How Exhaust Emissions Drive Diesel Engine Fuel Efficiency

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Diesel Aftertreatment
Once it has “emerged”…

...\( NO_x \) aftertreatment has the potential to improve diesel engine fuel economy over current state-of-the-art
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NOx Adsorber Fuel Penalties

Assuming

- Hydrogen to carbon ratio in the fuel = 1.85 [mole/mole]
- NO\textsubscript{x} Rate = 2.5 [gm NO\textsubscript{2}/bHp/hr]
- Air to Fuel Ratio = 25:1 [lbm/lbm]
- bsfc = 0.350 [lb/bHp/hr]
- lean:rich adsorption cycle = 30:1 [sec/sec]

Yields a fuel penalty of

- adsorber NO\textsubscript{x} chemistry = 0.405%
- O\textsubscript{2} consumption using exhaust reductant = 2.408%
- HC slip = 0.088%
- total = 2.9%
NOx Adsorber Chemistry

Adsorption

\[ 2 \text{NO} + \text{O}_2 \rightarrow 2 \text{NO}_2 \]
\[ 2 \text{NO}_2 + \text{MO} + \frac{1}{2} \text{O}_2 \rightarrow \text{M(NO}_3)_2 \]

overall
\[ 2 \text{NO} + \frac{3}{2} \text{O}_2 + \text{MO} \rightarrow \text{M(NO}_3)_2 \]

Desorption with CO

\[ \text{M(NO}_3)_2 + 3 \text{CO} + \frac{3}{2} \text{O}_2 \rightarrow \text{MO} + 2 \text{NO} + 3 \text{CO}_2 \]

Reduction with CO

\[ 2 \text{NO} + 2 \text{CO} \rightarrow \text{N}_2 + 2 \text{CO}_2 \]

\[ \therefore \text{five moles of CO are required to desorb and reduce two moles of NO} \]
NOx Adsorber Chemistry (cont.)

Adsorption

$$2\text{NO} + \frac{3}{2}\text{O}_2 + \text{MO} \rightarrow \text{M(NO}_3)_2$$

Desorption with CH$_{1.85}$

$$\text{M(NO}_3)_2 + 1.02564\text{ CH}_{1.85} \rightarrow \text{MO} + 2\text{NO} + 1.02564\text{ CO}_2 + 0.94872\text{ H}_2\text{O}$$

Desorption and reduction with CH$_{1.85}$

$$\text{M(NO}_3)_2 + 1.7094\text{ CH}_{1.85} \rightarrow \text{MO} + \text{N}_2 + 1.7094\text{ CO}_2 + 1.5812\text{ H}_2\text{O}$$

∴ 0.8547 moles of CH$_{1.85}$ are required to convert one mole of NO.
NOx Chemistry Fuel Penalty

NOX ≡ NO_x reduction rate [gm NO_2/bHp/hr]

\[ \frac{\text{NOX}}{46} \] mole NO_2/bHp/hr environment

\[ \frac{\text{NOX}}{46} \] mole NO/bHp/hr engine exhaust

stoichiometry → \( \frac{\text{NOX} \times 0.8547}{46} \) mole CH_{1.85}/bHp/hr

\( \frac{\text{NOX} \times 13.85 \times 0.8547}{46} \) gm CH_{1.85}/bHp/hr

\( \frac{\text{NOX} \times 13.85 \times 0.8547}{46} / 454 \) lb CH_{1.85}/bHp/hr

∴ NO_x chemistry fuel penalty (as a percentage):

\[ \frac{0.0567 \times \text{NOX}}{\text{BSFC}} \] [%]

∴ Example: To remove 2.5 gm of NO_x at 0.350 bsfc:

\[ 0.0567 \times 2.5 / 0.350 = 0.405\% \]
NOx Chemistry Is Minor Factor

% fuel penalty vs. NOx Reduction [gm/bHp/hr]

bsfc [lbm/bHp/hr]

0.25, 0.27, 0.29, 0.31, 0.33, 0.35, 0.37, 0.39, 0.41, 0.43, 0.45, 0.47, 0.49
HC Slip Fuel Penalty

