Low Temperature Regeneration of NOx Adsorber System

Diesel Engine Exhaust Reduction Workshop

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Objectives

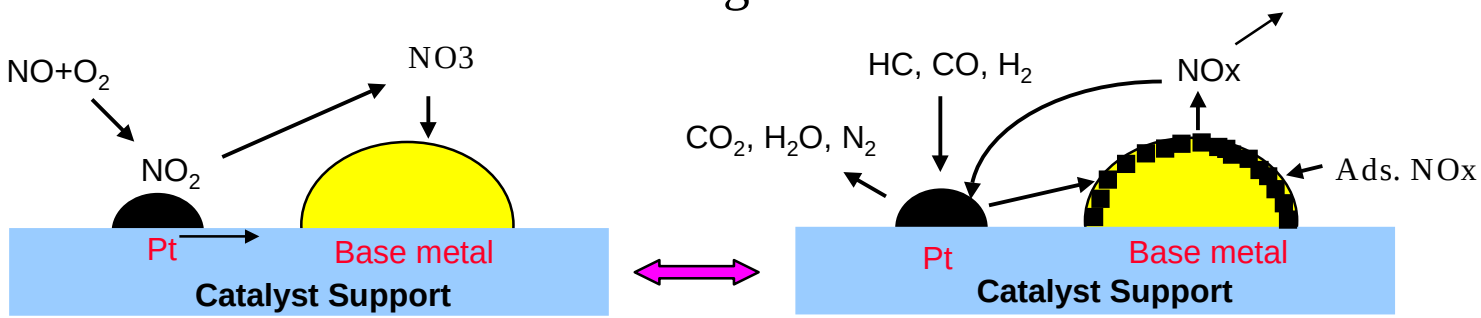
Low temperature performance of NOx adsorber systems seems to be an issue.

The objectives of this study are:

- to identify the optimal reductant for adsorber regeneration
- to understand the trade-off between efficiency improvement and fuel penalty at low temperatures

NOx Adsorber Concept

- Three-way catalyst is only good for gasoline exhaust in near stoichiometric A/F, not functional for diesel exhaust in standard lean A/F operation mode
- NOx Adsorber requires cyclic operation:
  - → Store NOx in lean operation
  - → Reduce the stored NOx during rich transient



Lean Operation
(NOx Trapping)

Rich Transient
(Reduce Stored NOx)

NOx Adsorber Functional Chemistry

- **Oxidation of NO to NO_2**
  - → over PM or metal oxides (Pt is the more active)
- **NO_x Storage**
  - → as surface nitrates on Pt/BMO interface
  - → as nitrates and NO_2 (ads) on BMO
- **NO_x Release**
  - → thermodynamics, desorption, displacement

$$M(NO3)_2 \longrightarrow MO + 2\,NO_2 + 1/2\,O_2$$

$$NO_2 \longrightarrow NO + 1/2\,O_2$$

$$NO_2\,(ads) + HC \longrightarrow NO + 1/2\,O_2$$

- **NO_x Reduction to N_2**
  - → H2, CO, reductants over the PM and PM/BMO interface

