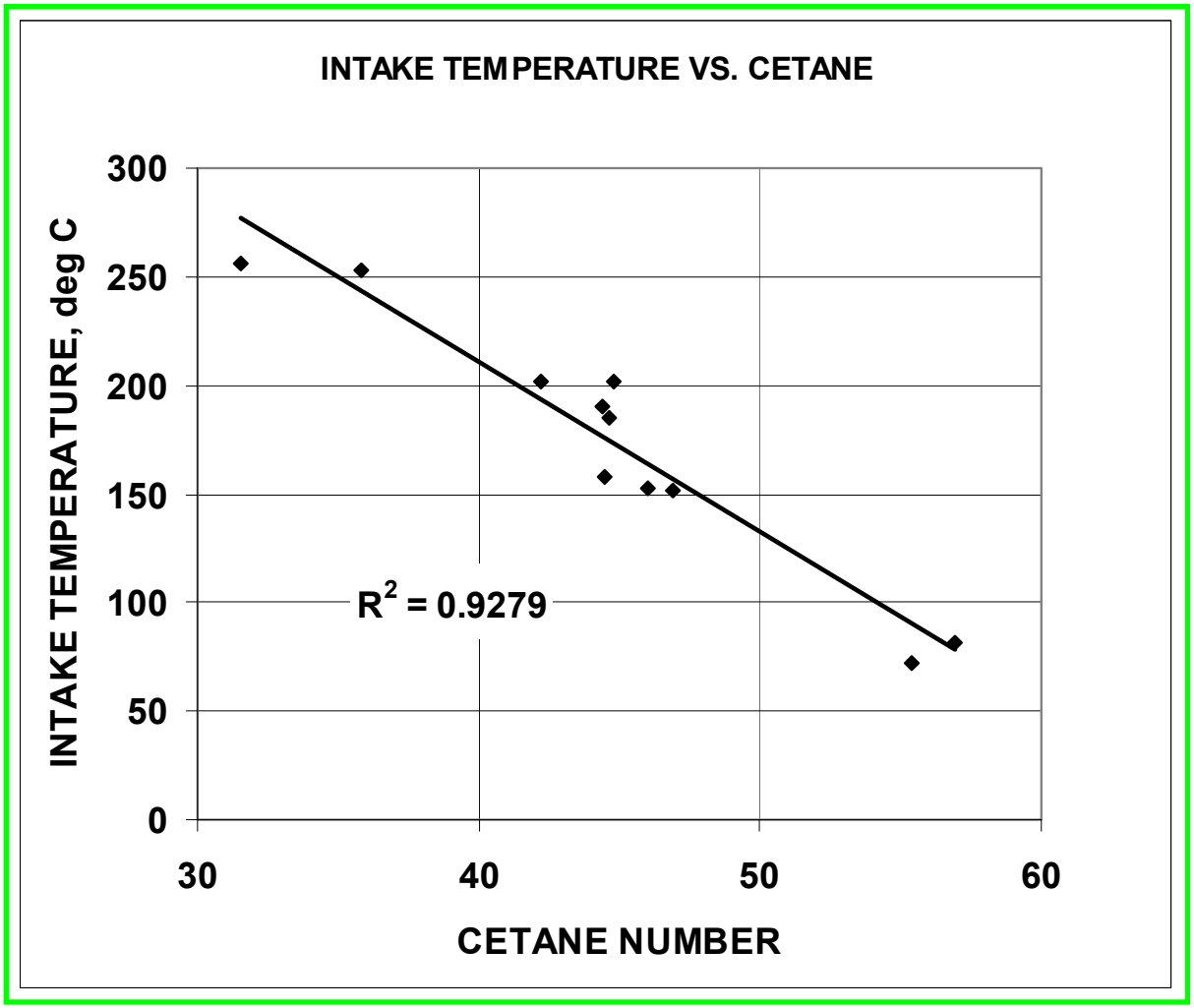
Diesel fuel blends, response of ISFC and ITE to fuel properties related to 'heavy fuels'

