Using an Inexpensive NOx/O2 Concentration Sensor to Screen Tailpipe Emissions

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Executive Summary

NO_x/O_2 concentration sensors can be used as a relatively inexpensive method to screen and estimate tail pipe emission performance of light-duty vehicles in the real world, in conjunction with OBD data or along with basic fuel flow and distance measurements. This approach can be employed as an initial step to assess the effectiveness of the emission control features such as the Cold Start Emission Reduction Strategy (CSERS), to verify Auxiliary Emission Control Device (AECD) definitions (fuel enrichment authority), or even to detect defeat devices.

To demonstrate the potential of this method firsthand, our testing focused on CSERS performance for a gasoline and diesel vehicle as well as on the operational enrichment range for a gasoline vehicle under extended driving conditions. Differences in the estimation of NOx emissions using different calculation approaches were also explored.

In the gasoline vehicle, the CSERS strategy was only activated following fully soaked start conditions, and poor NOx CSERS performance for intermediate soak conditions. The range of fuel enrichment measured in the gasoline vehicle for some extended drive-cycle conditions was found to be within the allowed tolerance range during both open and closed loop conditions. We found that the diesel vehicle we tested also only applied the CSERS strategy to a cold-soaked vehicle. However, unlike the gasoline vehicle, the cold-soaked condition when CSERS was active produced the high NOx emissions; NOx emission generally improved with shorter soak periods that had higher initial catalyst temperatures.

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Introduction

In-use real-world vehicle emissions are under increased scrutiny by regulators world-wide. Manufacturers are subject to heavy monetary fines and consent decrees agreed to by manufactures as a result of civil and criminal investigations related to defeat devices or un-approved AECDs that operate outside of the test-cycle conditions. Differences between measurements of real-world emission performance and that stated in certification documents have triggered further investigation by regulators. A Portable Emission Measurement System (PEMS) can be employed to acquire accurate emissions measurements in the real-world, however, such approach is costly, as PEMS systems cost around $300k USD. As an alternative method, several researchers in this field have presented data generated with NOx sensors to estimate NOx tailpipe emissions. This approach has been applied with success, specifically in light-duty and heavy-duty diesel vehicles, by either measuring with an external NOx/O2 concentration sensor (Bernard, German, Kentroti, Muncrief, 2019) or with an on-board downstream NOx sensor (Tan et all., 2019; Vermeulen, Ligterink, Vonk, Baarbé, 2012). An externally mounted NOx/O2 concentration sensor with an independent control module, has an advantage to an on-board NOx sensor, relative to capturing cold start emissions, since sensor heater control strategies associated with on-board NOx sensors inhibit sensor heating during cold starts until the exhaust gas temperature dew point is reached to avoid damage to the sensor due to water condensation. Whereas an externally mounted NOx/O2 sensor can be heated independently and capture cold start emissions. This is applicable to both gasoline and diesel vehicles. Also, a NOx/O2 concentration sensor measures O2 concertation simultaneously with NOx, which is useful for investigating enrichment strategies in gasoline vehicles.

This paper describes the tests performed on two passenger vehicles (fitted with a NOx/O2 concentration sensor to evaluate their tailpipe emissions), the test hardware used, sample data generated, calculation techniques, and the conclusion reached.

Vehicles Tested

The following in-use light-duty vehicles were used to demonstrate the capability to assess and screen tailpipe emissions with a NOx/O2 concentration sensor:

- 2014 Volkswagen 2.0L TSI gasoline vehicle using a 3-way catalyst (2.0L I4 turbocharged)
- 2012 Mercedes-Benz S350 BlueTec diesel vehicle with SCR system (3.0L V7)

Both vehicles are certified to Tier 2 BIN5 and in California to LEV-II (ULEV) which have a full useful life NOx standard of 0.07 g/mile. The gasoline vehicle had a mileage of roughly 45,000 miles and the diesel vehicle had roughly 123,000 miles. The details of these vehicles are mentioned in Appendix 1.

A diagnostic report of the diesel vehicles was clean and showed no active trouble, or fault codes present in Mode[1] $07 (pending trouble code), Mode $03 (confirmed trouble code), or Mode $0A (permanent trouble code). The gasoline vehicle did not have any active, pending, or confirmed fault codes, but did have an active permanent P0299- Turbo Under boost fault code in the Mode $0A memory (permanent fault). Also, PID $30, number of warm-up since DTC cleared reporting 75 and PID[2] $31, distance traveled since DTC cleared, at 1426 miles. Since the permanent fault code was still in memory, the P0299 monitor failed to make a PASS decision on 3 subsequent driving cycles. Although at the end of the testing, the permanent fault code was cleared since 80 warm-up cycles had passed. Ideally, vehicles that are screened should not have any permanent fault codes present, to eliminate the possibility that the higher-than-expected NOx emissions could be due to a malfunction of an emission control related component. However, since the primary objective of this test is to exercise and demonstrate the potential of the screening method, the presence of a permanent code was not of concern.

Setup and Equipment

A commercially available NOx/O2 concentration sensor was installed in a custom exhaust tailpipe fixture which allowed for real-time monitoring of NO2, O2, and AFR data with at least 1-hertz resolution. This data was captured on a laptop running the sensor supplier's software. Additional measurements were taken by recording Mode $01 PID data with an OBD2

[1] Mode refers to one of the ten (10) OBD-II diagnostic test modes required to be supported by manufactures.
[2] PID is a Parameter Identifier which are defined in the SAE J1979 Standard. https://en.wikipedia.org/wiki/OBD-II_PIDs

scanner device that supported most OBDII communication with software that could record user-selected PIDs. Additional details are provided in Appendix 2 and Appendix 3.