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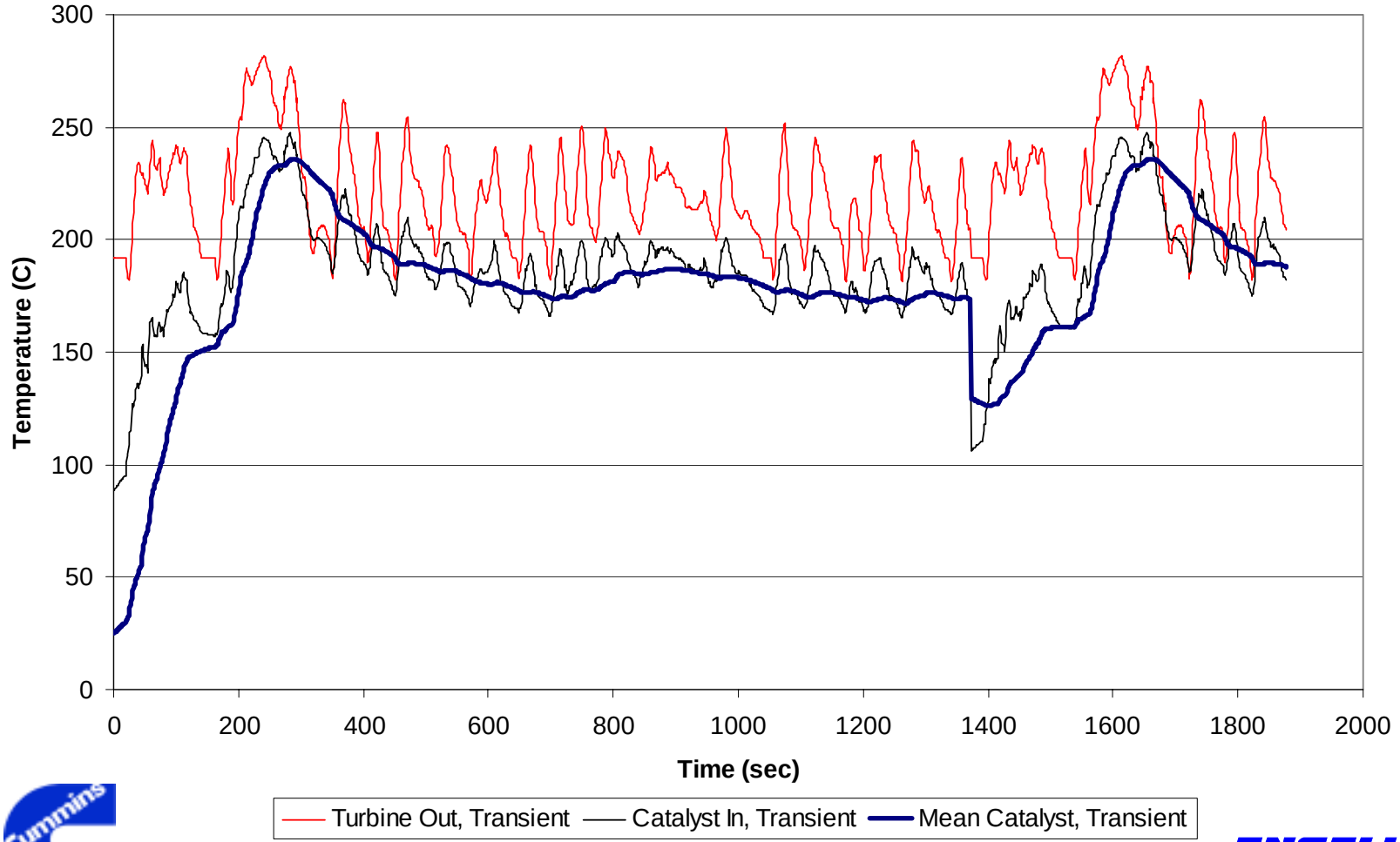
