Effects of Methyl Ester Biodiesel Blends on NOx Emissions

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Background

Impact of methyl ester biodiesel on regulated emissions:

- Reduces particulate matter
- Reduces unburned hydrocarbons
- **Effects on NOx vary in magnitude and even direction across multiple studies**

This study focused on B20 for adequate NOx response

Cause of Change in NOx Emissions Due to B20

Fundamental combustion effects due to fuel chemistry and fluid dynamics

- Generally engine independent

Interaction of the lower specific energy content of the biodiesel with the **engine control system**

- Interaction is engine specific

Approach

Gather an accurate **experimental data** set using a single cylinder engine operating on two commercial diesel fuels and B20 blends of those fuels.

Calibrate the KIVA combustion CFD **model**.

Investigate the fundamental combustion impact of B20.

Calculate the engine controls impact of B20.

Calculate the net impact of B20 on NOx over several key duty cycles.

Test Fuels

CN44	DF2 – higher aromatics
CN48	CN44 + 20% biodiesel
CN51	DF2 – lower aromatics
CN52	CN51 + 20% biodiesel

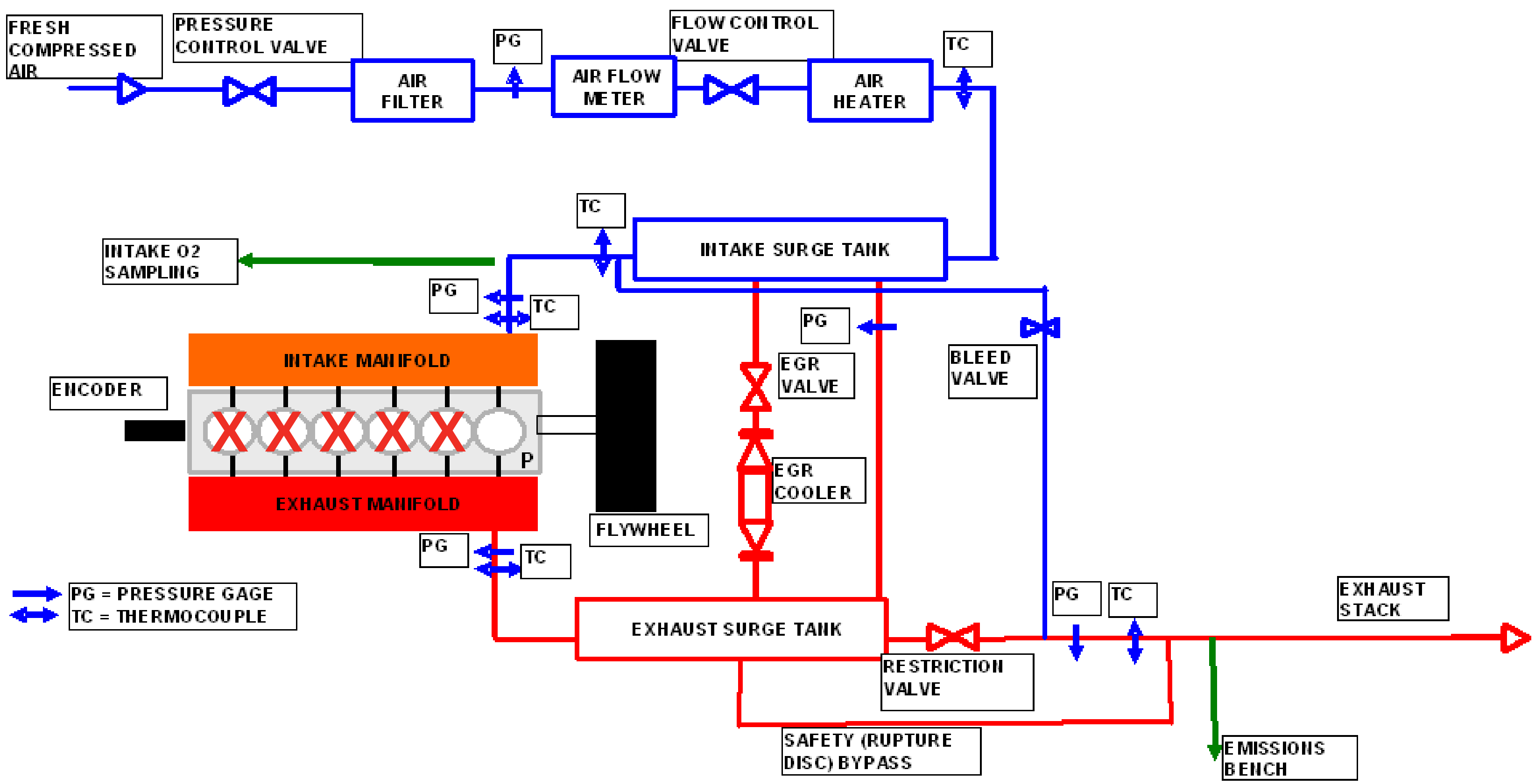
Fuel Properties

	Aromatics	Sulfur	Specific	Viscosity	Cetane
	(%)	ppm	Gravity	cSt	No
Method ASTM	**D5186**	**D5453**		**D445**	**D613**
High Aromatics Fuel - DF2 (CN44)	31.4	8	0.84	2.25	44.4
Low Aromatics Fuel - DF2 (CN51)	8.4	0	0.83	2.41	51
B20/High Aromatics - B20 (CN48)	25.1	6	0.85	2.54	48
B20/Low Aromatics - B20 (CN52)	6.7	0	0.84	2.63	51.5
B100	0	0	0.89	4.14	51.6

- **Cetane number is generally correlated with aromatic content.**
- **Higher aromatic fuels generally have lower cetane numbers.**

