DEER 2004

Session 1 – Emerging Diesel Technology

Diesel Aftertreatment

How Exhaust Emissions Drive Diesel Engine Fuel Efficiency

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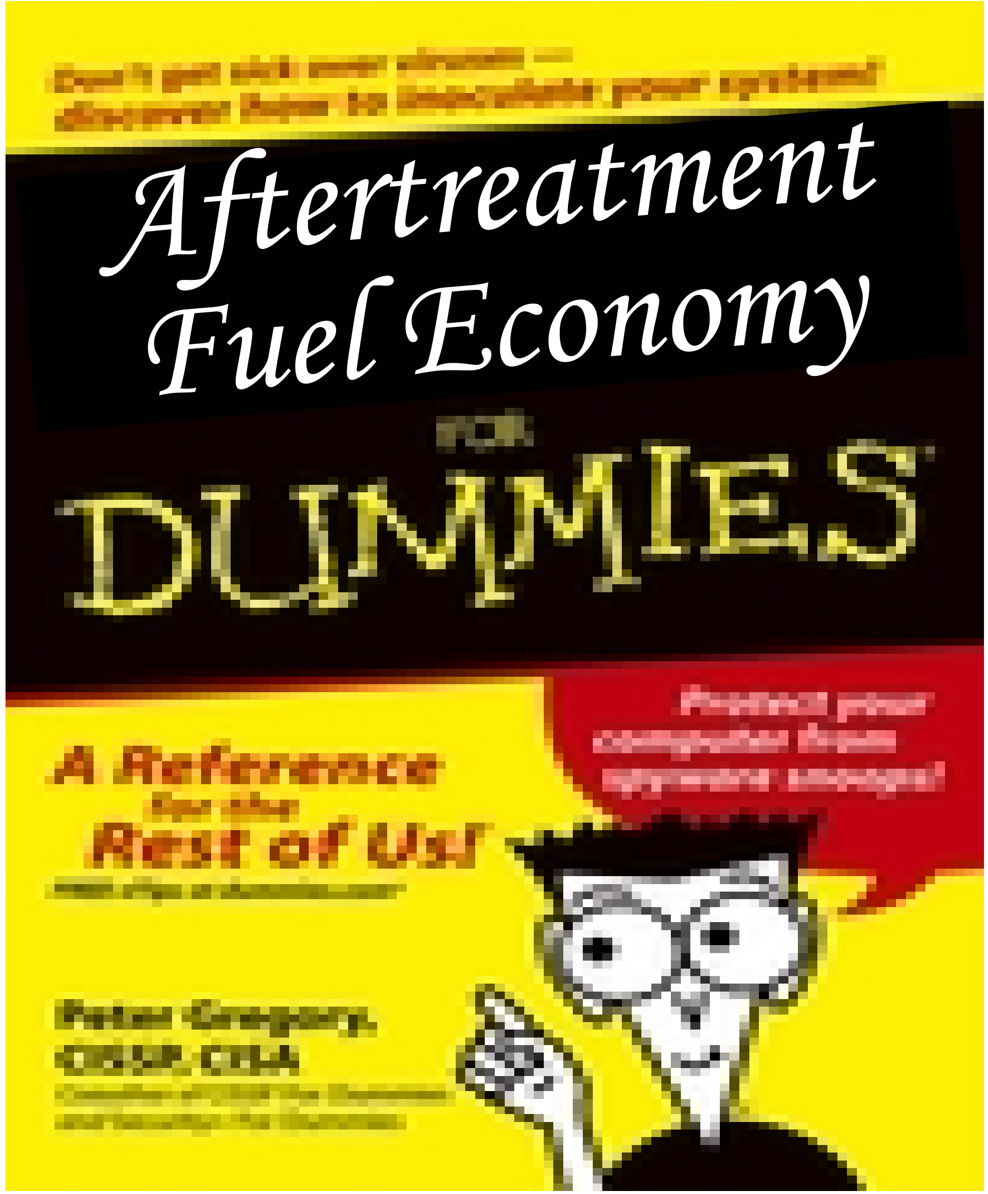
Once it has "emerged"…

…NO_x aftertreatment has the potential to improve diesel engine fuel economy over current state-of-the-art


Aftertreatment
Fuel Economy
FOR
DUMMIES
A Reference for the Rest of Us!
Peter Gregory,
CISSP, CISA

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NO_x Adsorber 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 [lb/bHp/hr]
lean:rich adsorption cycle	= 30:1 [sec/sec]

Yields a fuel penalty of

adsorber NO_x chemistry	= 0.405%
O_2 consumption using exhaust reductant	= 2.408%
HC slip	= 0.088%
total	= **2.9%**

NO_x Adsorber Chemistry

Adsorption

$$2\ NO + O_2 \rightarrow 2\ NO_2$$

$$2\ NO_2 + MO + \frac{1}{2} O_2 \rightarrow M(NO_3)_2$$

overall

$$2\ NO + {}^3/_2\ O_2 + MO \rightarrow M(NO_3)_2$$

Desorption with CO

$$M(NO_3)_2 + 3\ CO + {}^3/_2\ O_2 \rightarrow MO + 2\ NO + 3\ CO_2$$

Reduction with CO

$$2\ NO + 2\ CO \rightarrow N_2 + 2\ CO_2$$

∴ **five moles of CO are required to desorb and reduce two moles of NO**

NO_x Adsorber Chemistry –cont-

Adsorption

$$2\ NO + {}^{3}/_{2}\ O_2 + MO \rightarrow M(NO_3)_2$$

Desorption with $CH_{1.85}$

$$M(NO_3)_2 + 1.02564\ CH_{1.85} \rightarrow$$
$$MO + 2\ NO + 1.02564\ CO_2 + 0.94872\ H_20$$

Desorption and reduction with $CH_{1.85}$

$$M(NO_3)_2 + 1.7094\ CH_{1.85} \rightarrow$$
$$MO + N_2 + 1.7094\ CO_2 + 1.5812\ H_20$$