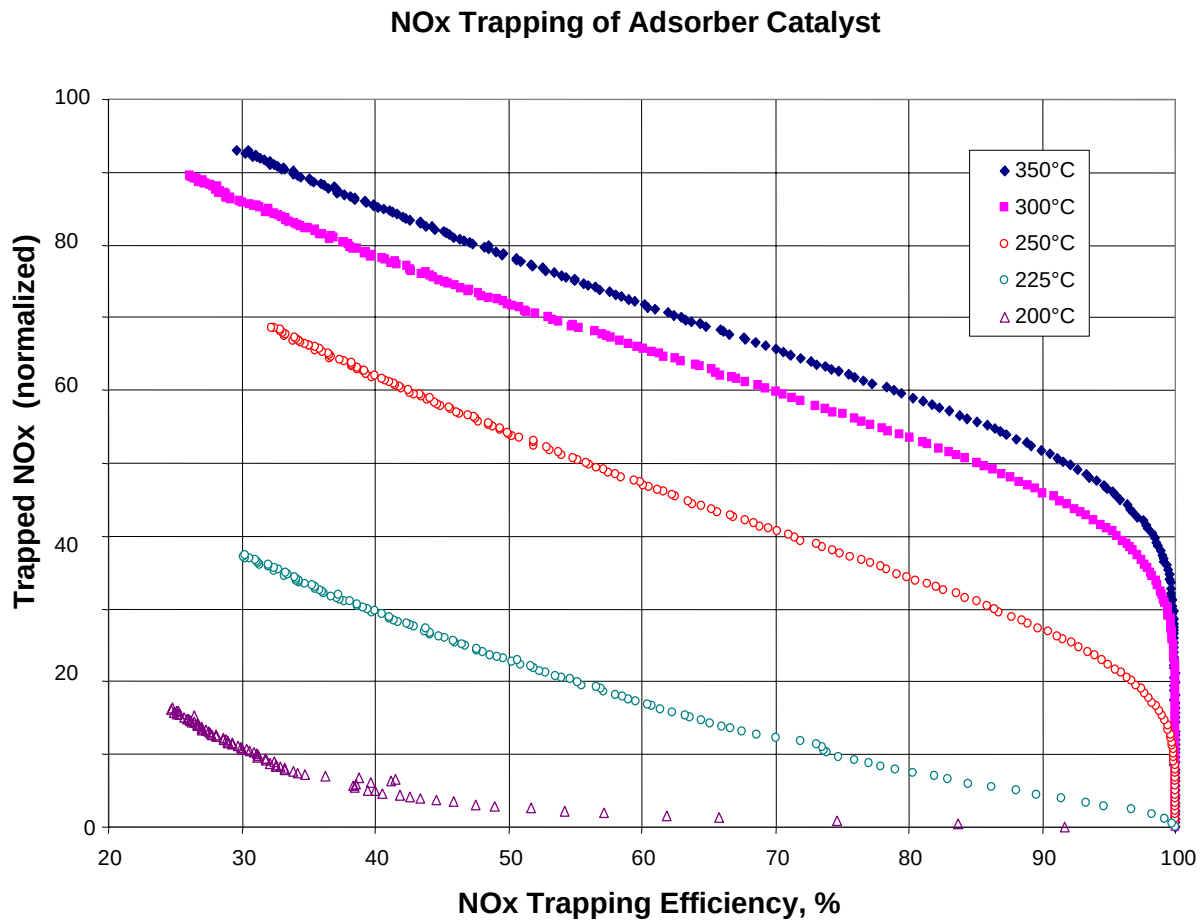
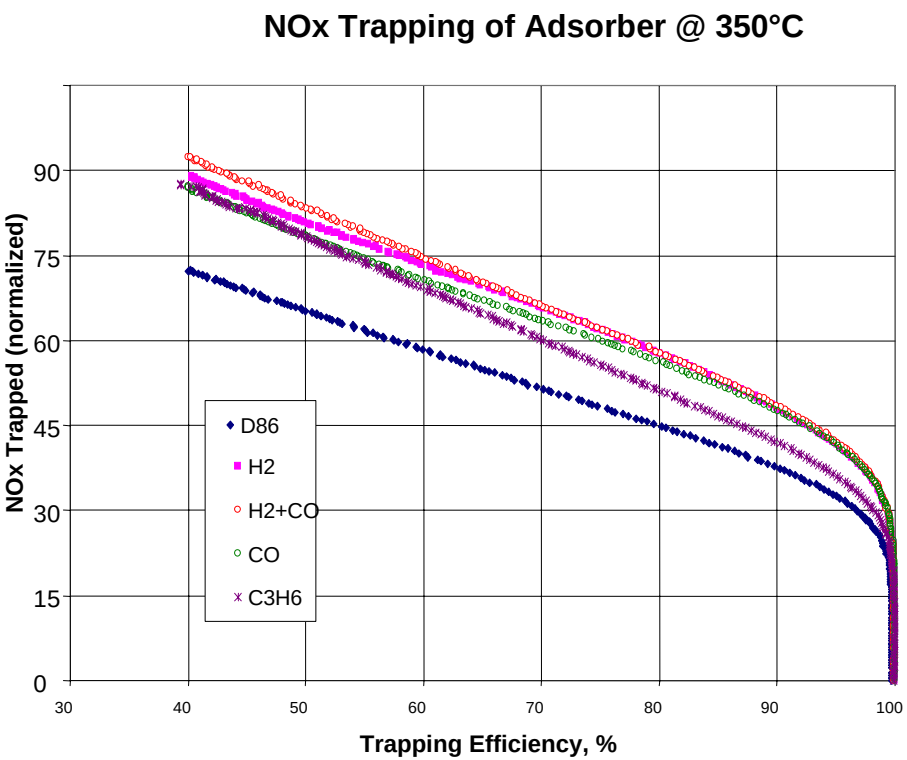
LDV Engine Out Gas Temperature (FTP-75 Cycle)