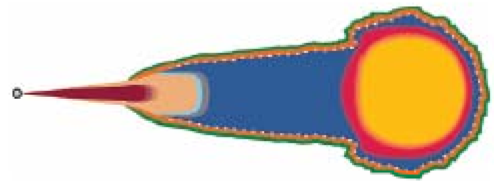
Single Cylinder Engine Test Setup

→ **CoV of Fuel Specific NOx<0.5%**



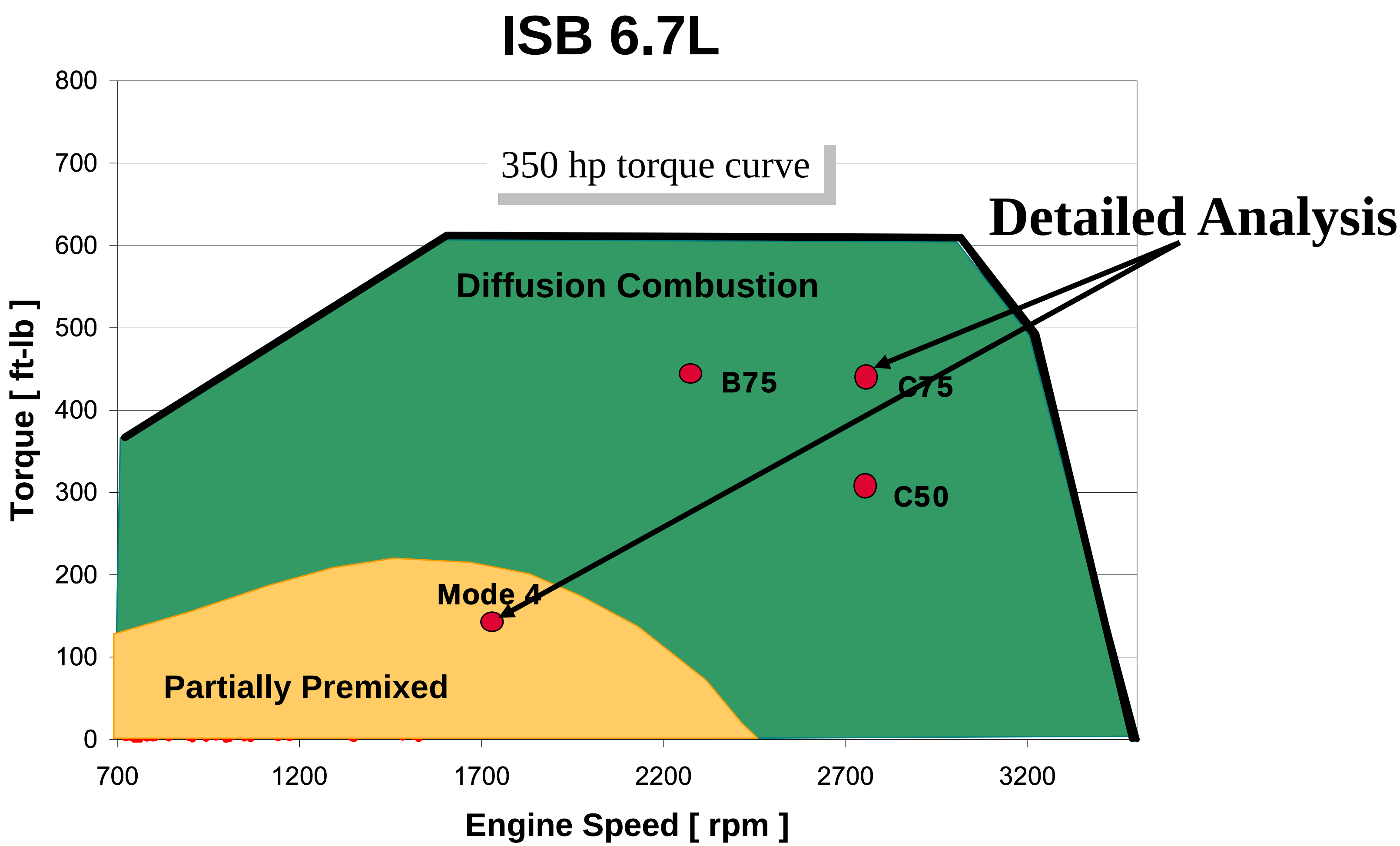
Combustion Modeling

KIVA3-RIF CFD Code



- Enables use of extensive biodiesel kinetics mechanisms
- Methyl butanoate selected for biodiesel mechanism
- Mixture of n-decane and α-methylnaphthelene for DF2
- 252 non-steady state species
- Surrogate fuel mixtures selected to match experimental autoignition characteristics of the blends

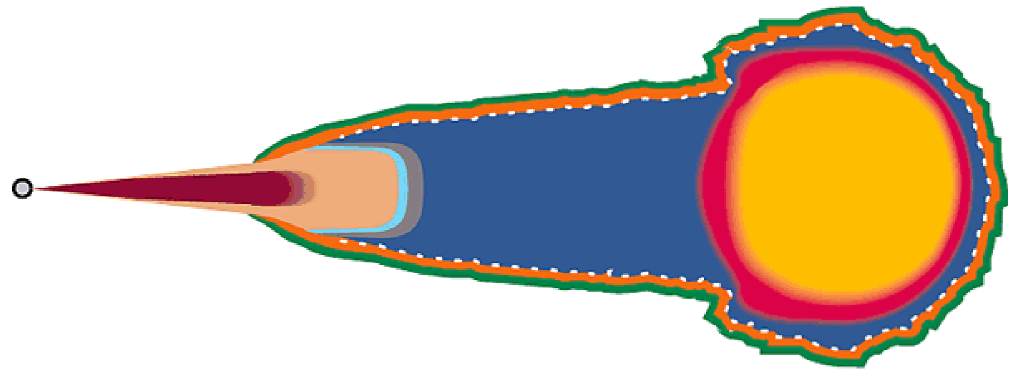
Engine Operating Conditions Used for Single Cylinder Testing