FUEL EFFICIENCY WORSE WITH FUELS HAVING HIGHER DENSITY, MORE POLYAROMATICS, AND LOWER HEATING VALUE

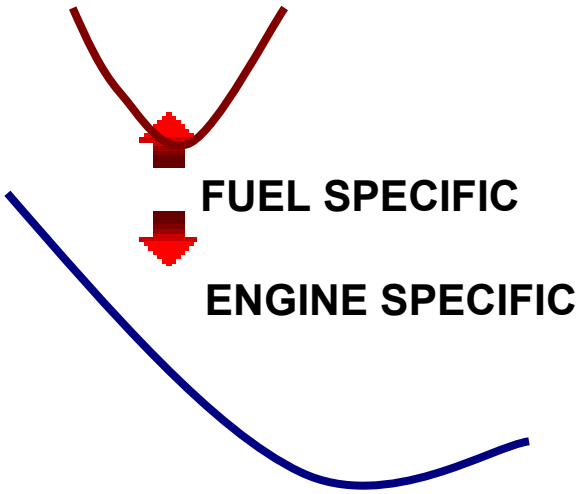
CETANE NUMBER WAS NOT A STRONG CORRELATION

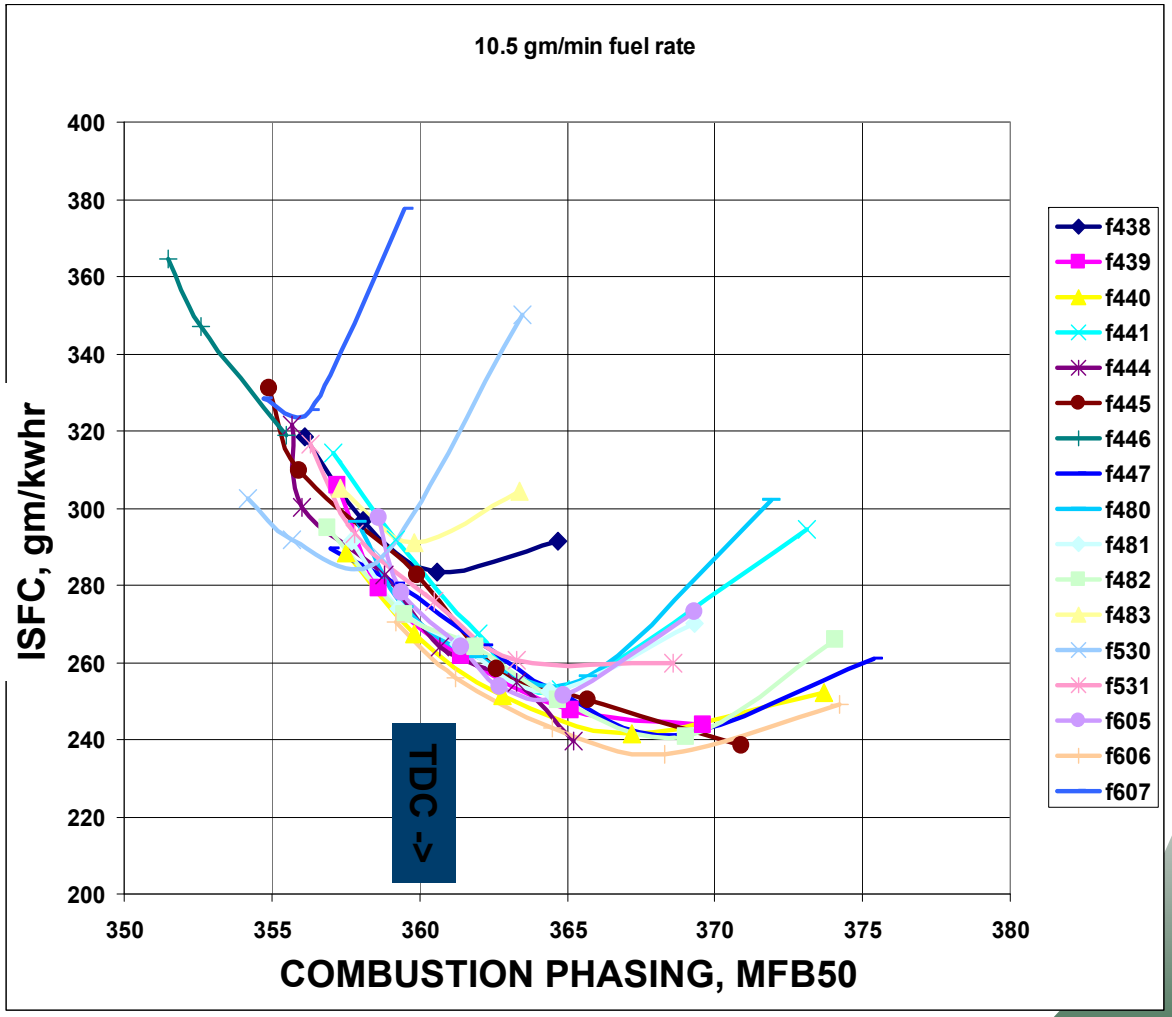


Diesel fuel blends - higher cetane fuels required lower intake temperature to maintain constant combustion phasing