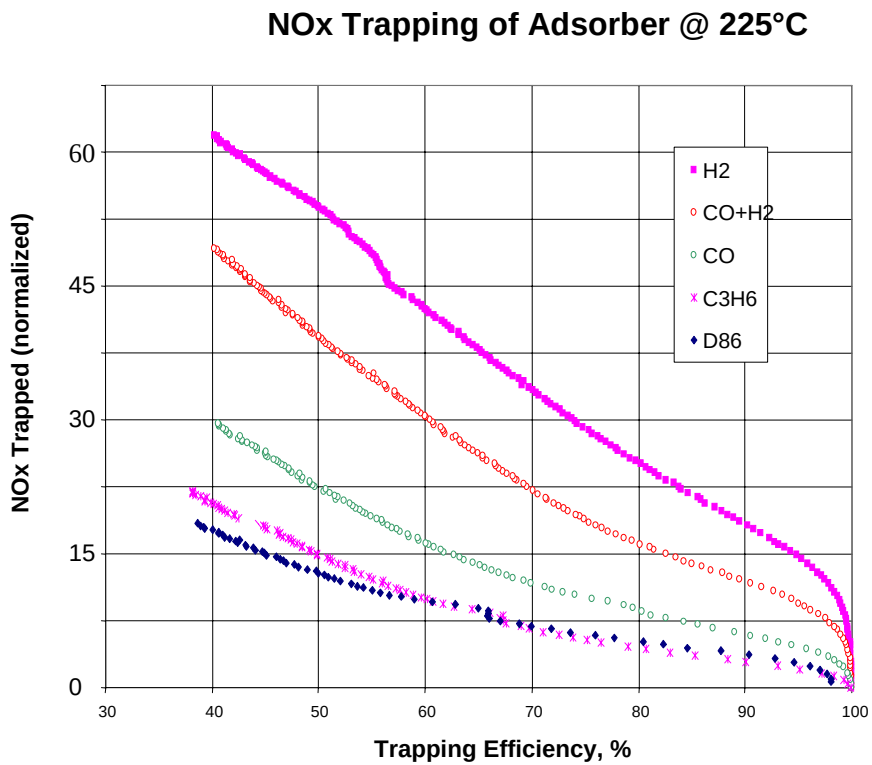


Adsorber Catalyst Performance as a Function of Temperature

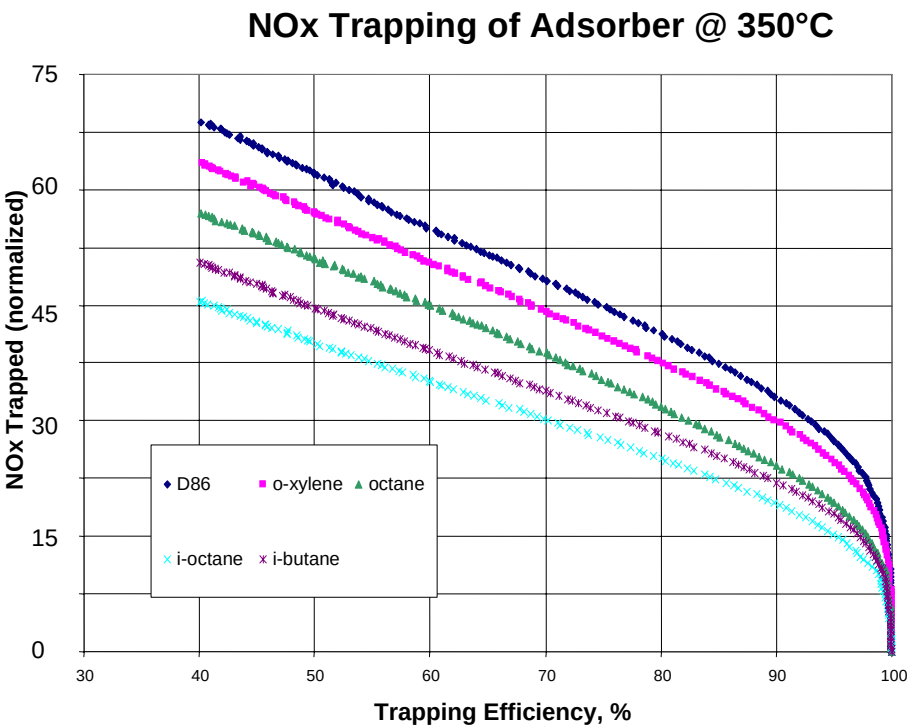


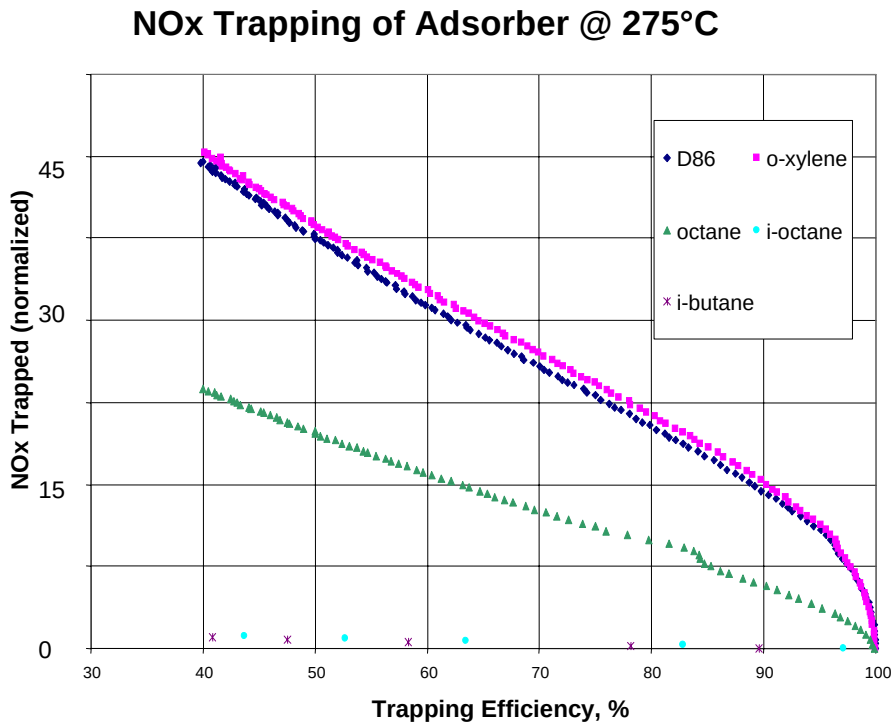