Fundamental Combustion Effects

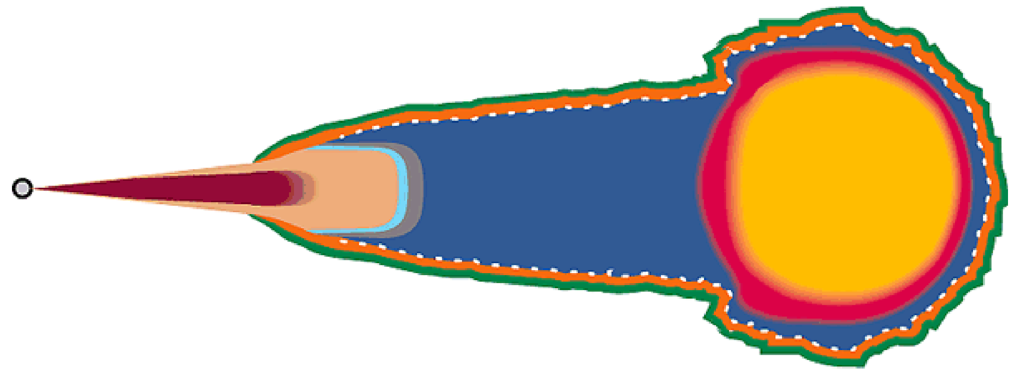
NOx ~ Temperature

Diesel Combustion



- Initial fuel injected into hot combustion air
- Fuel and air mix before combustion starts
- Initial combustion of pre-mixed fuel
  (lower temperature → lower NOx)
- Continued mixing and diffusion combustion
  as the rest of the fuel is injected
  (higher temperature → higher NOx)