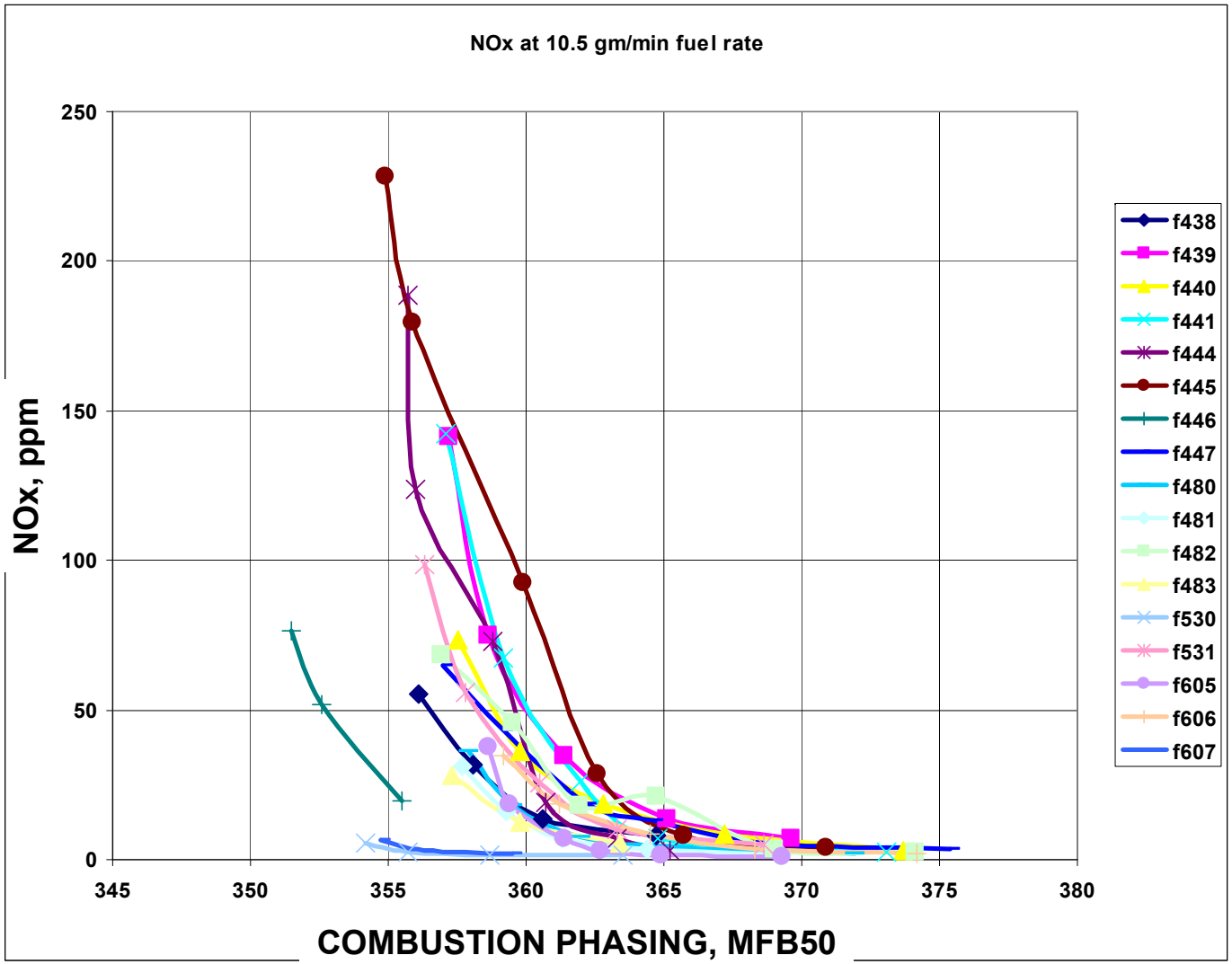


Oil sands derived, shows both engine related and fuel related trends





Ability to advance timing is limited by NOx, dP/dCA, peak pressure, noise, etc.



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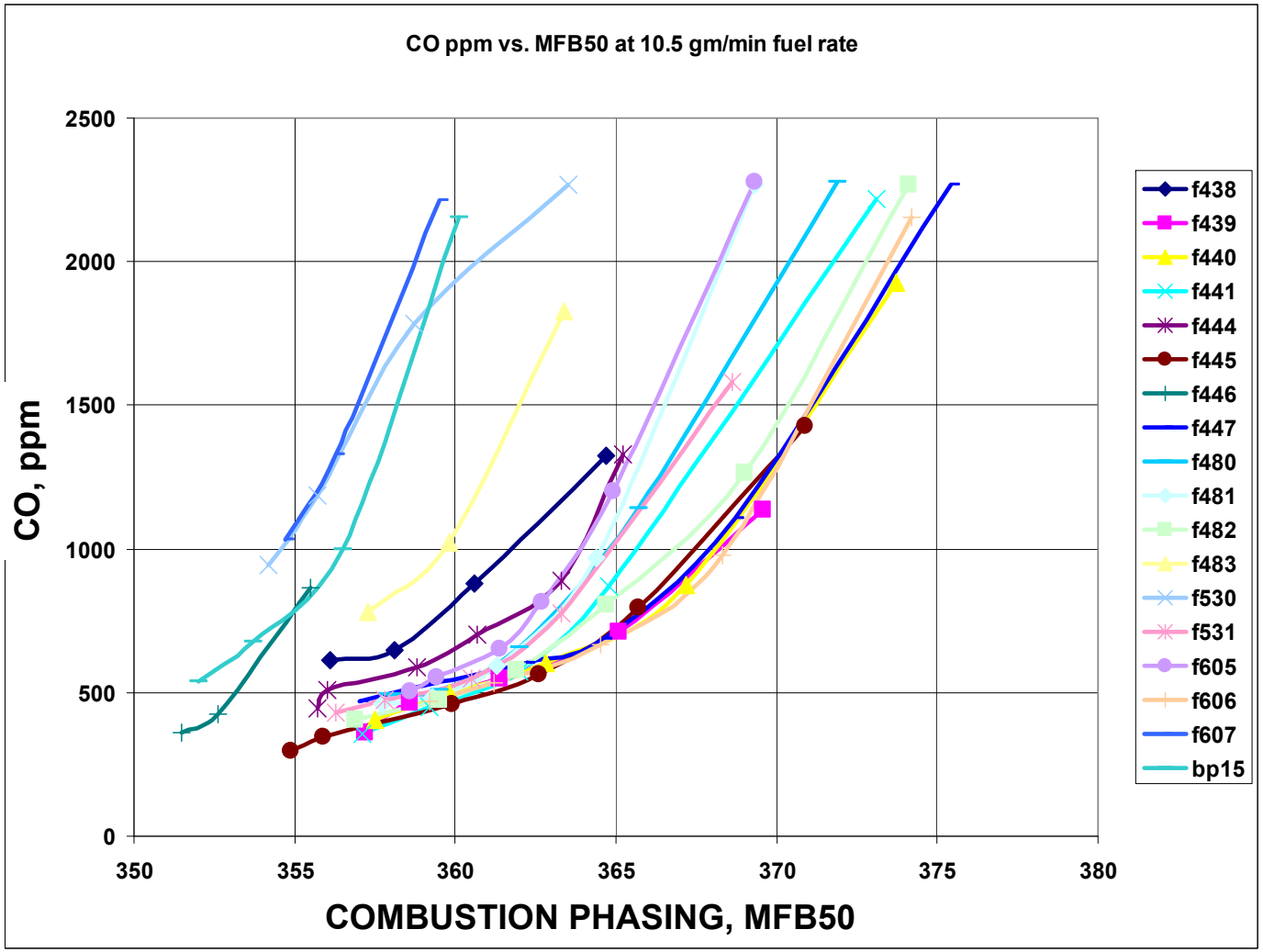
Ability to retard timing is limited by incomplete burning, high CO, high HC



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Oil sands derived - parametric control study

- Open loop (constant intake temperature)
  - Mono-aromatics improve fuel economy by retarding combustion phasing
  - N-paraffins increase NOx by increasing combustion rate
- Closed loop control (constant MFB50 @ 5°ATDC)
  - Mono-aromatics require higher intake temperature for constant phasing
  - This raises NOx and lowers HC, CO, and smoke
  - ISFC improved by higher intake temperature combined with retarded combustion
- 'Magic fuel sensor' (finds best ISFC for each fuel)
  - Measurement not defined yet
  - ISFC improved by later combustion phasing, which also decreases smoke
  - Mono-aromatics enable later combustion phasing