∴ **0.8547 moles of $CH_{1.85}$ are required to convert one mole of NO**

NO_x Chemistry Fuel Penalty

$\mathcal{NOX}$ **≡ NO_x reduction rate [gm NO_2/bHp/hr]**

$= \{\mathcal{NOX}/46\}$ [mole NO_2/bHp/hr] environment

$= \{\mathcal{NOX}/46\}$ [mole NO/bHp/hr] engine exhaust

stoichiometry $\rightarrow \{\mathcal{NOX}*0.8547/46\}$ [mole $CH_{1.85}$ /bHp/hr]

$= \{\mathcal{NOX}*13.85*0.8547/46\}$ [gm $CH_{1.85}$ /bHp/hr]

$= \{\mathcal{NOX}*13.85*0.8547/46/454\}$ [lb $CH_{1.85}$ /bHp/hr]

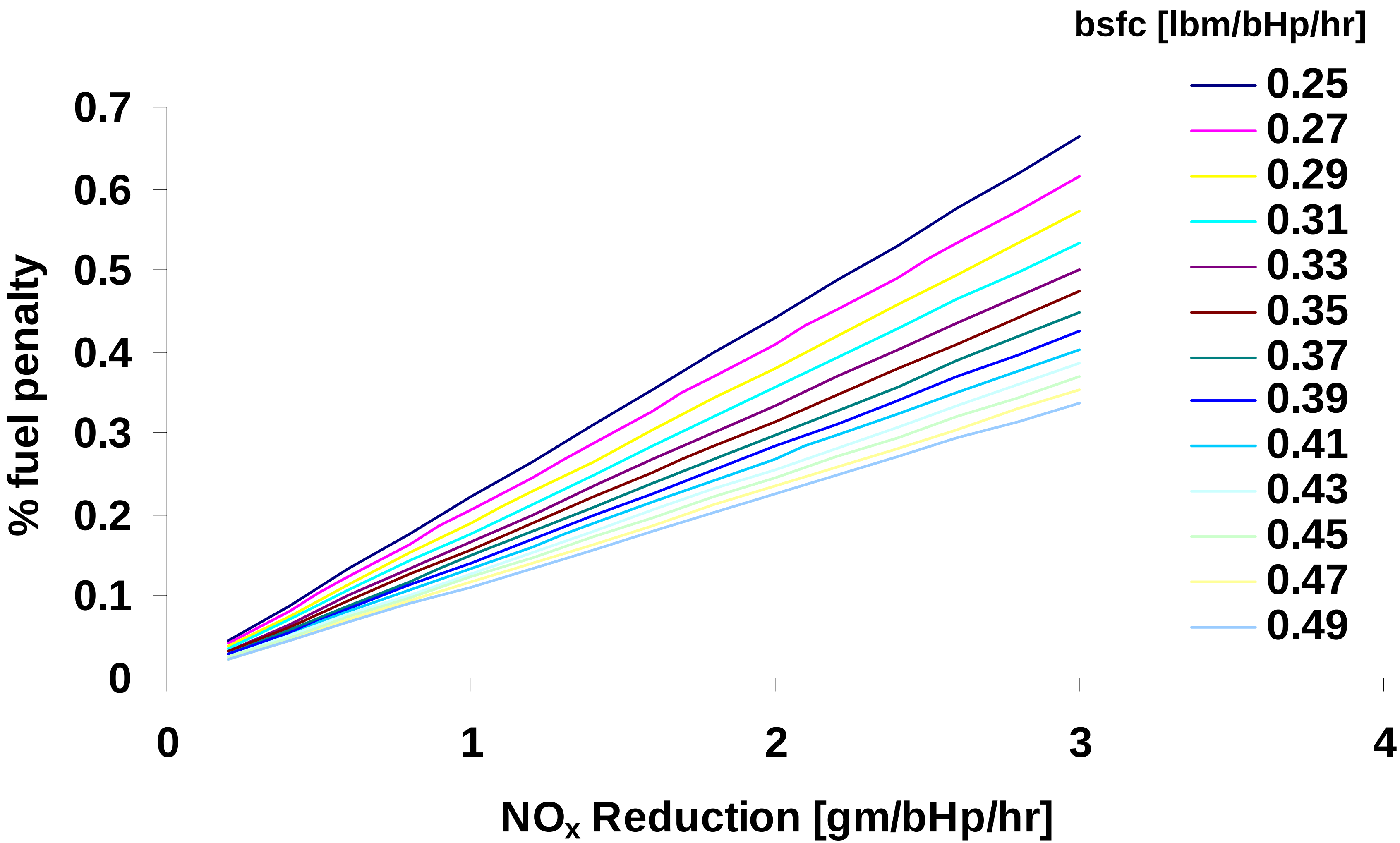
∴ **NO_x chemistry fuel penalty (as a percentage):**

$\{0.0567*\mathcal{NOX} / \mathcal{BSFC}\}$ [%]

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

0.0567*2.5/0.350 = **0.405%**

NO_x Chemistry is Minor Factor



HC Slip Fuel Penalty

$\mathcal{NMHC}$ ≡ **Non-Methane Hydrocarbon reduction rate**

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

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

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

∴ **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 $CH_{1.85}$

$O_2 + 0.68376\ CH_{1.85} \rightarrow 0.68376\ CO_2 + 0.63248\ H_20$

$\therefore$ stoichiometry = 0.68376 [mole $CH_{1.85}$/mole O_2]

Lean oxidation of $CH_{1.85}$

$(0.2095\ O_2 + 0.7905\ N_2) + \mathit{phi}\ CH_{1.85} \rightarrow (0.2095 - 5.85/4*\mathit{phi})\ O_2$
$+ 0.7905\ N_2 + \mathit{phi}\ CO_2 + (1.85/2)\ \mathit{phi}\ H_20$

$\therefore$ exhaust oxygen concentration:

$\{(0.2095 - 1.4625*\mathit{phi})/(1.0 + 0.4625*\mathit{phi})\}$ [mole O_2 /mole exh]

O_2 Consumption Fuel Penalty –cont-

AFR ≡ **Air to Fuel Ratio** [lbm air/lbm $CH_{1.85}$]

= {28.96/*phi*/13.85} [gm air/gm $CH_{1.85}$]

ExO2 ≡ **O_2 concentration in the exhaust** [mole O_2 /mole exh]

= {(0.2095**AFR*–3.0581)/(*AFR*+0.9670)} [mole O_2 /mole exh]

Please note the following relationship for exhaust flow rate:

(exhaust flow rate)/(fresh air flow rate) = {1.0 + 1.0/*AFR*} [lb /lb]

O_2 Consumption Fuel Penalty –cont-

Putting it all together…

[mole $CH_{1.85}$ / mole exhaust] →
{*ExO2* * 0.68376}

[gm $CH_{1.85}$ /gm exhaust] →
{*ExO2* * 0.68376*13.85/28.8} see note

[lbm $CH_{1.85}$ /lbm intake air] →
{*ExO2* * 0.68376*13.85/28.8*(1.0 + 1.0/*AFR*)}

[lbm $CH_{1.85}$ /lbm engine fueling] →
{*ExO2* * 0.68376*13.85/28.8*(*AFR* + 1.0)}

Note: exhaust gas molecular weight was assumed to be 28.8

O_2 Consumption Fuel Penalty –cont-

…yields the oxygen depletion fuel penalty:

[lbm $CH_{1.85}$ / lbm engine fueling] →

{(0.2095*$\mathcal{AFR}$–3.058)/($\mathcal{AFR}$+0.967)*0.684*13.85/28.8*($\mathcal{AFR}$+ 1)}

or approximately…

[lbm $CH_{1.85}$ / lbm engine fueling] →

{(0.2095*$\mathcal{AFR}$–3.058)*0.684*13.85/28.8}

Finally, accounting for rich-lean cycling:

{(6.89*$\mathcal{AFR}$ - 100)/(*lean:rich*)} [%]

∴ **Example:** To remove exhaust O_2 at 25 AFR and 30:1 lean rich yields a fuel penalty of**:** (6.89*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