NMHC ≡ Non-Methane Hydrocarbon reduction rate

\[
NMHC \, [gm \, CH_{1.85}\,/bHp/hr] = \{NMHC \, /454\} \, [lbm \, CH_{1.85}\,/bHp/hr]
\]

HC slip fuel penalty (as a percentage) is simply the ratio:

\[
\{100*NMHC \, /454/ \, BSFC \} \, [%]
\]

∴ Example: Assuming 2007HD NMHC level of 0.14g/bHp/hr and 0.350 bsfc:

fuel penalty = 100*0.14/454/0.350 = 0.088%

Note: 0.088% assumes that no tailpipe HC are methane and that no stored (on the catalyst) HC are oxidized during the lean operating period
Oxygen Consumption Fuel Penalty

Stoichiometric Oxidation of CH$_{1.85}$

\[ O_2 + 0.68376 \text{ CH}_{1.85} \rightarrow 0.68376 \text{ CO}_2 + 0.63248 \text{ H}_2\text{O} \]

\[ \therefore \text{ stoichiometry} = 0.68376 \text{ [mole CH}_{1.85}/\text{mole O}_2] \]

Lean oxidation of CH$_{1.85}$

\[ (0.2095 \text{ O}_2 + 0.7905 \text{ N}_2) + \phi \text{ CH}_{1.85} \rightarrow (0.2095 - 5.85/4*\phi) \text{ O}_2 + 0.7905 \text{ N}_2 + \phi \text{ CO}_2 + (1.85/2) \phi \text{ H}_2\text{O} \]

\[ \therefore \text{ exhaust oxygen concentration:} \]

\[ \{(0.2095 - 1.4625*\phi)/(1.0 + 0.4625*\phi)\} \text{ [mole O}_2/\text{mole exh]} \]
O2 Consumption Fuel Penalty (cont.)

AFR \equiv \text{Air to Fuel Ratio} \ [\text{lbm air/lbm CH}_{1.85}] \\
= \{28.96/\phi /13.85\} \ [\text{gm air/gm CH}_{1.85}]

ExO2 \equiv \text{O}_2 \text{ concentration in the exhaust} \ [\text{mole } \text{O}_2/\text{mole exh}] \\
= \{(0.2095*\text{AFR} –3.0581)/(\text{AFR} +0.9670)\} \ [\text{mole } \text{O}_2/\text{mole exh}]

Please note the following relationship for exhaust flow rate:

(exhaust flow rate)/(fresh air flow rate) = \{1.0 + 1.0/\text{AFR}\} \ [\text{lb }/\text{lb}]
O2 Consumption Fuel Penalty (cont.)

Putting it all together…

\[ \text{[mole CH}_{1.85} / \text{mole exhaust]} \rightarrow \{\text{ExO}_2 \cdot 0.68376\} \]
\[ \text{[gm CH}_{1.85} / \text{gm exhaust]} \rightarrow \{\text{ExO}_2 \cdot 0.68376 \cdot 13.85/28.8\} \text{ see note} \]
\[ \text{[lbm CH}_{1.85} / \text{lbm intake air]} \rightarrow \{\text{ExO}_2 \cdot 0.68376 \cdot 13.85/28.8 \cdot (1.0 + 1.0/\text{AFR})\} \]
\[ \text{[lbm CH}_{1.85} / \text{lbm engine fueling]} \rightarrow \{\text{ExO}_2 \cdot 0.68376 \cdot 13.85/28.8 \cdot (\text{AFR} + 1.0)\} \]

**Note:** exhaust gas molecular weight was assumed to be 28.8
O2 Consumption Fuel Penalty (cont.)

...yields the oxygen depletion fuel penalty:

\[
\text{[lbm CH}_{1.85}/\text{lbm engine fueling]} \rightarrow \frac{(0.2095 \times \text{AFR} - 3.058)}{(\text{AFR} + 0.967) \times 0.684 \times 13.85/28.8 \times \text{AFR} + 1)}
\]

or approximately...