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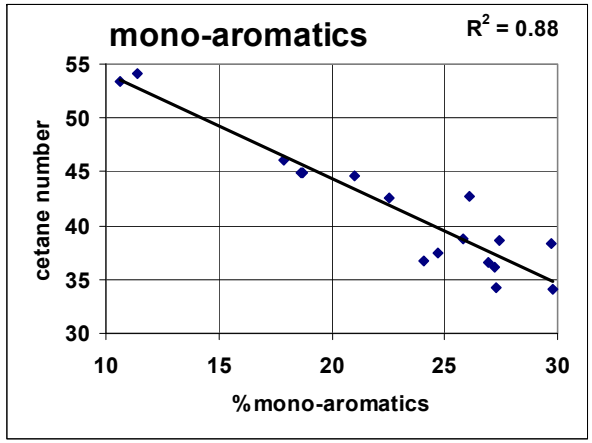
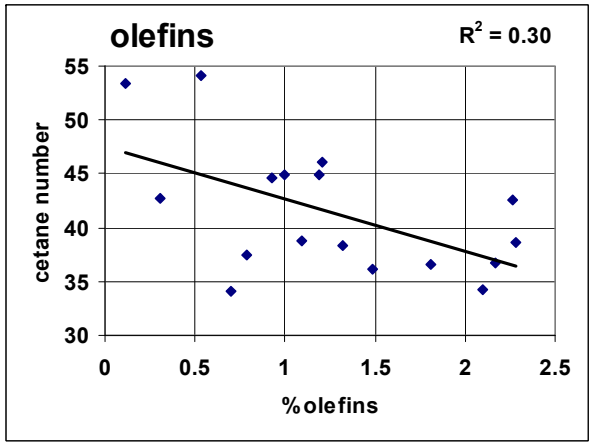
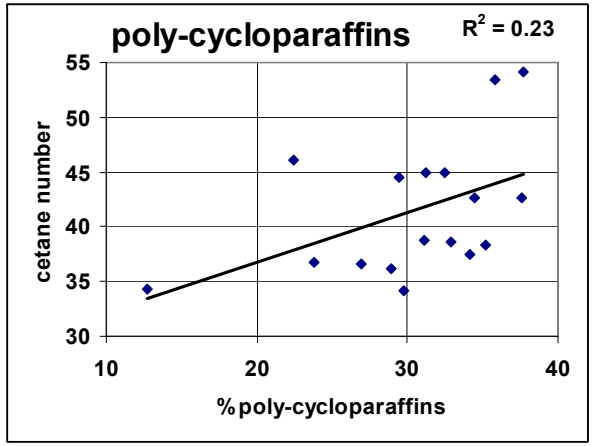
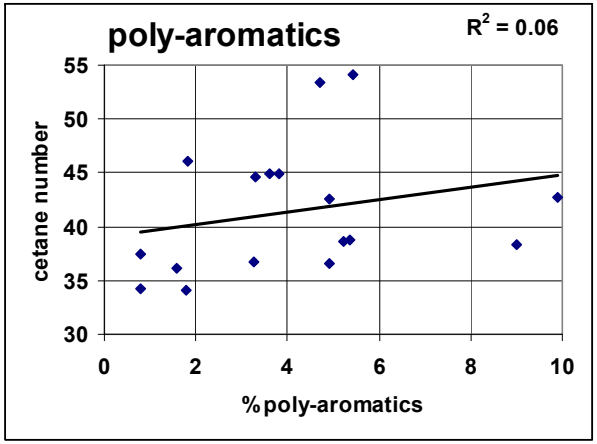
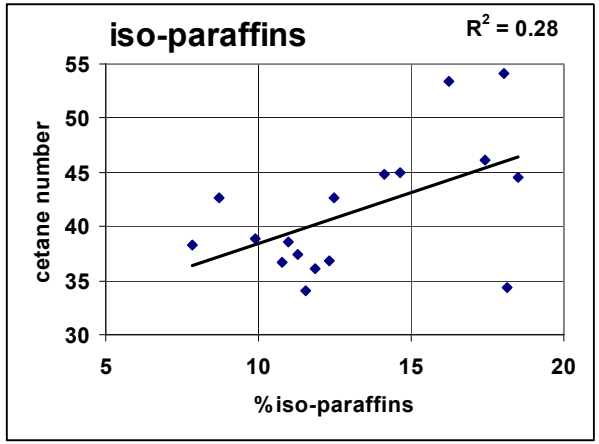
Oil sands derived-cetane and fuel chemistry