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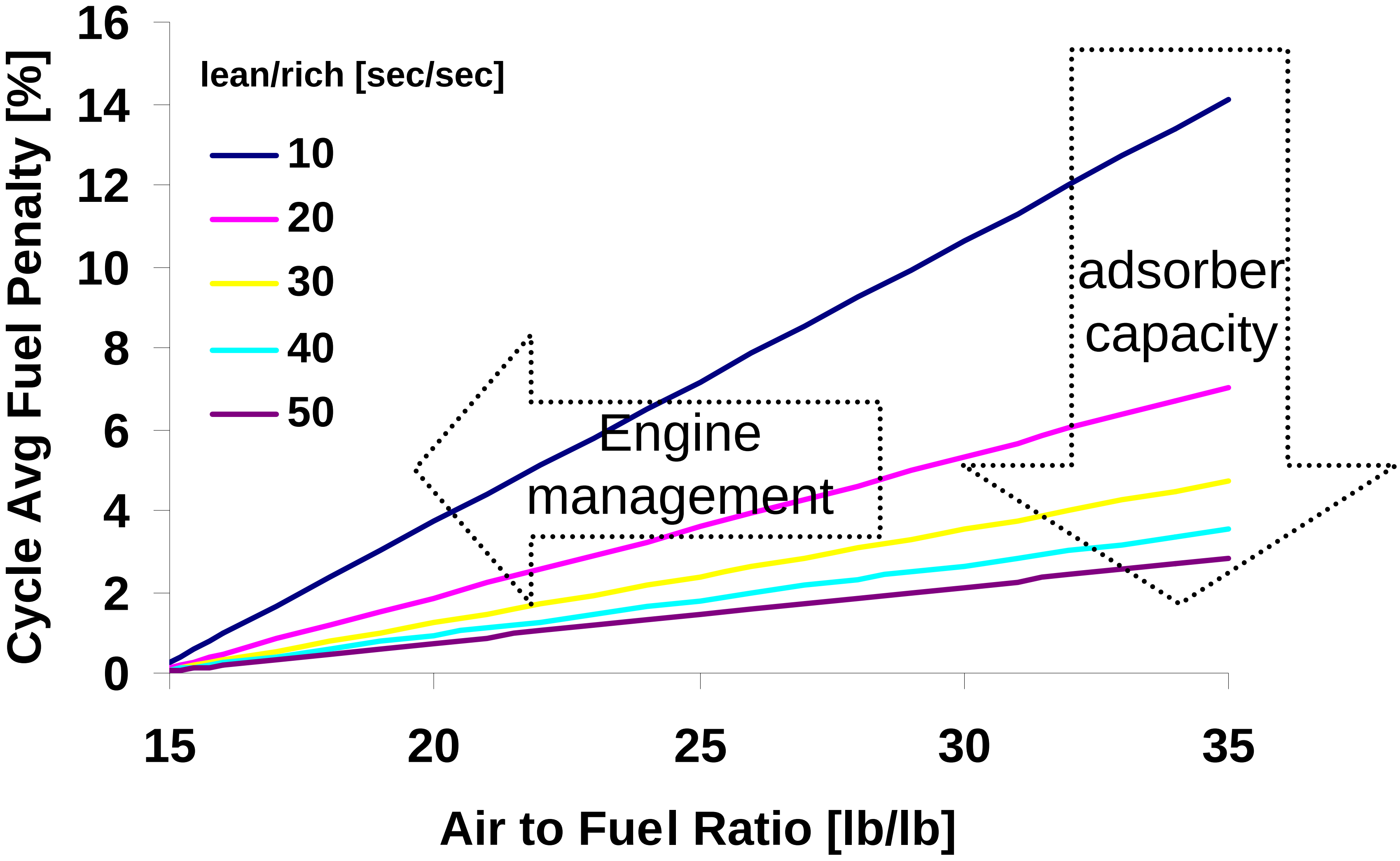
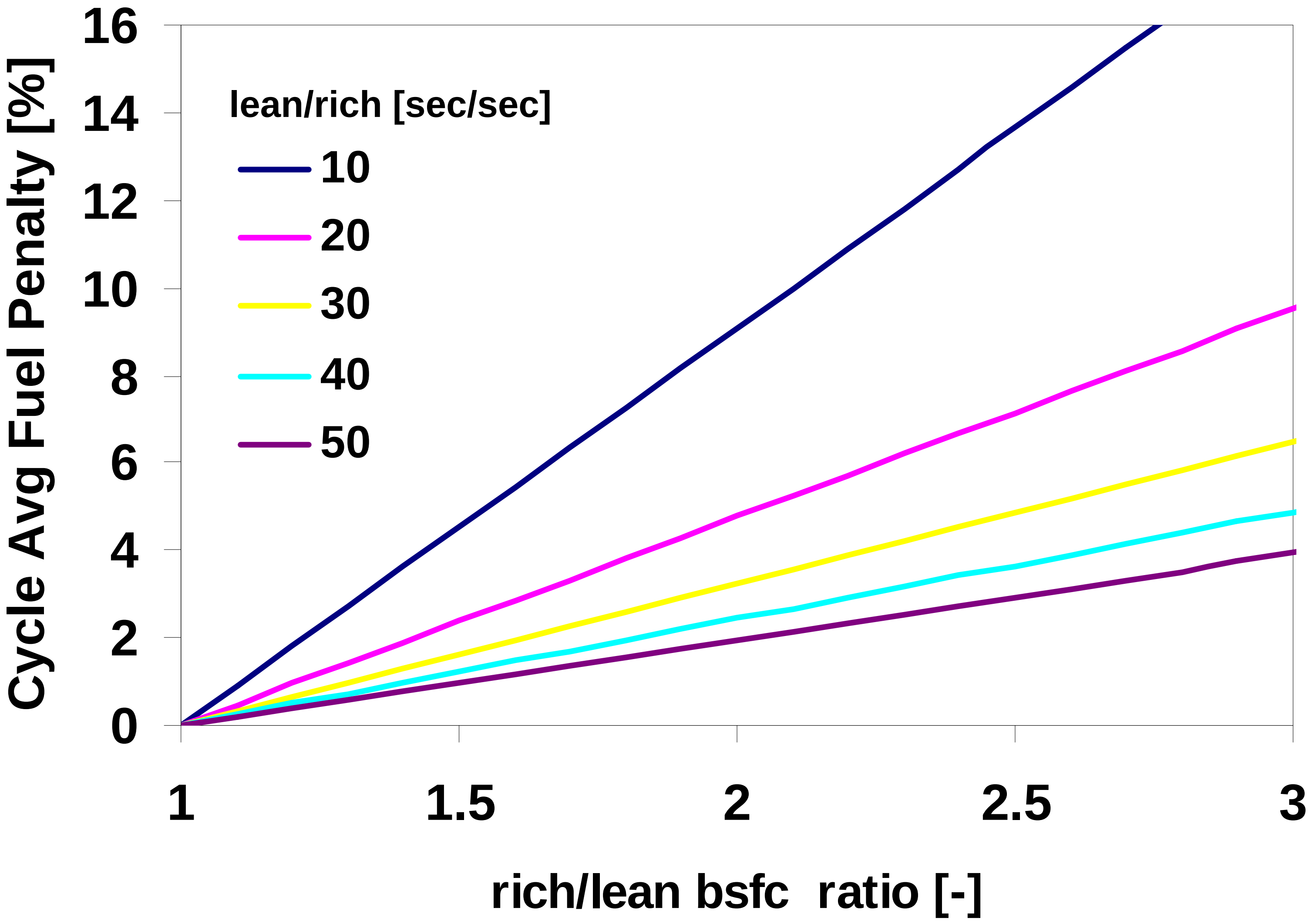
Oxygen Depletion