\[
\text{[lbm CH}_{1.85}/\text{lbm engine fueling]} \rightarrow \frac{(0.2095 \times \text{AFR} - 3.058) \times 0.684 \times 13.85/28.8}{(\text{lean:rich})} \%
\]

Finally, accounting for rich-lean cycling:

\[
\frac{(6.89 \times \text{AFR} - 100)}{(\text{lean:rich})} \%
\]

**Example:** To remove exhaust O₂ at 25 AFR and 30:1 lean rich yields a fuel penalty of:

\[
\frac{(6.89 \times 25 - 100)}{30} = 2.41\%
\]
Oxygen Consumption Fuel Penalty

Three approaches:

– reduce exhaust flow to the catalyst w/bypass
  • analysis done but not included (available on request)

– increase adsorption/regeneration time ratios

– operate the engine at low air/fuel ratios
  • throttle the engine (decrease air)
  • increase EGR rates (decrease air)
  • destroy efficiency (increase fuel)
Oxygen Consumption Fuel Penalty

Three approaches:

- reduce exhaust flow to the catalyst w/bypass
  - analysis done but not included (available on request)
- increase adsorption/regeneration time ratios
- operate the engine at low air/fuel ratios
  - throttle the engine (decrease air)
  - increase EGR rates (decrease air)
  - destroy efficiency (increase fuel)
In-Cylinder Enrichment

Cycle Avg Fuel Penalty [%]

lean/rich [sec/sec]
- 10
- 20
- 30
- 40
- 50

rich/lean bsfc ratio [-]
Adsorber Fuel Penalty Equation

penalty [%] =

\{100 \times (0.000567) \times \text{NOX} / \text{BSFC} \} + \\
\{100 \times \text{NMHC} / 454/ \text{BSFC} \} + \\
\{(0.206 \times \text{AFR} - 3.058) / (\text{AFR} + 0.967) \times \\
0.684 \times 13.85 / 28.8 \times (\text{AFR} + 1.0) / \\
(\text{lean:rich})\}
Conclusion #1

With maturity NO$_x$ Adsorbers will allow engine retune

- 2.5 gm NO$_x$ → 2.9% fuel penalty
- 5.0 gm NO$_x$ → 3.3% fuel penalty

**Note:** this argument is not unlike the case some are making for urea-SCR (primarily in Europe)

Key science need – better understanding of the desorption/regeneration phenomenon
Aftertreatment will save fuel!

A Classic NO\textsubscript{x} & BSFC Curve

Adsorber tradeoff curve
Conclusion #2

Given that $O_2$ depletion is the biggest piece of the fuel penalty and the strong relationship with Air-to-Fuel ratio,

$$\frac{(6.89 \times \text{AFR} - 100)}{\text{(lean:rich)}} \%$$

$\text{NO}_x$ Adsorbers will have a relatively larger fuel penalty under lighter load operating conditions.

- 2.4% penalty at 25:1 AFR
- 10.5% penalty at 60:1 AFR
- 20% penalty at 100:1 AFR

Which implies one of two strategies:

- (massive) EGR rates for AFR reduction
- dual mode w/HCCI-like combustion at light loads
EGR Effect on Oxygen Concentration

![Graph showing the effect of EGR rate on oxygen concentration for different oxygen concentrations (16%, 17%, 18%, 19%, 20%) and fresh A/F ratios (15 to 85).](01MunteanGeorge.ppt)
HCCI(like) Combustion and NOx Adsorbers

- Exhaust system enrichment
- In-cylinder enrichment
- HCCI mode

Engine Speed [RPM]

BMEP [bar]

FTP75
Overview

**NO\textsubscript{x} Adsorbers**
- NO\textsubscript{x} chemistry
- HC slip
- Oxygen depletion

**Lean NO\textsubscript{x}**
- NO\textsubscript{x} chemistry
- Selectivity
- Activity

**Particulate Filters**
- Backpressure
- Regeneration (Enthalpy)
HC Lean NOx Fuel Penalties

Assuming

- Hydrogen to carbon ratio in the fuel = 1.85 [mole/mole]
- NO_x Rate = 2.5 [gm NO_2/bHp/hr]
- Air to Fuel Ratio = 25:1 [lbm/lbm]
- bsfc = 0.350 [lbm/bHp/hr]
- C:N (typical optimum for lean NO_x) = 6 [m CH_{1.85}/m NO]