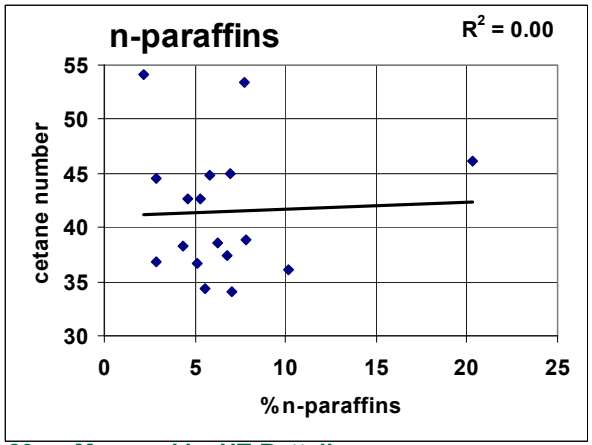


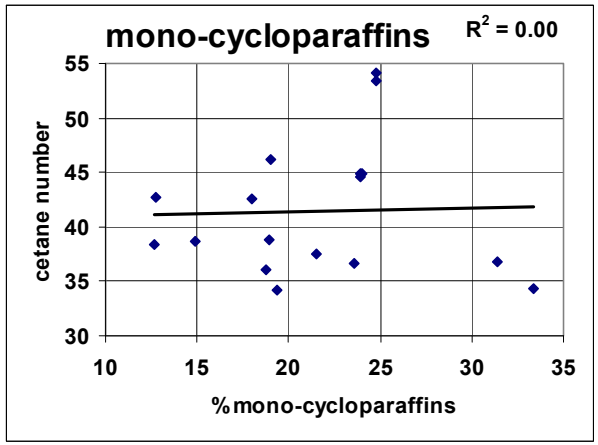












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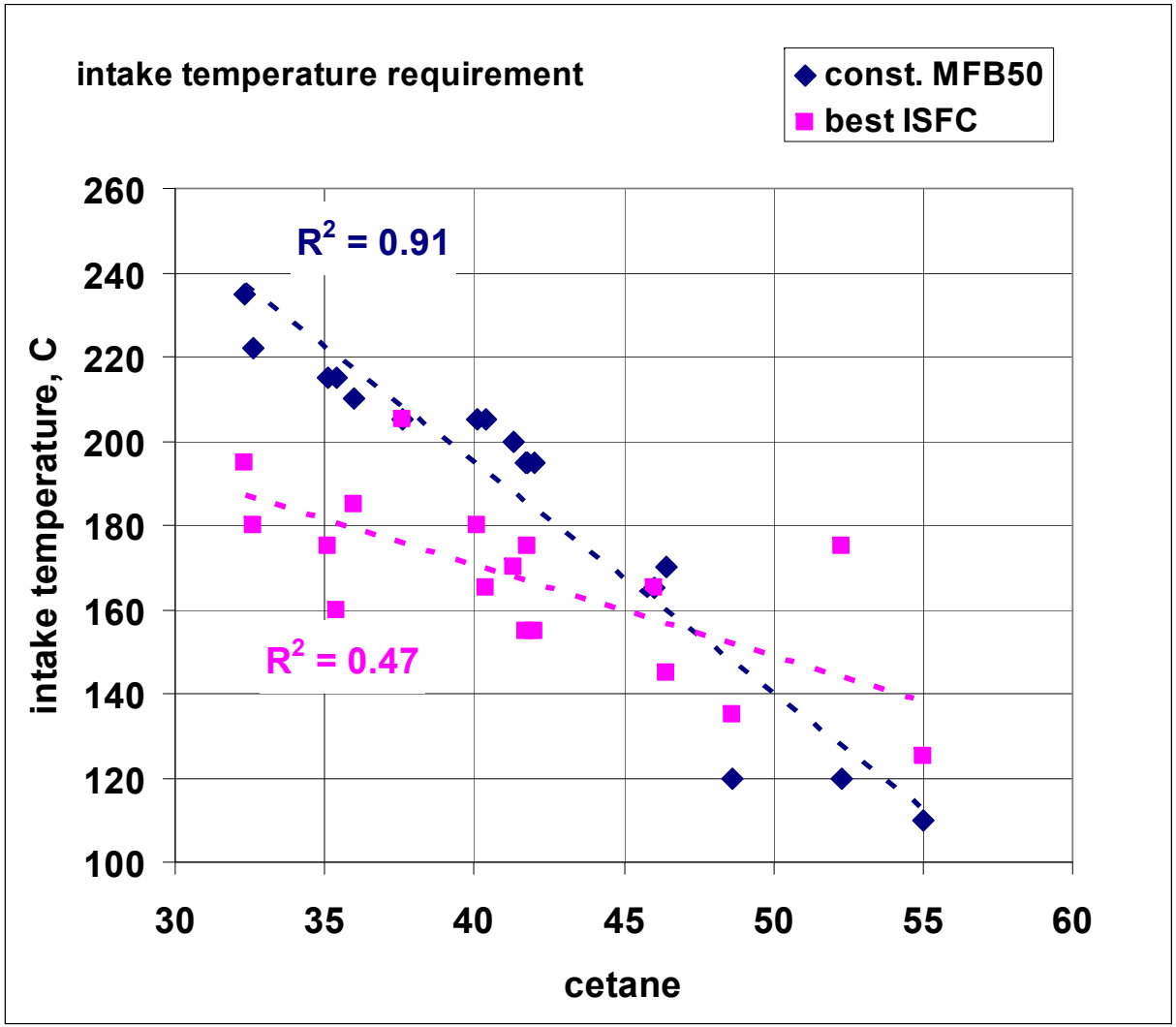