In-Cylinder Enrichment



Adsorber Fuel Penalty Equation

penalty [%] =

{100*(0.000567)*$\mathcal{NOX}$ / $\mathcal{BSFC}$} +

{100*$\mathcal{NMHC}$/454/ $\mathcal{BSFC}$} +

{(0.206*$\mathcal{AFR}$–3.058)/($\mathcal{AFR}$+0.967) *

0.684*13.85/28.8*($\mathcal{AFR}$+ 1.0) /

(*lean:rich*)}

Conclusion #1

With maturity NO_x Adsorbers will allow engine retune

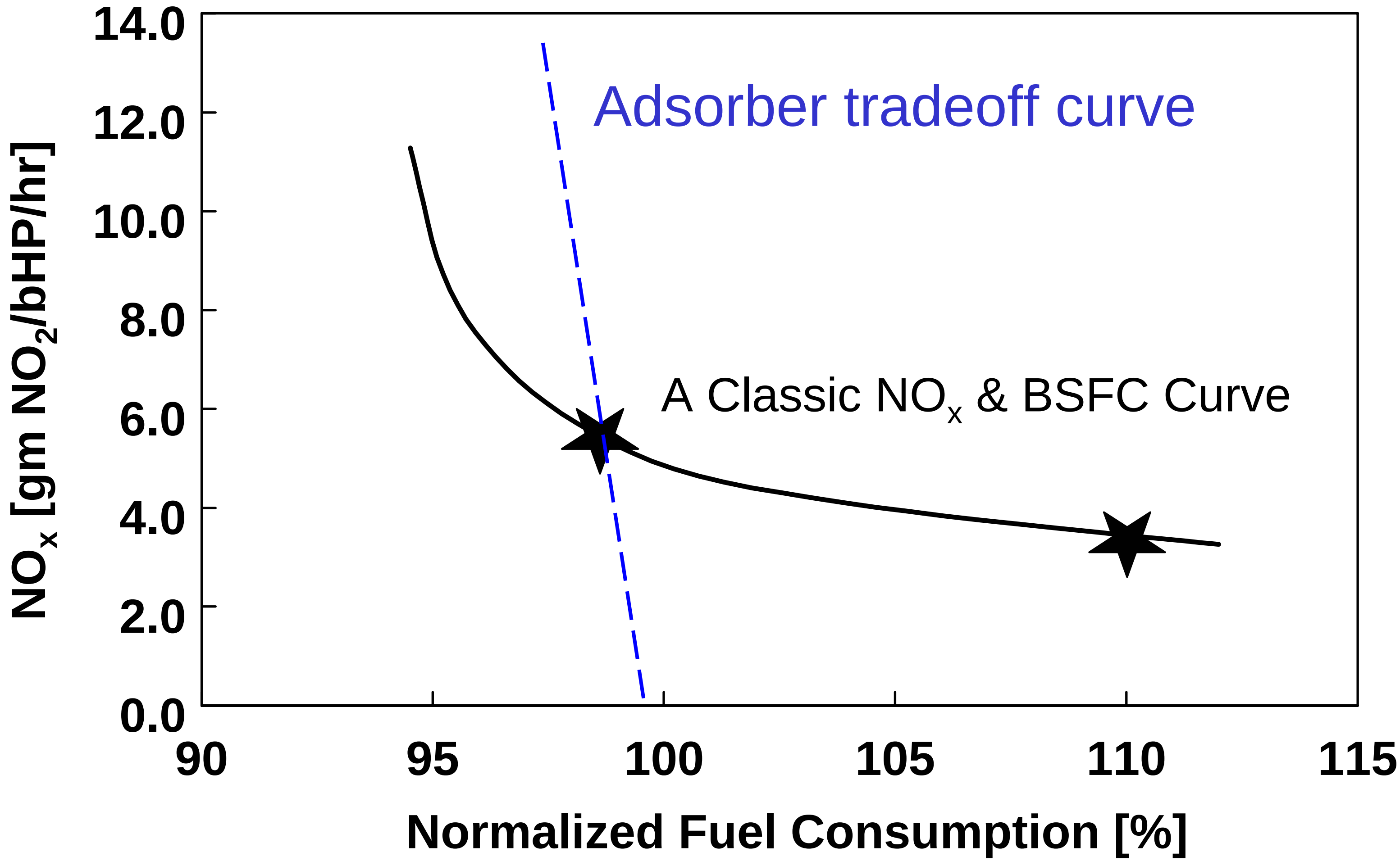
2.5 gm NO_x → 2.9% fuel penalty

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!



Conclusion #2

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

{(6.89*$\mathcal{AFR}$ - 100)/(lean:rich)} [%]

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

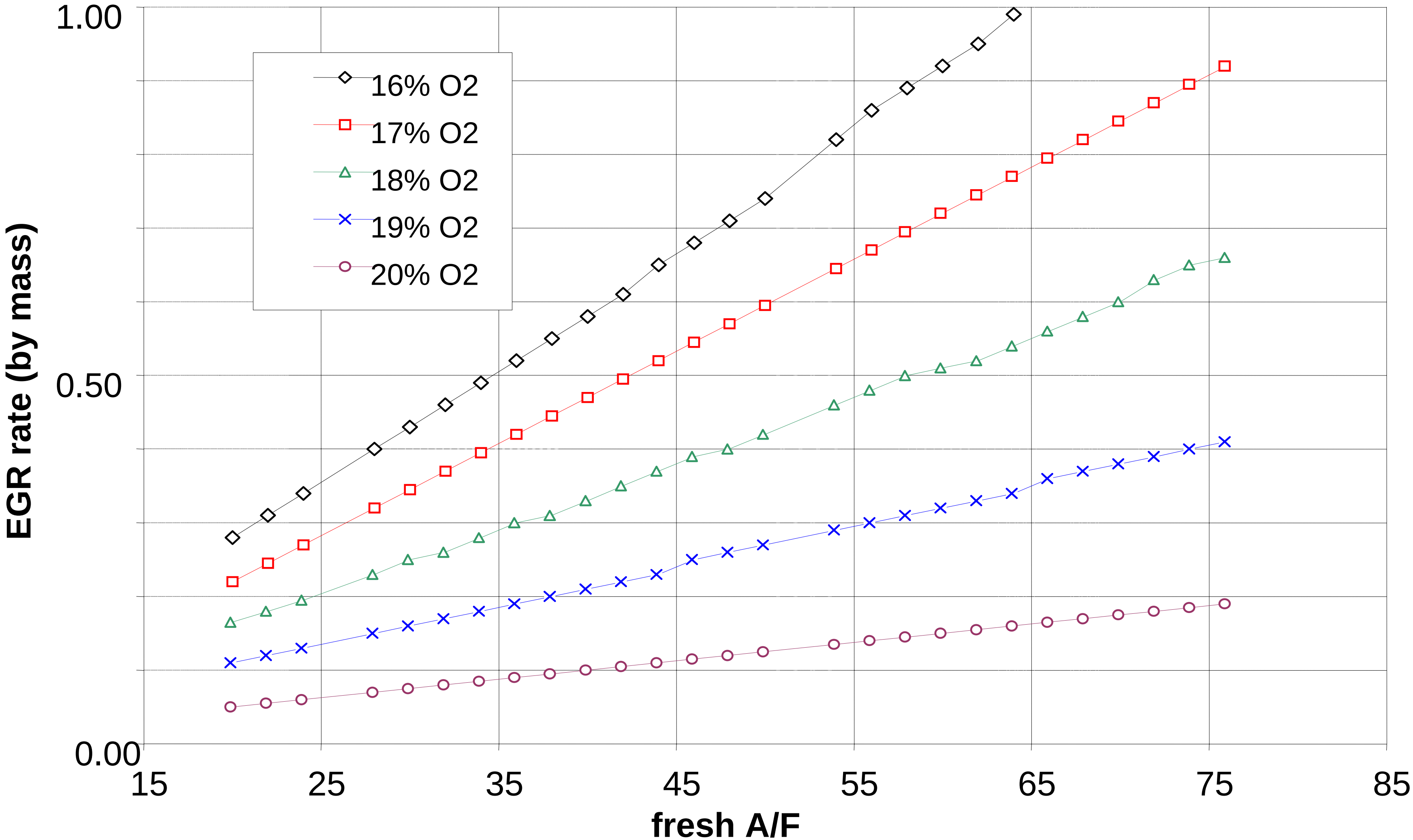
20% penalty at 100:1 AFR

Which implies one of two strategies:

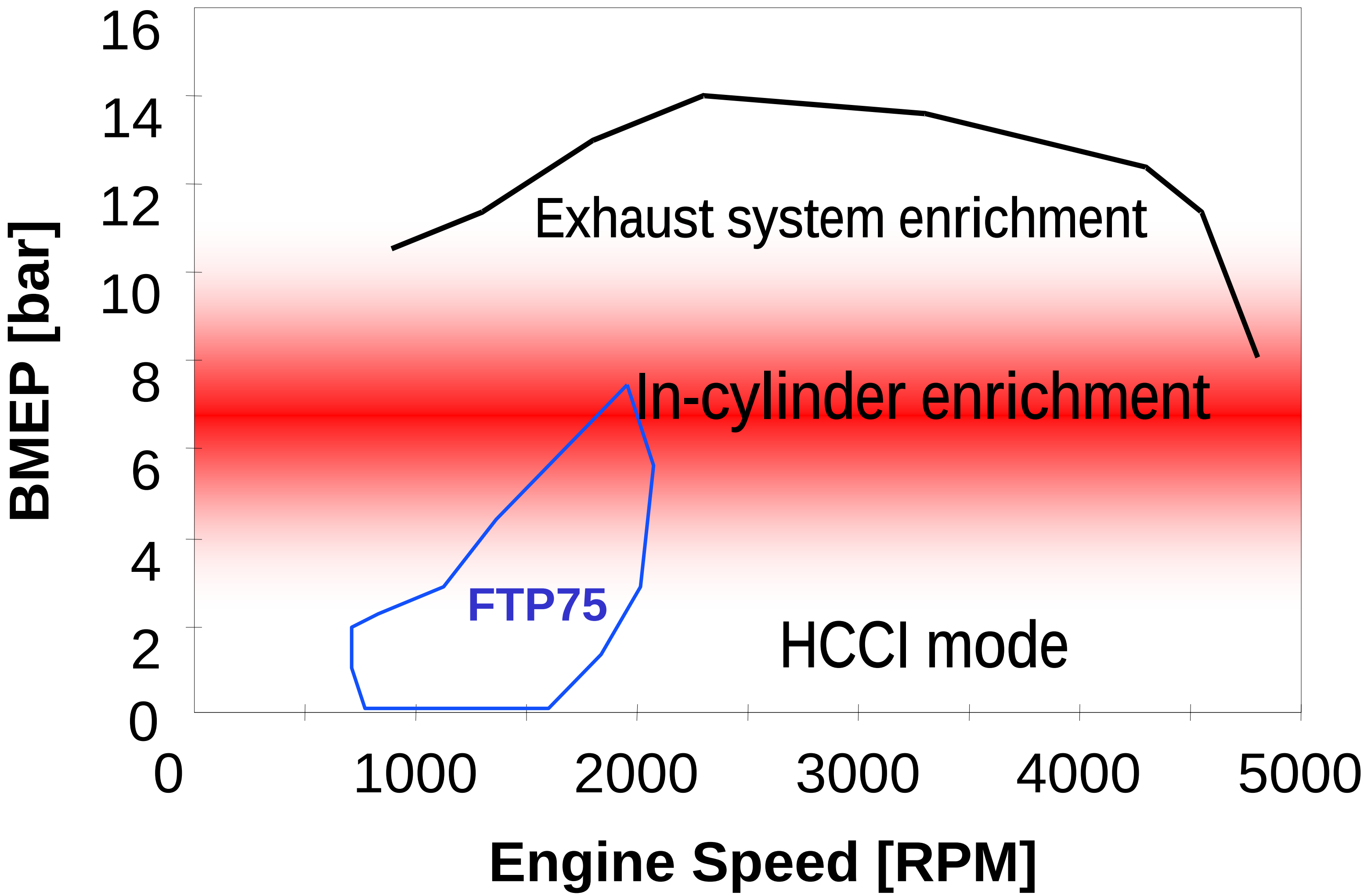
(massive) EGR rates for AFR reduction

dual mode w/HCCI-like combustion at light loads

EGR Effect on Oxygen Concentration



HCCI(like) Combustion & NO_x adsorbers



Overview

NO_x Adsorbers

- NO_x chemistry
- HC slip
- Oxygen depletion

Lean NO_x

- NO_x chemistry
- Selectivity
- Activity

Particulate Filters

- Backpressure
- Regeneration (Enthalpy)

HC lean NO_x 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 NO_x Chemistry

Ideal NO_x reduction with $CH_{1.85}$

$$NO + 0.3419\ CH_{1.85} \rightarrow \tfrac{1}{2}\ N_2 + 0.3419\ CO_2 + 0.3162\ H_20$$

∴ 0.3419 moles of $CH_{1.85}$ are required to convert one mole of NO

From ideal lean NO_x chemistry

= $\mathcal{NOX}$ [gm NO_2/bHp/hr]

stoichiometry → {$\mathcal{NOX}$*0.3419/46} [mole $CH_{1.85}$ /bHp/hr]

= {$\mathcal{NOX}$*13.85*0.3419/46/454} [lb $CH_{1.85}$ /bHp/hr]

∴ **Ideal fuel penalty (as a percentage):**

{100*13.85*0.3419/46/454*$\mathcal{NOX}$ / $\mathcal{BSFC}$} [%]