Diesel Combustion



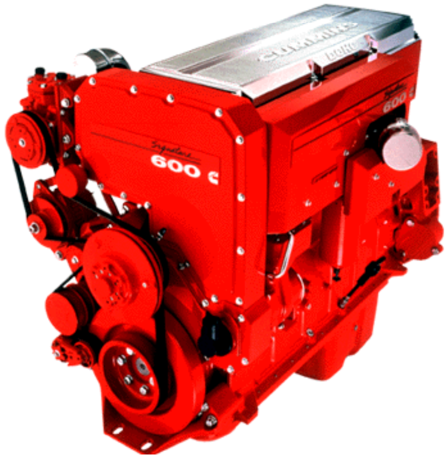
1. Premixed – depends on ignition delay

2. Diffusion controlled – dominant at high load

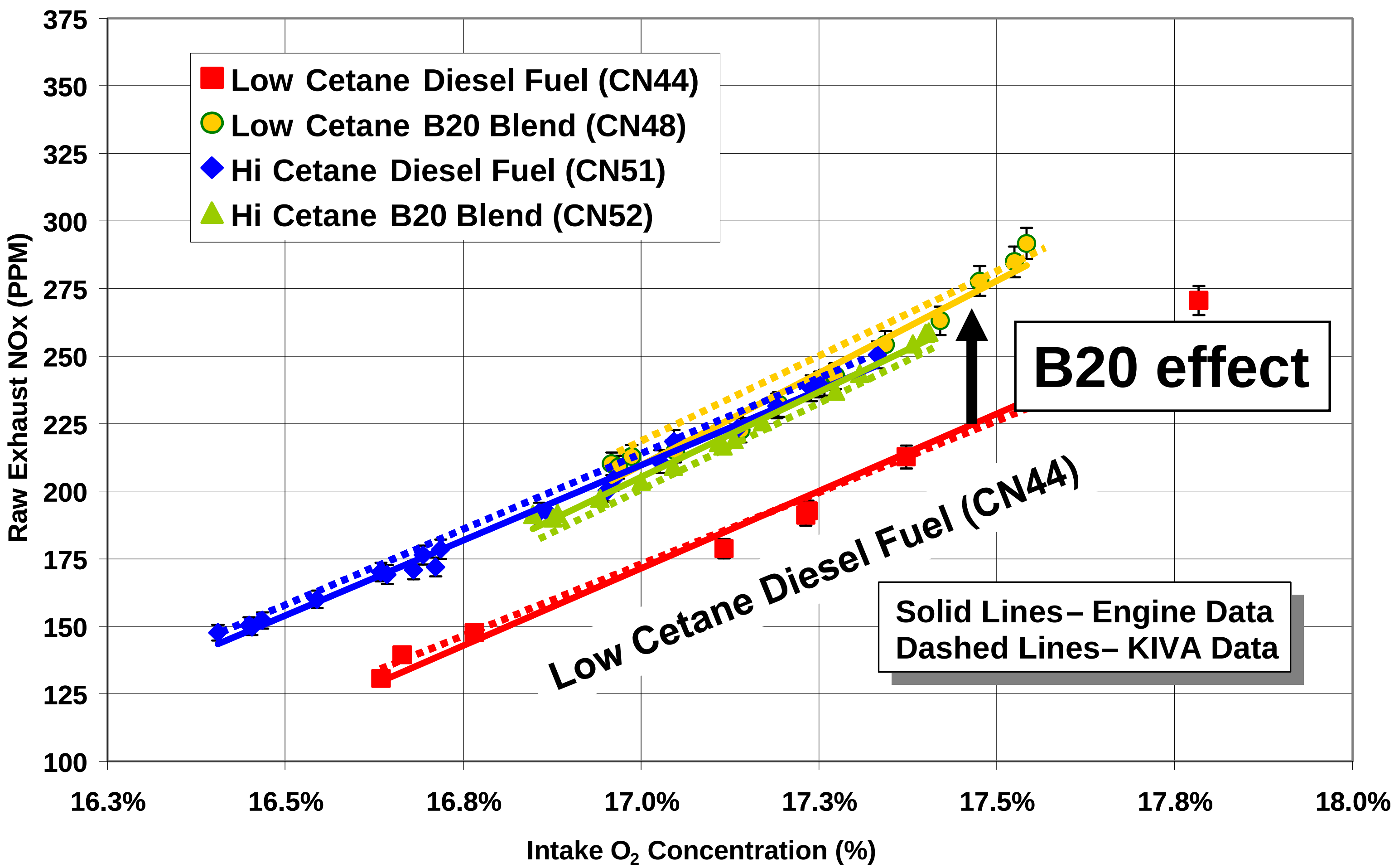
Fuel Effects on Combustion / NOx

Premixed fraction / Ignition delay is driven by cetane number (aromatics)

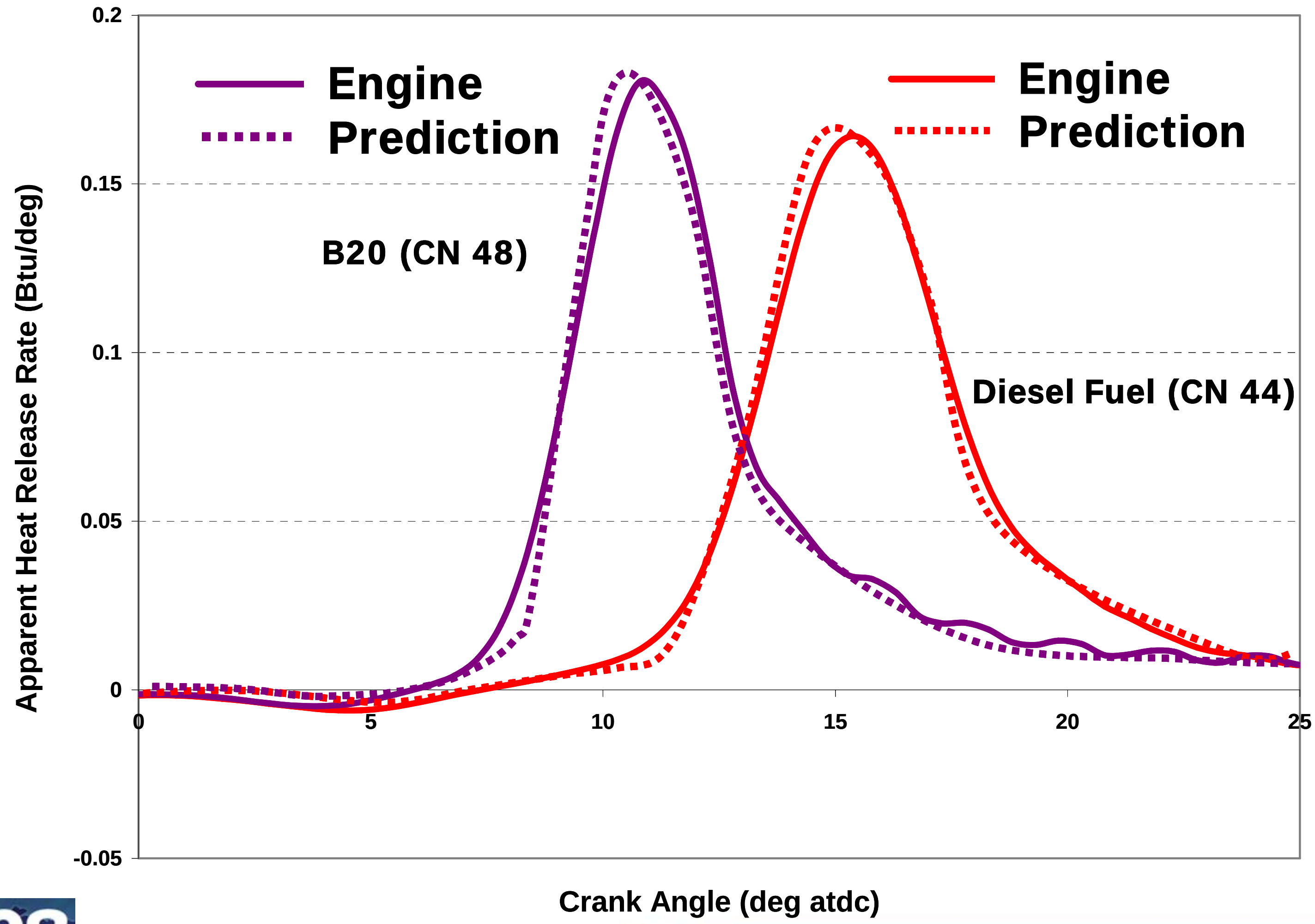
- Lower cetane → longer ignition delay → more premixing → lower NOx
- Not a linear effect – higher cetane fuels show less difference
- More important at lighter loads (a greater fraction of the fuel burns premixed)



Combustion at Mode 4 (Light Load)



Effect of Biodiesel on Ignition Delay



Combustion Effect at Low Load

Low cetane → longer ignition delay → more premixing → lower NOx

B20 blend has higher cetane number than its base fuel

B20 has a larger effect on NOx at **low load** with **low cetane fuels**

- B20 causes ~ 5% increase in NOx with lower cetane fuel on average across pre-mixed combustion zone