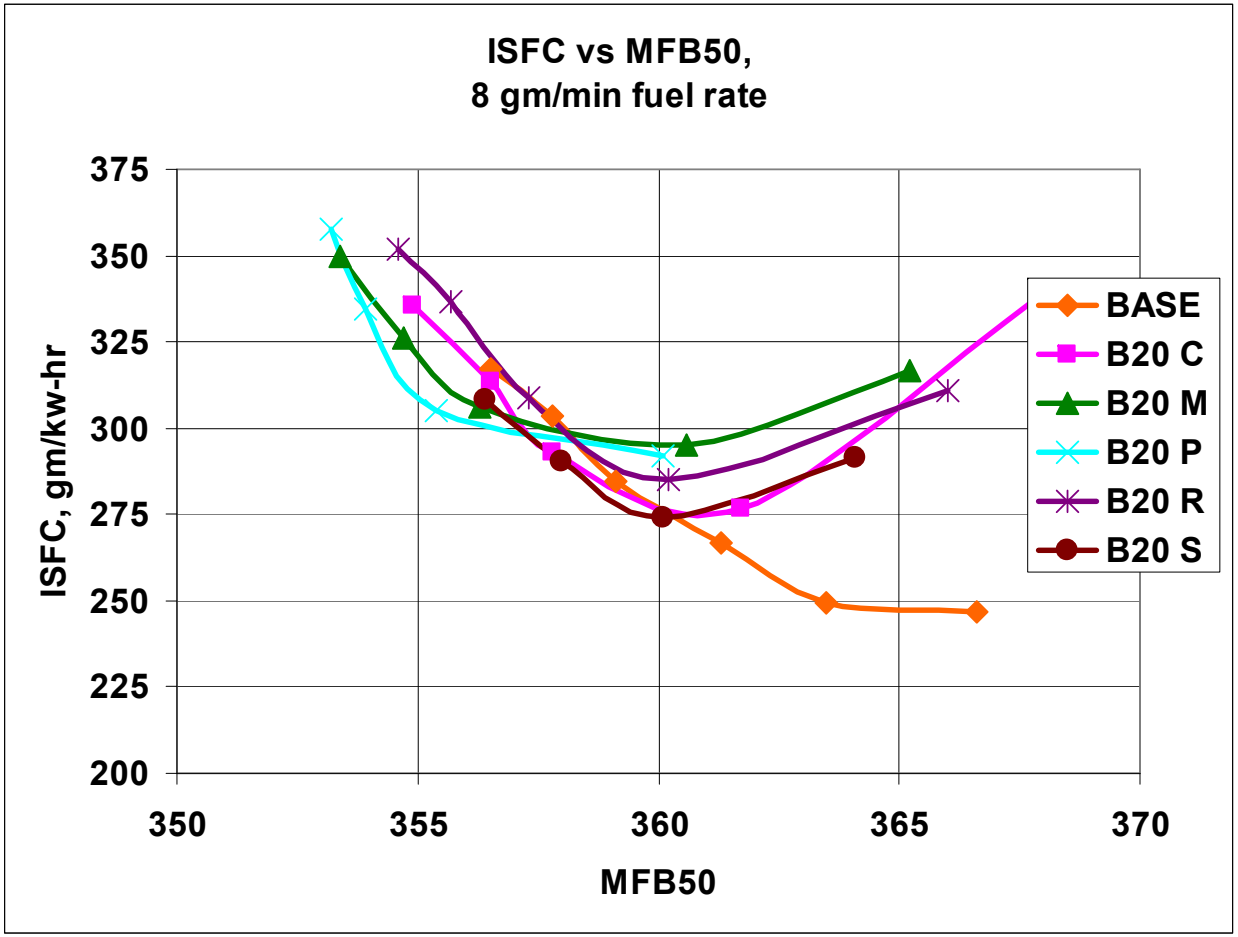
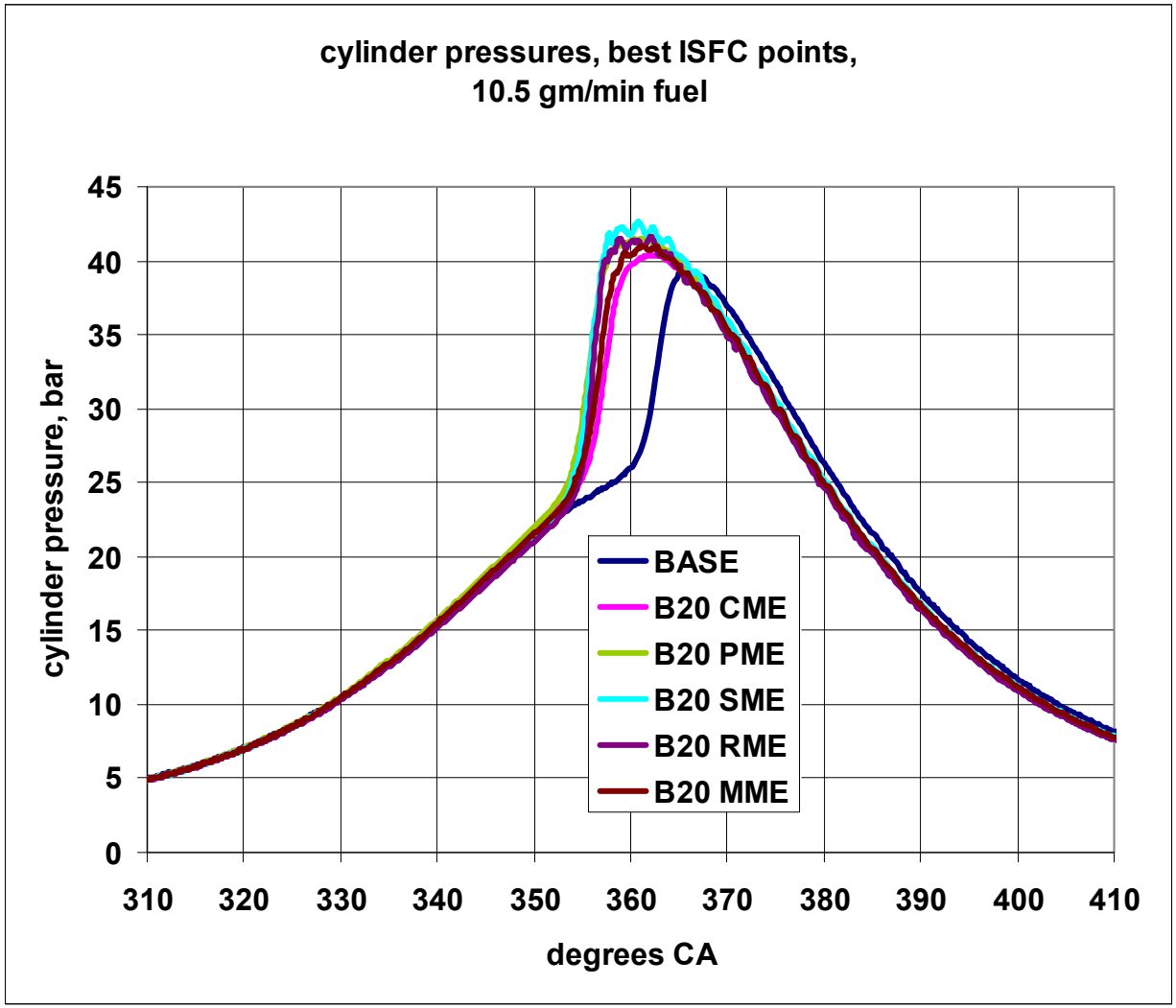
Oil sands derived - large control changes are necessary, cetane number remains a major variable