Hydrogen Appears To Be The Most Reactive Reductant





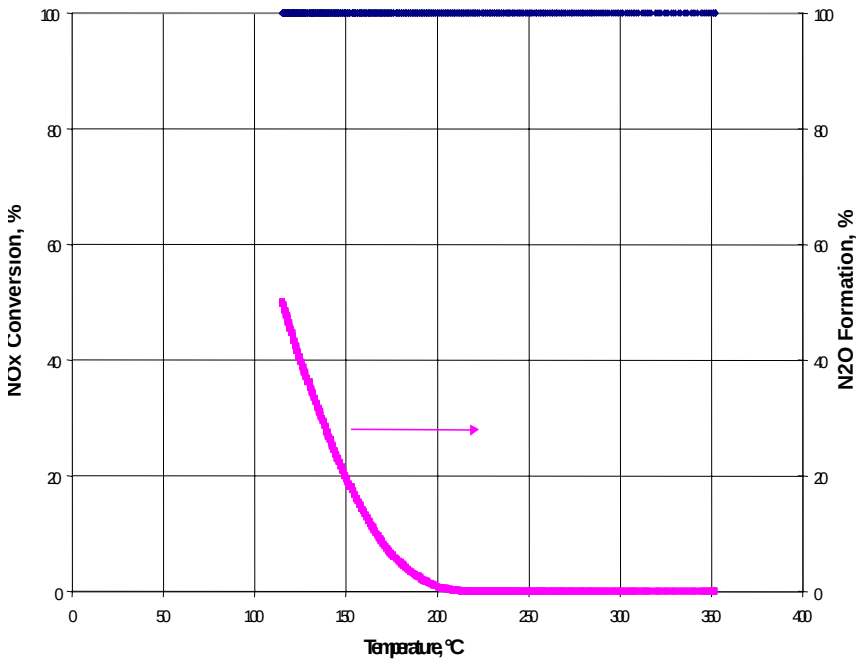
Most of the Cracking Products from Diesel Prove to be Less Active