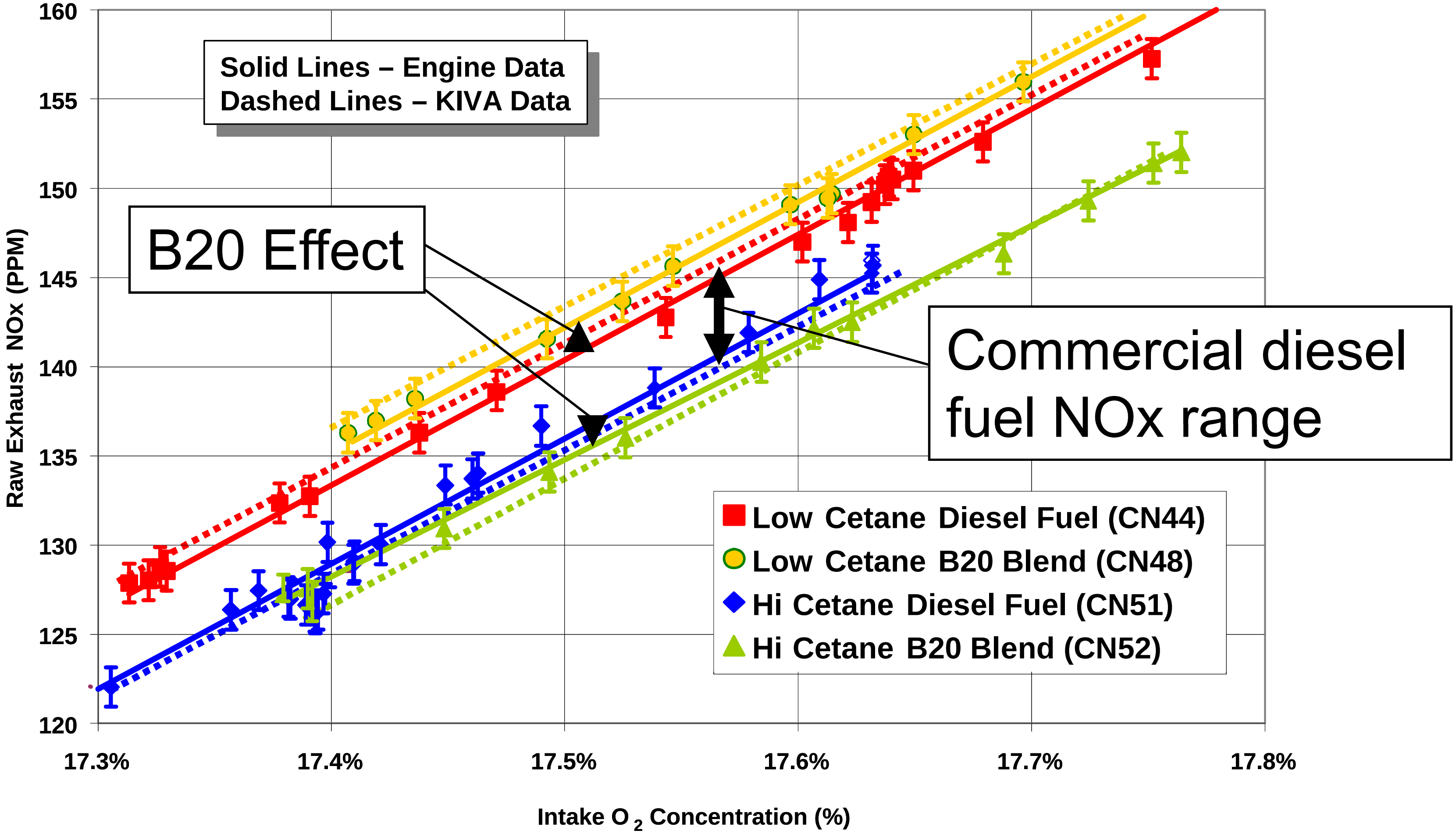
Small effect for higher cetane fuels

Fuel Effects on Combustion / NOx

NOx from **Diffusion Controlled Combustion** is driven by details of fuel chemistry

- Higher aromatics → higher T
- Double bonds in methyl-ester biodiesel → higher T
- Mono and Polyalkylbenzene reactivity is affected by methyl esters
  - Effect is larger for high aromatic fuels
  - Recent understanding

Diffusion Flame Combustion
C75 Condition (High Load)



Combustion Effect at High Load

High aromatic diesel fuels produce more NOx

B20 blends have a small effect on NOx (1%)

- Competing chemical mechanisms offset

Fundamental combustion effect of B20 on NOx at high load is less than the NOx difference measured between commercially available fuels