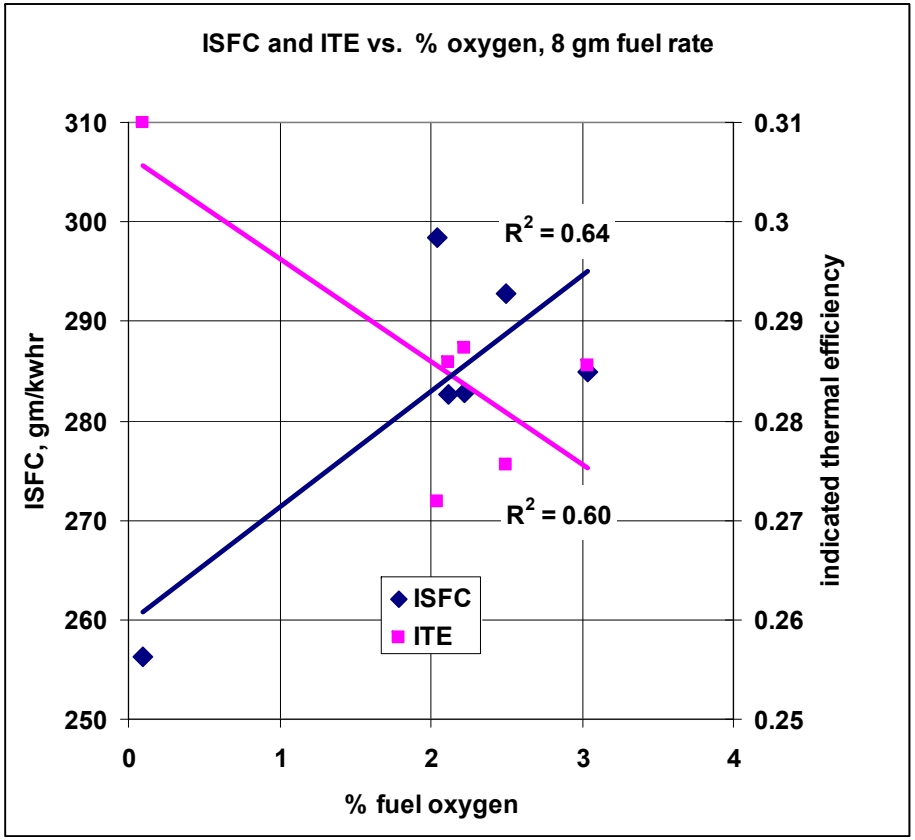
Biodiesels - ISFC response to combustion phasing