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

100*0.000227*2.5/0.350 = **0.162%**

Real Lean NO_x Chemistry

$\mathcal{C}:\mathcal{N}$ ≡ **carbon to NO_x molar ratio - unit conversion**

$\mathcal{C}:\mathcal{N}$ [moles $CH_{1.85}$/moles NO] → {$\mathcal{C}:\mathcal{N}$*13.85/46} [gm HC/gm NO_2]

SELECTIVITY: lean NO_x reduction competes with direct oxidation

$$NO + (5.85/4 * \mathcal{C}:\mathcal{N} - 1/2)\ O_2 + (\mathcal{C}:\mathcal{N})\ CH_{1.85} \rightarrow$$

$$\tfrac{1}{2}\ N_2 + \mathcal{C}:\mathcal{N}\ CO_2 + (\mathcal{C}:\mathcal{N} * 1.85/2)\ H_20$$

∴ **Selectivity** = {100*0.3419/$\mathcal{C}:\mathcal{N}$} [%]

∴ **Fuel penalty (as a percentage):**

{100*13.85/46/454*$\mathcal{C}:\mathcal{N}$*$\mathcal{NOX}$/$\mathcal{BSFC}$} [%]

∴ **Example:** To remove 2.5 gm of NO_x at 0.350 bsfc with a C:N of 6:

0.06632*6*2.5/0.350= **2.84%**

(w/selectivity of: 100*0.3419/6 = **5.70%**)

Real Lean NO_x Chemistry –cont-

ACTIVITY: lean NO_x reduction is not yet 100% efficient

$$NO + (5.85/4*\mathcal{C}:\mathcal{N} - act/2)\ O_2 + (\mathcal{C}:\mathcal{N})\ CH_{1.85} \rightarrow$$

$$(1-act)\ NO + (act/2)\ N_2 + \mathcal{C}:\mathcal{N}\ CO_2 + (\mathcal{C}:\mathcal{N}*1.85/2)\ H_20$$

∴ **Activity impacts selectivity.**

Selectivity = {100*act*0.3419/$\mathcal{C}:\mathcal{N}$} [%]

∴ **Example:** To remove NO_x at 50% efficiency with a C:N of 6 yields a selectivity of {100*0.5*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_x Adsorbers

- NO_x chemistry
- HC slip
- Oxygen depletion

Lean NO_x

- NO_x chemistry
- Selectivity
- Activity

Particulate Filters

- Backpressure
- Regeneration (Enthalpy)

Particulate Filter Fuel Penalties

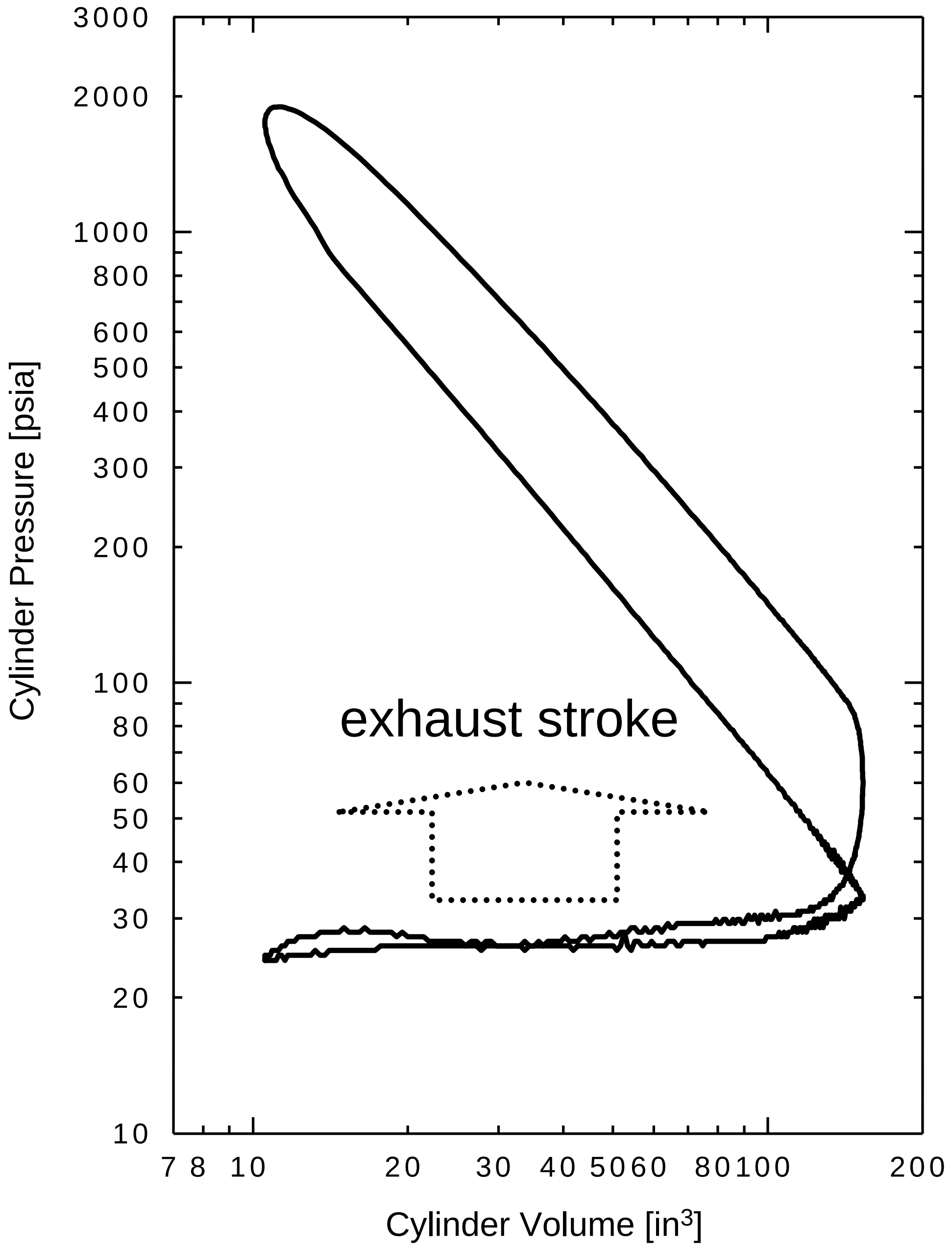
Assuming

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 avgerage regeneration penalty	= 0.34%
Total penalty	= **1.34%**