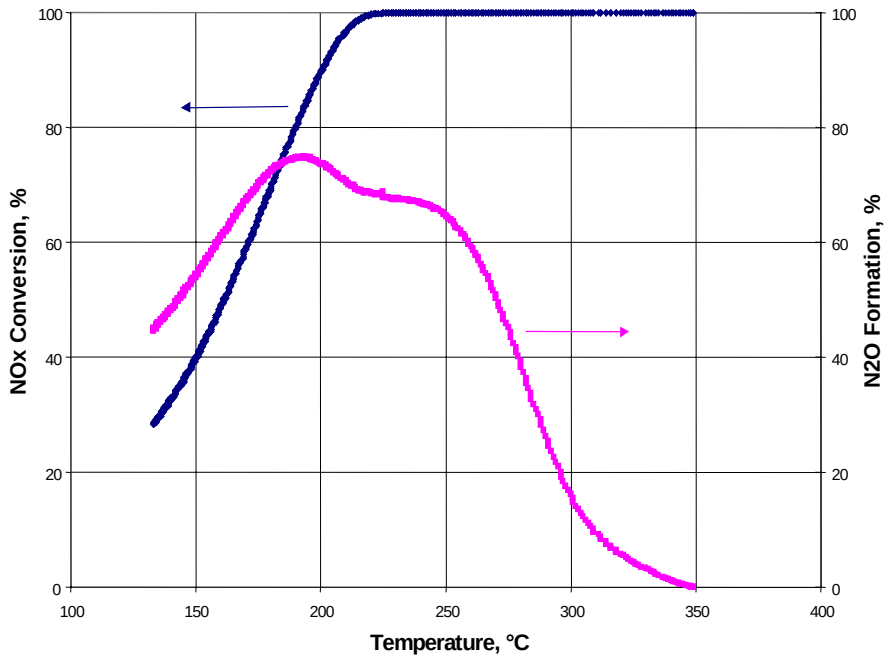


NO Reduction Shows Selectivity Issues

NO Reduction With H2 Over Adsorber



NO Reduction With CO Over Adsorber



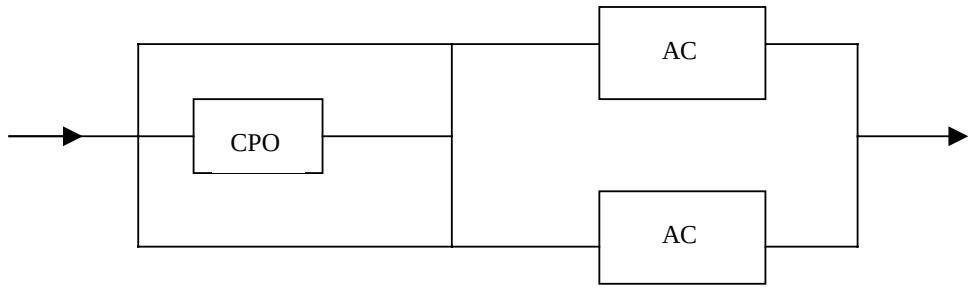
Fuel Reformation

Reformers have been primarily used for Fuel Cell applications

Fuel reformation may be useful for Aftertreatment application

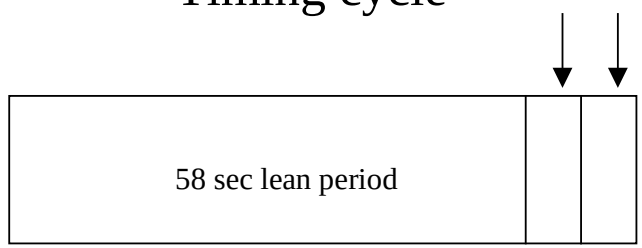
- → CO production is not an issue
- → Space velocity should be high (> 100 K)
- → Reformer temperature should be higher than 650 C
- → Need O2/C < 0.5 to generate CO
- → Operation is not continuous
- → High instantaneous production requirement
- → Coking may be an issue but could be burnt during lean period