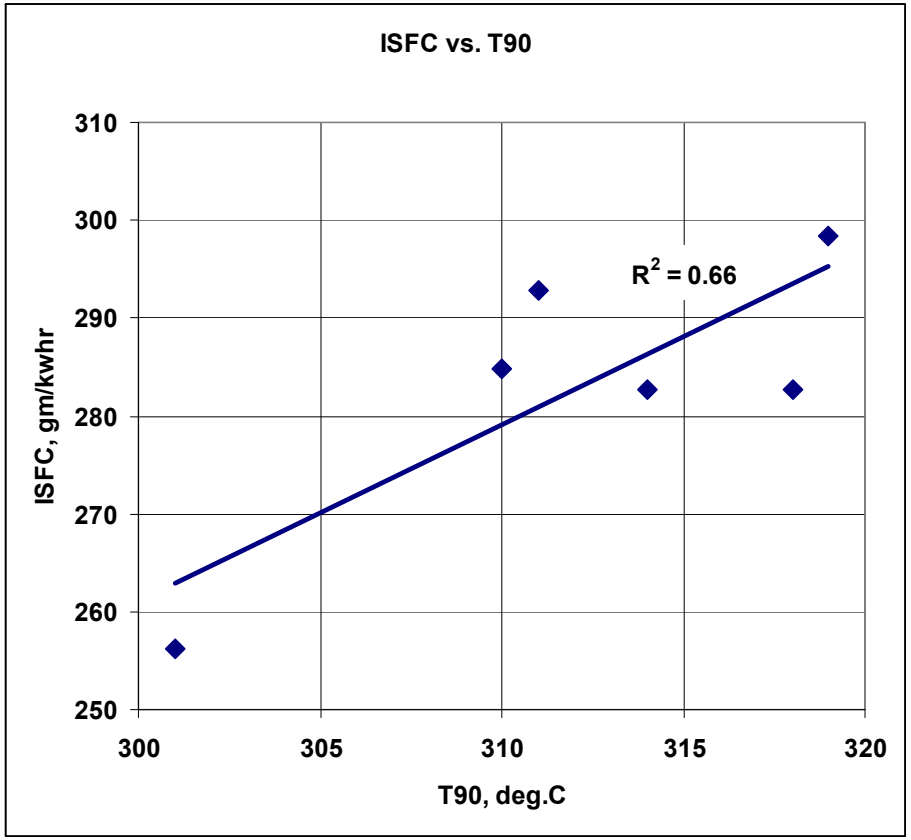


Biodiesel blends all require more advanced timing for optimum fuel efficiency



Examples of correlations





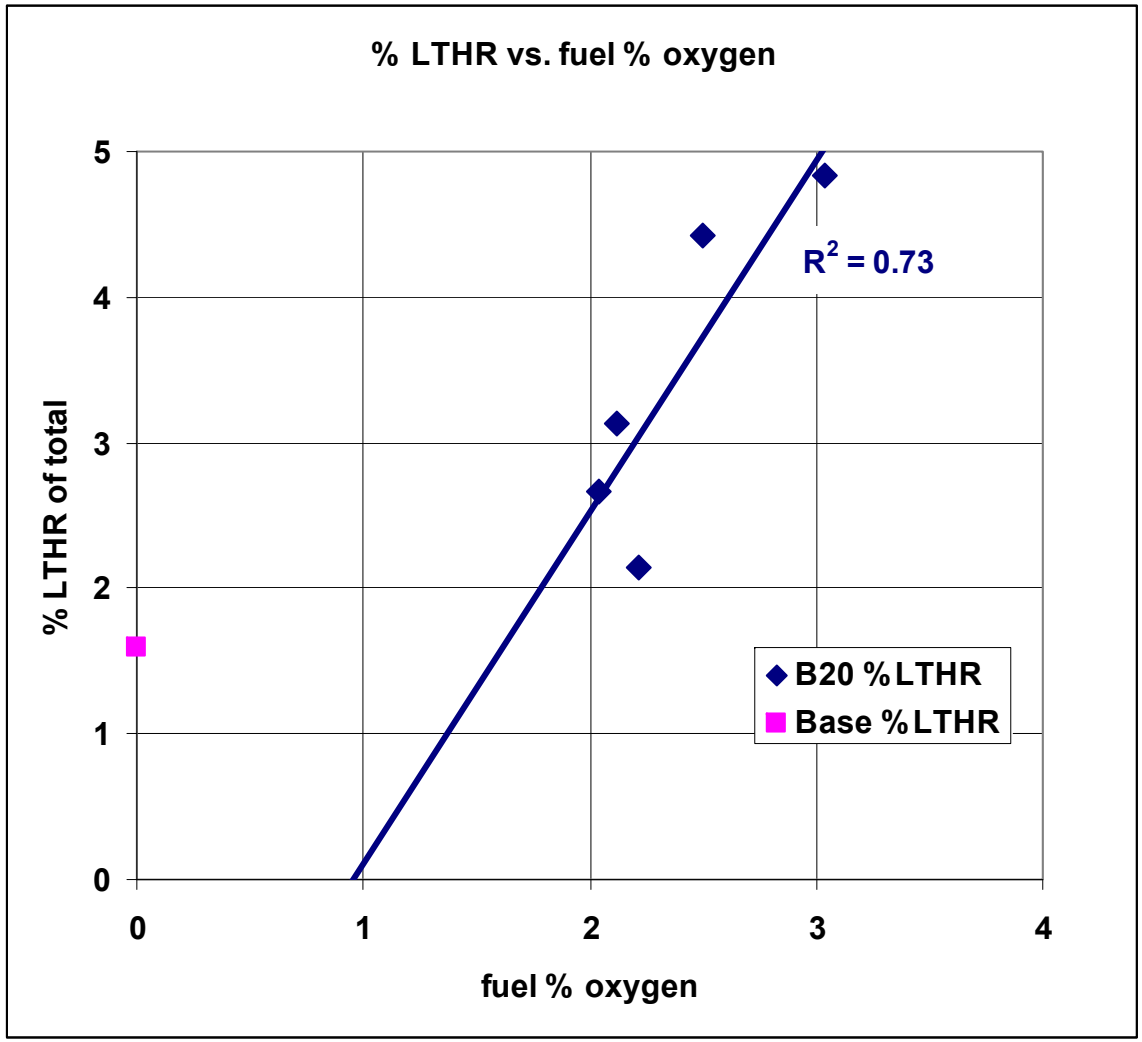
When contrasting B20 blends to base fuel

ISFC and ITE are worse with higher % O2 and with higher T90

But, when contrasting only B20 blends

ISFC does not correlate to % O2 or T90

% LTHR is higher for B20 blends and increases with % O2



Conclusions – diesel fuel set

- Most any fuel can be optimized to a maximum fuel efficiency
- Heavier fuels, with higher density, polyaromatics, and T50 and lower energy content produce worse ISFC and worst ITE
- Cetane can upset the balance between a fuel and an engine, but within limits can be compensated for by tuning changes
- Our models typically predict ISFC with a 95% confidence limit of ±11 gm/kWh or ±5 percent
  - Adequate for studying gross fuel effects variables on ISFC
  - Not adequate for final answer on fuel selection or engine tuning
- Larger fuel sets and further analysis will needed to resolve finer differences in fuel performance and engine matching

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Conclusions - oil sands derived

- Cetane number remains a major variable for predicting ignition behavior
- Major chemistry variable controlling cetane number is reverse relationship to mono-aromatics
  - Olefins also decrease cetane
  - Cetane increases slightly with boiling points
- Mixed cyclo-paraffins do not appear to possess unique chemistry for affecting cetane number or combustion characteristics

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Conclusions – biodiesel

- Probably explanation for worst ISFC of B20 blends
  - Increased low temperature heat release → Improved ignition
  - Lower intake temperature required → Possible fuel condensation in intake
  - Lower peak cylinder temperature → More prone to expansion stroke quenching
  - Earlier combustion phasing required → Moves us away from optimum for engine
- Bio-diesels from various fat sources are not interchangeable
  - Boiling point distribution, % oxygen, % unsaturated
  - Control changes required

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Some qualifiers on conclusions

- The conclusion that lower cetane improves HCCI engine performance has also been demonstrated by others but needs to be evaluated in more complex and flexible production-intent advanced combustion engines
- The conclusions relative to chemistry and property effects with these fuels is limited by number of fuels and inherent correlations between fuel properties and chemistry
- Chemistry effects of mixed refining streams may not be the same as chemistry effects of individual molecules

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Future work

- Compare HCCI and PCCI results to determine if same rules apply
- Deeper dive into chemistry and property relationships for fuels
- Compare combustion and performance of mixed-stream, refinery-derived fuels and simple surrogate blends to determine additional ways to optimize fuels
- Study fuel sensing and engine performance measurement correlations with goal of maintaining optimum engine performance across a slate of fuels
- Additional fuel sets
  - Biodiesel fuels with more variations in boiling point, oxygen content, and un-saturation
  - FACE diesel fuels
  - 'Optimum' fuel blends to confirm parametric conclusions
  - Oil shale derived fuel set – chemistry and boiling points
  - Additional refinery based fuels and intermediates
  - Model Fuels Consortium diesel surrogate blends
- Continue similar program for gasoline range fuels

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