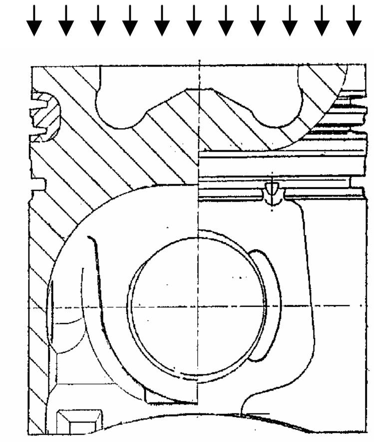
Note: These penalties are highly duty cycle dependant!



Backpressure

BMEP is directly impacted by backpressure

pressure = work



Backpressure

Assuming

BMEP = 100 [psi]

Backpressure = 1 [psi]

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 = {100*backpressure/bmep} [%]

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

{100*1.0/100} = **1.0%**

Enthalpy

Assuming

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

From dH = C_p dT

18500 [Btu/lbm supl. fuel] = 0.2412 [Btu/lbm exhaust/deg F] *
$\mathcal{dT}$ [deg F] * ($\mathcal{AFR}$ + 1) [lbm exh/lbm fueling] *
(1/efficiency) [lbm fueling/lbm supl. Fuel]

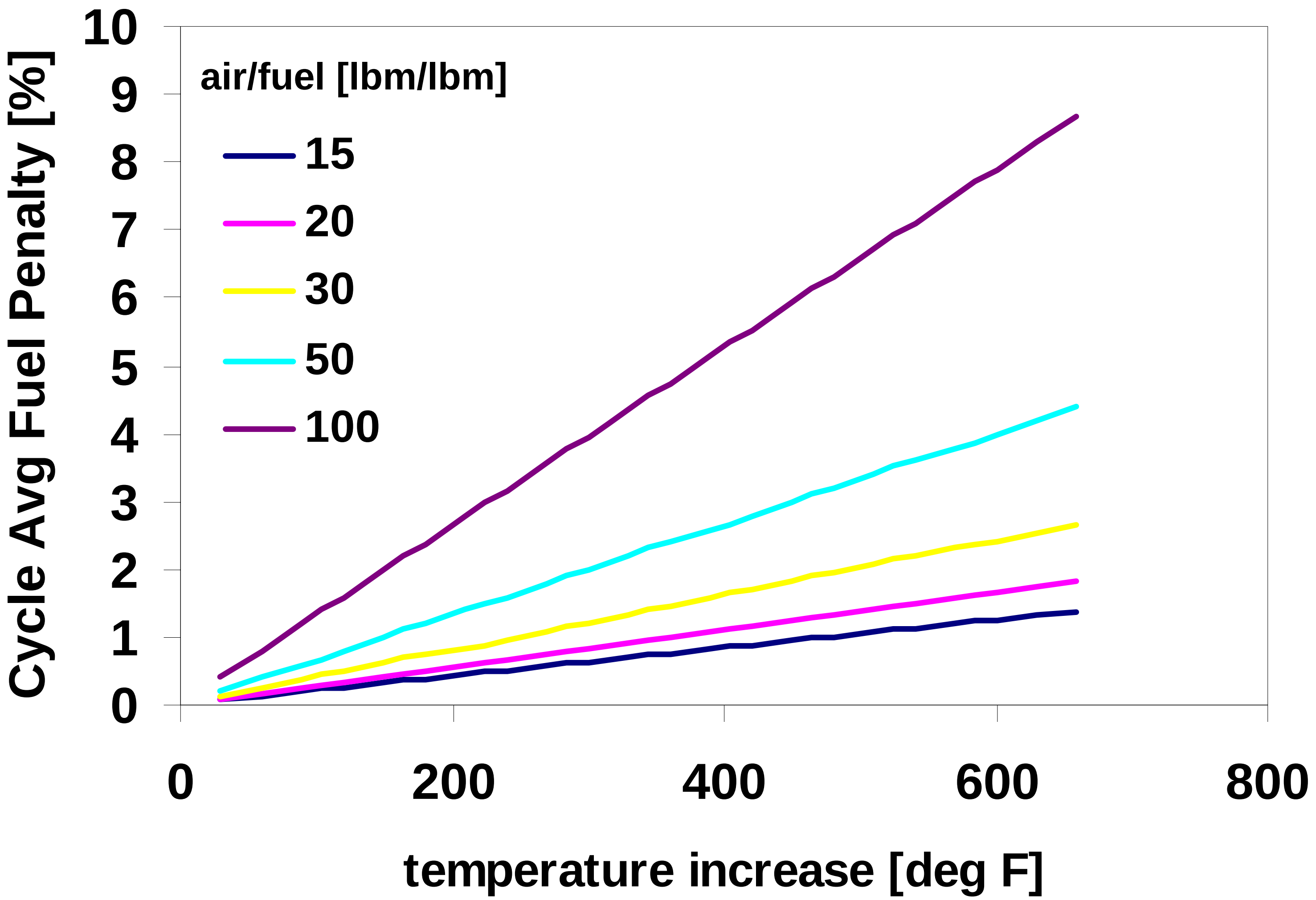
∴ **fuel penalty during regen is…**

{(1+AFR)*0.2412*dT/18500*$\mathcal{DC}$} [%]

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

(1+25)*0.2412*100/18500*10 = **0.34%**

DPF penalty w/10% duty cycle



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”…

…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?