Yields fuel penalties of

- Ideal lean NO_x chemistry = 0.162%
- Actual lean NO_x chemistry = 2.84%
- Current system selectivity = 2.85%

Note: Higher C:N yields better reduction but with diminishing returns
Ideal Lean NOx Chemistry

Ideal NO\textsubscript{x} reduction with CH\textsubscript{1.85}

\[ \text{NO} + 0.3419 \text{ CH}_{1.85} \rightarrow \frac{1}{2} \text{ N}_2 + 0.3419 \text{ CO}_2 + 0.3162 \text{ H}_2\text{O} \]

∴ 0.3419 moles of CH\textsubscript{1.85} are required to convert one mole of NO

From ideal lean NO\textsubscript{x} chemistry

\[ \text{NOX} \text{ stoichiometry} \rightarrow \text{NOX} \times 0.3419 \times 46 \text{ [mole CH}_{1.85} \text{ /bHp/hr]} \]

\[ \text{NOX} \times 13.85 	imes 0.3419 \times 46 \times 454 \text{ [lb CH}_{1.85} \text{ /bHp/hr]} \]

∴ Ideal fuel penalty (as a percentage):

\[ \{100 \times 13.85 \times 0.3419 \times 46 \times 454 \times \text{NOX} / \text{BSFC} \} \% \]

∴ Example: To remove 2.5 gm of NO\textsubscript{x} at 0.350 bsfc:

100 \times 0.000227 \times 2.5 / 0.350 = 0.162\%
Real Lean NOx Chemistry

C:N ≡ carbon to NO\textsubscript{x} molar ratio - unit conversion

\[ \text{C:N} \ [\text{moles CH}_{1.85}/\text{moles NO}] \rightarrow \{\text{C:N } \times 13.85/46\} \ [\text{gm HC/gm NO}\textsubscript{2}] \]

SELECTIVITY: lean NO\textsubscript{x} reduction competes with direct oxidation

\[ \text{NO} + (5.85/4\times\text{C:N} - 1/2) \text{O}_2 + (\text{C:N} ) \text{CH}_{1.85} \rightarrow \]
\[ \frac{1}{2} \text{N}_2 + \text{C:N} \text{ CO}_2 + (\text{C:N} \times 1.85/2) \text{H}_2\text{O} \]

∴ Selectivity = \[100 \times 0.3419/\text{C:N}\] [%]

∴ Fuel penalty (as a percentage):

\[\{100 \times 13.85/46/454*\text{C:N} \times \text{NOX }/\text{BSFC}\}\]

[%]

∴ Example: To remove 2.5 gm of NO\textsubscript{x} at 0.350 bsfc with a C:N of 6:

\[0.06632 \times 6 \times 2.5/0.350 = 2.84\%
\]

(w/selectivity of: \[100 \times 0.3419/6 = 5.70\%\])
Real Lean NOx Chemistry (cont.)

ACTIVITY: lean NO\textsubscript{x} reduction is not yet 100% efficient

\[ \text{NO} + \left( \frac{5.85}{4} \times \text{C:N} - \text{act} /2 \right) \text{O}_2 + \left( \text{C:N} \right) \text{CH}_{1.85} \rightarrow \]
\[ (1-\text{act}) \text{NO} + \left( \frac{\text{act}}{2} \right) \text{N}_2 + \text{C:N} \ \text{CO}_2 + \left( \text{C:N} \times \frac{1.85}{2} \right) \text{H}_2\text{O} \]

∴ Activity impacts selectivity.