Summary of Fundamental Combustion Effects

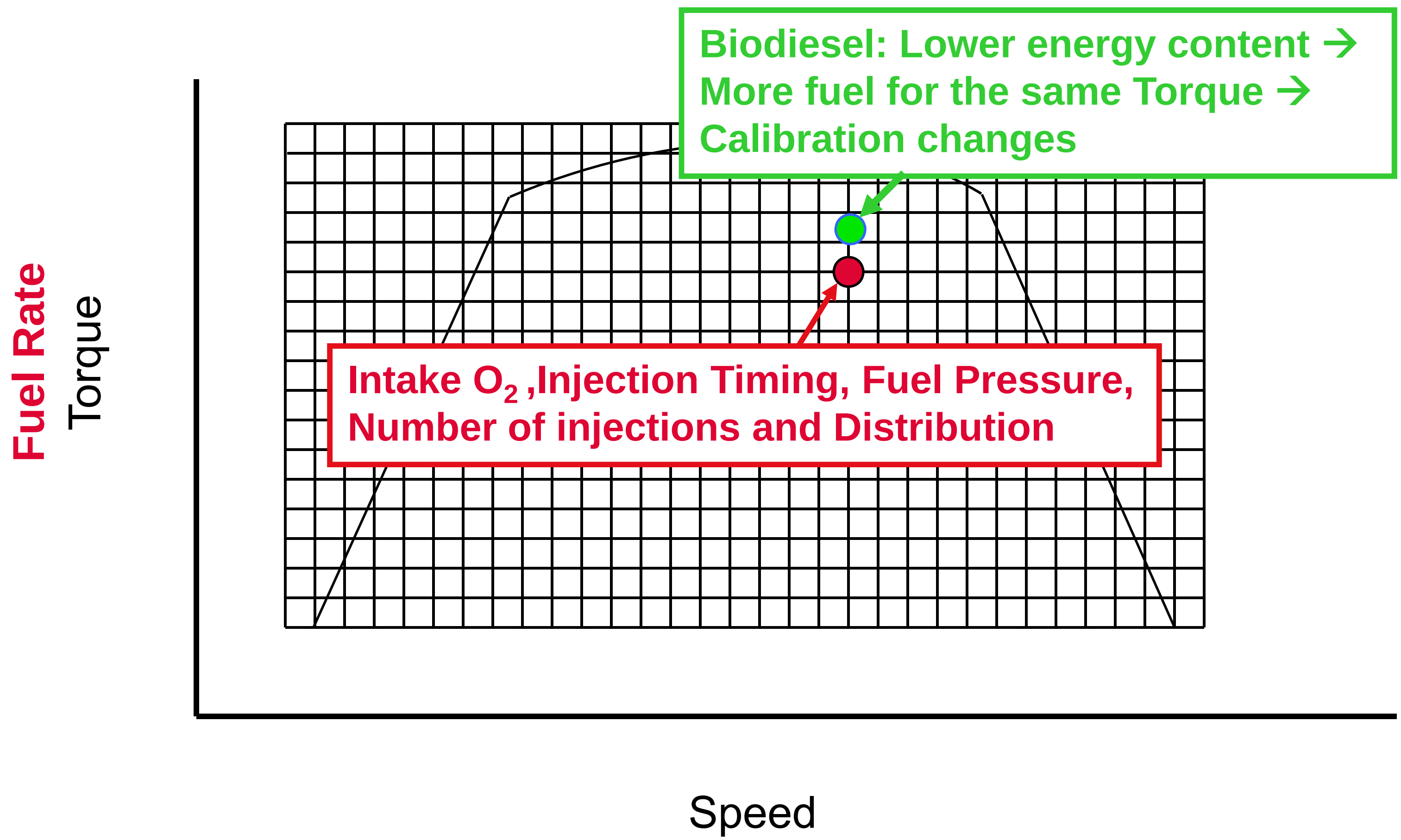
- Light load, lower cetane base fuel
→ B20 increased NOx ~ 5%

- Everywhere else: little effect

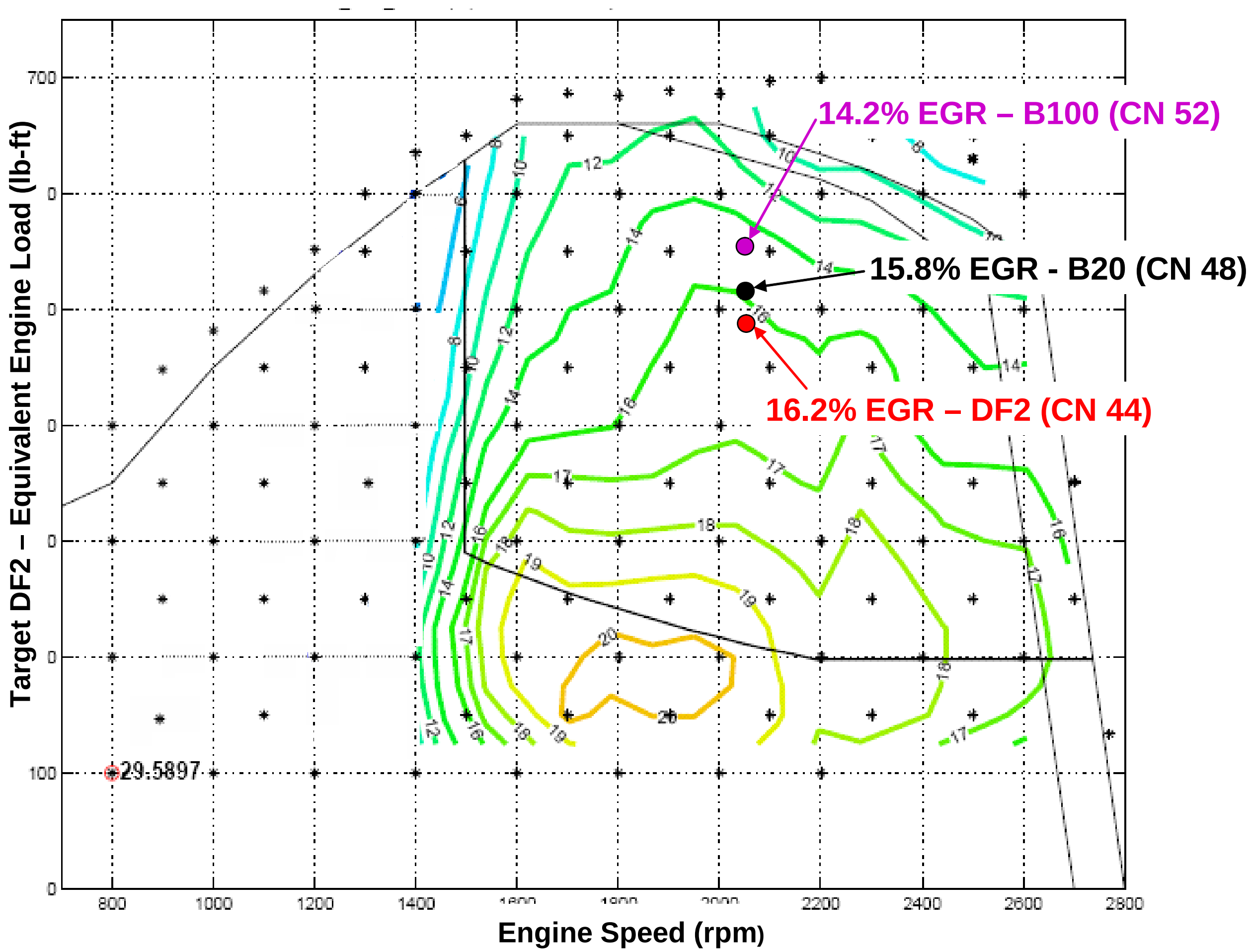
Interaction With Engine Controls

Controls effects are ***engine specific***…
so these observations and conclusions are for current Cummins electronic engines. With knowledge of controls calibration, similar calculations can be made for any engine.