Reformer Schematic



Lean	50-50 flow	58 sec
Rich	20-80 flow	1 sec
Rich	80-20 flow	1 sec

Timing cycle



Assumptions for the Analysis Tool

Average Diata FTP-75 conditions

CPO requirements
- T > 650C
- $O_2/C < 0.4$
- $H_2O/C > 2$
- SV > 100K/hr

Energy Requirements for CPO

A Radiation + Convection loss from external surface

B Convection loss from flow inside CPO
(during regeneration and slip flow to burn coke)

C Theoretical input energy (sensible heat to combust reactants)

D Fuel to electrical energy conversion efficiency, 0.3

Fuel required to keep CPO running = (A+B+C)/D

Flow through CPO and Adsorber during regeneration = 20%

Based on average Diata conditions O_2 in exhaust = 10%

Assumptions for the Analysis Tool

H_2O in exhaust = 6.5%
CPO size = 4.66" D X 1" L

Based on this, CPO requirements achieved in system,

$O_2/C \sim 0.3$
$H_2O/C \sim 0.2$*
SV ~ 118 K/hr

*Since H_2O/C ratio is not met coking is expected
Coking Factor = 0.8 (i.e., 25% more D2 required to generate desired H_2)
Slip flow during lean period to burn coke = 2.0%
Heat released during combustion of coke balances convective loss
$O_2 + H_2$ combustion efficiency = 100%
NOx + H_2 reaction efficiency = 50% (from Engelhard presentations)

CPO H_2 production efficiency is 35% based on heating value
CO production is not used in calculations (CO not as active + buffer)

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Fuel Penalty Calculation for Reformer

a H_2 required to burn the oxygen in 20% of the exhaust flow

b H_2 required to reduce the loaded NOx

α HC required to produce the necessary H_2 for steps a and b

β HC required to keep the reformer running (A+B+C)/D

Total Fuel Penalty = $(\alpha * 2 + \beta)/(\text{engine fuel flow})$

Calculation Results

DIATA	rpm	torque	AFR	FUEL lb/hr	AIR lb/min	NOx ppm	NOx g/hr	Cat_in T, K	NOx g/hp hr
	1475	**15**	**31.5**	**2.736**	**1.44**	**164.5**	**10.53**	**450**	**2.5**
	AC brick size		L	2.5					
	Reformer flow rate								
excess air		kg/hr	20.86						
H2 req. for desired AF ratio	0.122 kg/hr	in g/s	0.034						
H2 req. during regeneration	g	0.034	HC req. to produce this H2	g	**0.354**				
NOx loading during Lean period	g	0.085							
Efficiency of NO and H2 react.	%	**50.00**							
H2 required for loaded NOx	g	0.015	heat rel. during coke comb. J/s		146.8328				
HC req. to produce the H2 for Loaded NOx		g	**0.155**						
	total HC required	g/injection	**0.509**						
	# of injections		2.000						
	HC flow rate	g/sec	0.01726	lb/hr	0.137				
Supplementary inj. penalty		%	**5.01**						
Sacrificial HC for reformer		g/sec	0.006021	lb/hr	0.048				
Reformer HC penalty		%	**1.75**						
Total fuel penalty FEP		%	**6.75**						

Electrical Heating (50% duty cycle) = ~6%

Conclusions

Issue

- Light duty vehicles and cold start conditions may create low temperature performance issues for adsorbers

Possible reasons for poor adsorber performance at low temperatures are

- Both the thermodynamic and desorption release of NOx is slow
- Diesel is not active @ T < 250°C

Possible solutions are

- Engine management to increase engine out temperature
- System configuration such external exhaust heating
- Fuel reformulation to improve regeneration efficiency at low temperatures
  - → H2 > H2+CO > CO > diesel > cracking components
- Analytical tool predicts < 7% fuel penalty with reformer

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