Selectivity = \{100 \times \text{act} \times 0.3419 / \text{C:N} \} \, [%]

∴ Example: To remove NO\textsubscript{x} at 50% efficiency with a C:N of 6 yields a selectivity of \{100 \times 0.5 \times 0.3419 / 6\} = 2.85%

Note: I’m being somewhat loose with my definition of selectivity and activity.
Conclusion

Lean NO$_x$ catalysis is the ‘Holy Grail’ for diesel engines

- minimal complexity
- low impact on engine design
- potentially low cost
- potential for high durability and reliability

Like absorbers, if lean NO$_x$ catalysis can be made to work they WILL ultimately prove to be a fuel SAVINGS device.

However!

Key science - We need (HC) lean NO$_x$ to be *nearly* as selective and active as urea-SCR.
Overview

**NO\textsubscript{x} Adsorbers**
- NO\textsubscript{x} chemistry
- HC slip
- Oxygen depletion

**Lean NO\textsubscript{x}**
- NO\textsubscript{x} chemistry
- Selectivity
- Activity

**Particulate Filters**
- Backpressure
- Regeneration (Enthalpy)
Particulate Filter Fuel Penalties

Assuming

- BMEP = 100 [psi]
- Backpressure = 1 [psi]
- Air to Fuel Ratio = 25:1 [lbm/lbm]
- bsfc = 0.350 [lbm/bHp/hr]
- Temp rise in exhaust (dT) = 100 [deg F]
- Regeneration duty cycle (DC) = 10%

Yields fuel penalties of

- Backpressure fuel penalty = 1.0%
- Cycle average regeneration penalty = 0.34%
- Total penalty = 1.34%

Note: These penalties are highly duty-cycle dependent!
Backpressure

BMEP is directly impacted by backpressure

exhaust stroke

pressure = work

Cylinder Pressure [psia]

Cylinder Volume [in³]
Backpressure

Assuming

<table>
<thead>
<tr>
<th>BMEP</th>
<th>= 100 [psi]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Backpressure</td>
<td>= 1 [psi]</td>
</tr>
</tbody>
</table>

From simple reasoning

one psi backpressure removes one psi of useful work from the piston which must be recovered from increased fueling:

approx. fuel penalty = \( \frac{100 \times \text{backpressure}}{\text{bmep}} \) [%]

∴ **Example:** One psi backpressure at 100 psi bmep:

\[ \frac{100 \times 1.0}{100} = 1.0\% \]
Enthalpy

Assuming

- Diesel fuel heating value (higher) = 18500 [Btu/lbm]
- \( C_p \) = 0.2412 [Btu/lbm/F]
- Duty Cycle (DC) = 10 [%]

From \( dH = C_p \, dT \)

\[
18500 \text{ [Btu/lbm suppl. fuel]} = 0.2412 \text{ [Btu/lbm exhaust/deg F]} \times dT \text{ [deg F]} \times (AFR + 1) \text{ [lbm exh/lbm fueling]} \times (1/\text{efficiency}) \text{ [lbm fueling/lbm suppl. Fuel]}
\]

:: fuel penalty during regen is...

\[
\left\{ \frac{(1+AFR) \times 0.2412 \times dT}{18500 \times DC} \right\} \text{ [%]}
\]

:: Example: Penalty for 100 deg F rise at 25 AFR:

\[
(1+25) \times 0.2412 \times 100 \times \frac{1}{18500} \times 10 = 0.34\%
\]
DPF penalty w/10% duty cycle

Cycle Avg Fuel Penalty [%]

temperature increase [deg F]

air/fuel [lbm/lbm]

- 15
- 20
- 30
- 50
- 100
Conclusion

DPFs are unlikely to ever enhance a total system efficiency. Engine retune for efficiency will likely reduce DPF burden. Best one can hope for is to minimize the penalty.

Soot filter penalties are difficult to estimate
- # active regens required is entirely duty-cycle dependant
- backpressure is linked to regen history and flowrates
- soot oxidation characteristics are poorly understood

Key science – soot oxidation characterization, prediction and enhancement.
Once it has “emerged”…

\[ \text{NO}_x \] aftertreatment has the potential to improve diesel engine fuel economy over current state-of-the-art
And if you don’t believe it…

…consider where we have come in the last 25 years with TWC on gasoline engines!

Would you have believed that 30 years ago?