Typical Engine Control Structure



Impact of Engine Controls on EGR at High-Load Condition



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Impact of Engine Controls at High-Load Condition

	Units	DF2 (CN 44)	B20 (CN 48)	Impact on NOx	% NOx Change
Intake O_2	%	18.7	19.1	↑	8.0
Main SOI	deg btdc	3.5	3.0	↓	- 4.5
Rail Pressure	bar	1275	1280	↑	1
Post Quantity	mg/stroke	9.1	9.5	↓	-1
Pilot Quantity	mg/stroke	0.02	0.02	—	0
IMT	^oF	156	156	—	0

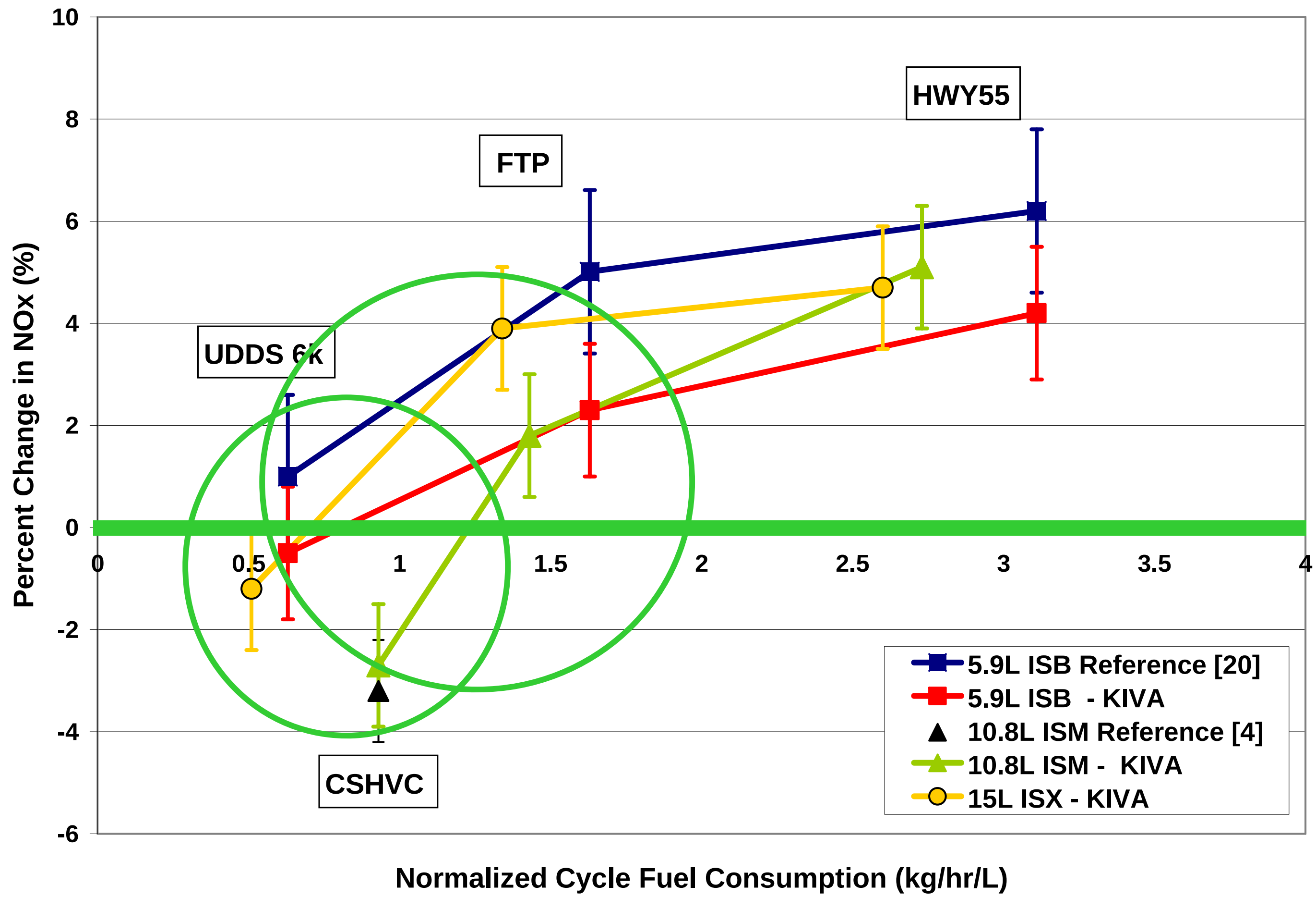
Combined NOx Impact for High-Load Operating Point

Impact of B20 on NOx at Constant Calibration (Combustion)	1.0%
Impact of B20 on NOx due to Engine Calibration	3.5%
Predicted Net NOx Increase	4.5%
Engine Data:	
DF2 (CN 44)	1.72 g/bhp-hr NOx
B20 (CN 48)	1.78 g/bhp-hr NOx
Net NOx Increase	3.5%

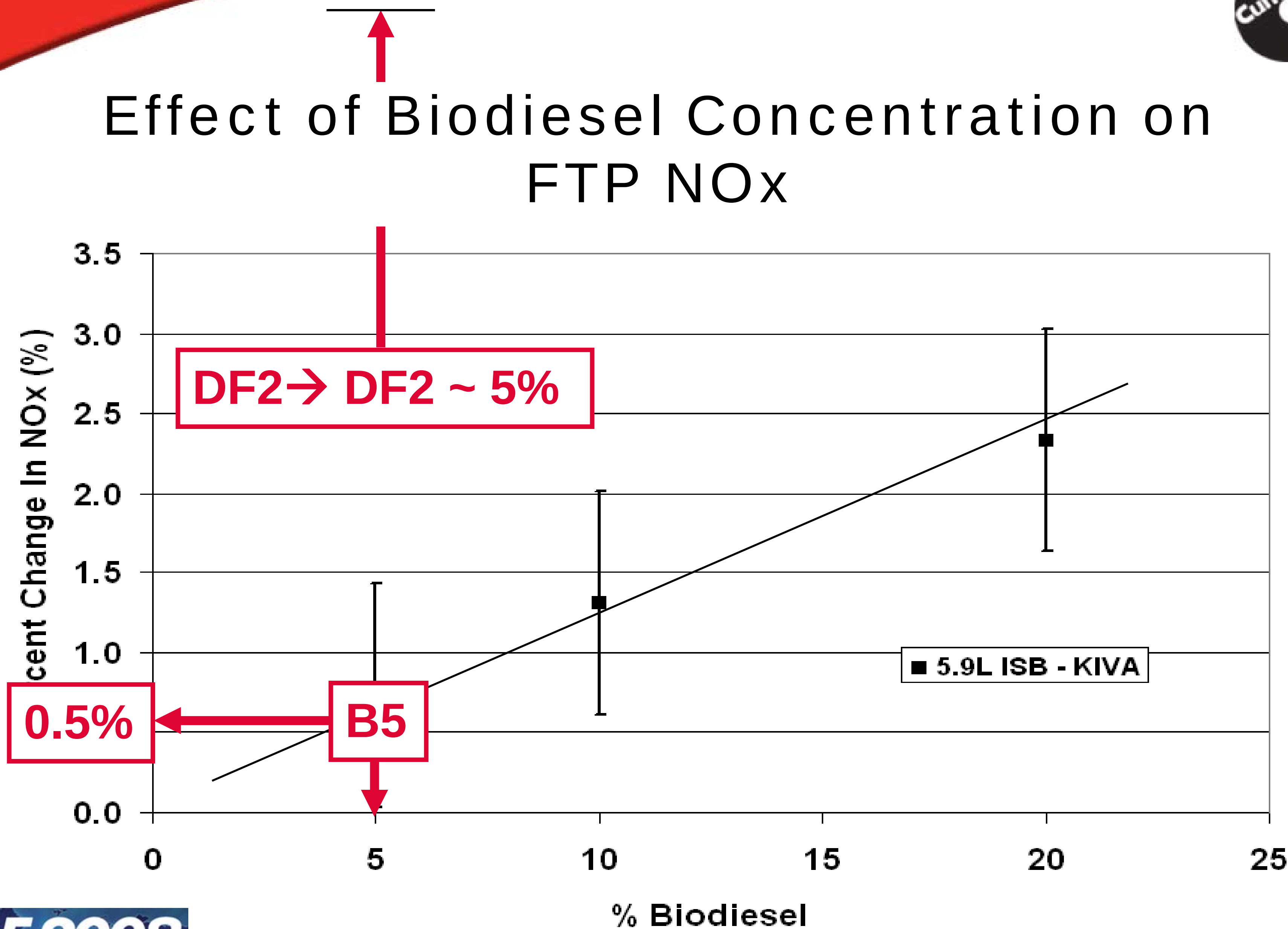
Combined NOx Impact for Low-Load Operating Point

Impact of B20 on NOx at Constant Calibration (Combustion)	5.3%
Impact of B20 on NOx due to Engine Calibration	-4.5%
Predicted Net NOx Increase	0.8%
Engine Data:	
DF2 (CN 44)	2.42 g/bhp-hr NOx
B20 (CN 48)	2.45 g/bhp-hr NOx
Net NOx Increase	1.3%

Change in NOx Emissions with B20 Blends for Several Engine Duty Cycles



Effect of Biodiesel Concentration on FTP NOx



Conclusions

Effect of B20 on NOx emissions is determined by **fundamental combustion** effects and interaction with **engine controls**. The experimentally observed "tailpipe NOX" effect is the sum of the two.

The net effect of combustion and engine controls on NOx at **low loads** depends on the cetane number of the blends: 1% increase with low cetane to a 5% decrease with high cetane.

The net effect of B20 on combustion and engine controls on NOx at **high loads** is a 4-5% increase. This is mostly due to engine controls.

Competing and contingent effects described in this paper explain the variation seen in published test results.

Summary: The Effects of B20 on NOx Emissions

APPLICATION		B20 EFFECT		
CETANE	LOAD	COMBUSTION EFFECT	CALIBRATION EFFECT	NET EFFECT
Low	Low	(+)	(-)	0
High	Low	0	(-)	(-)
Low	High	0	(+)	(+)
High	High	0	(+)	(+)

Conclusions

Expect an increase in NOx emissions at high average cycle power with B20 (~5%).

Expect equal or lower NOx emissions at low average cycle power.

Expect a small in-use NOx effect in urban duty cycles where biodiesel is generally used today.

The difference in NOx between a B20 blend and its base diesel fuel is less that the difference in NOx between two commercial diesel fuels within the range of fuels in the market today.

The NOx effect on the FTP varies linearly with biodiesel concentration from 0 to 20%. At B5 the net NOx effect is negligible.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