NOx Emission Estimations

NOx mass flow is typically calculated by measuring the exhaust mass flow, which can be accomplished by measuring the consumed air and fuel used in the combustion process. This data is already measured by the onboard vehicle sensors connected to the engine controller; and most likely are available directly from Mode $01 PID data as defined by the J1979 standard (if the specific PIDs are supported by the manufacturer, e.g., PID $5E (Engine Fuel Rate), PID $10 (Air Flow Rate), PIN $9E (Engine Exhaust Flow Rate), PID $66 (Mass Air Flow Sensor), PID $0D (Vehicle Speed)). The measured values can also be corrected for intake air temperate and humidity. This calculation is outlined in Appendix 4.

There is also an alternative method. NOx mass flow rate can be estimated based on the CO2 concentration, which can be determined directly from the O2 concentration measured by the NOx/CO2 concentration sensor. The NOx value (g/mile) can be estimated by calculating the mean NOx, mean CO2, total fuel consumed, and total distance traveled. It is also possible to apply this calculation to generate instantaneous NOx flow rate. This calculation is outlined in Appendix 5. During the test, NOx (g/mile) was estimated using the following methods:

(1) Use NOx concentration data and PID data (get engine exhaust mass flow and distance) to determine the instantaneous NOx mass flow and average NOx mass flow over the drive-cycle
(2) Use NOx and O2 (get CO2) concentration data and PID data (get fuel flow and distance) to determine the instantaneous NOx mass flow and average NOx mass flow over the drive-cycle
(3) Use NOx and O2 (get CO2) concentration data (get mean values), fuel consumption measured by refill events (to get total fuel consumed), and odometer readings (get total distance) to determine average NOx mass flow over the drive-cycle

The resulting data is shown in Table 1 which was not corrected for intake air temperature and humidity.

Calculation Method		Distance (miles)	Total Fuel Consumed (grams)	Total NOx (grams)	**Estimated Average NOx (g/mile)**
(1)	NOx Concentration + Exhaust Mass Flow and Vehicle Speed PIDs	23.54	-	0.9970	0.0424
(2)	NOx and O2 Concentration + Fuel Flow and Vehicle Speed PIDS	23.54	1826	0.9302	0.0395
(3)	NOx and O2 Concentration (from mean value) + Fuel via Refill data & Odometer readings	23.5	1811	0.8938	0.0380

Table 1 : Estimated Average NOx Emission (g/mile) for Volkswagen EOS over a 23.5-mile mixed cycle in the Real World using different calculation approaches (uncorrected – rough estimates)

Figure 1 displays the time resolved data used to determine the estimated average NOx emissions (g/mile) in Table 1. The instantaneous NOx mass flow using method (1) and (2) above are compared along with the cumulative mass of NOx (grams).

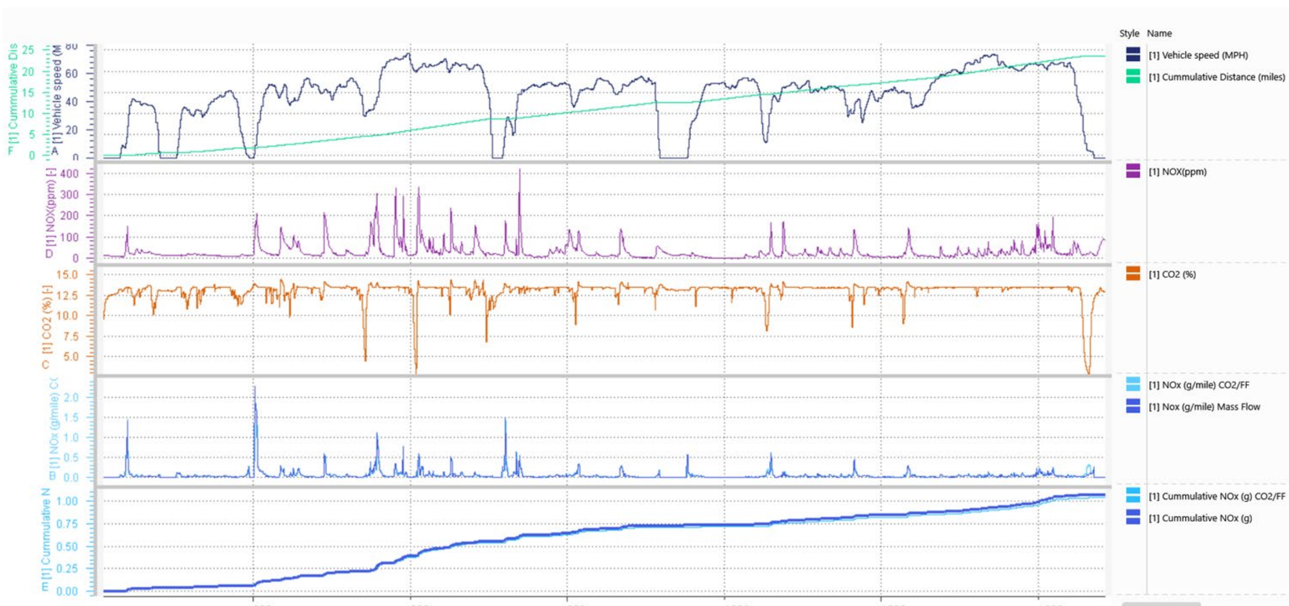

Figure 1 : Time resolved data used to calculate the estimated average NOx emissions (g/mile) for Volkswagen EOS over a 23.5-mile mixed cycle in the Real World

The data shows that method (1) and (2) are fairly well correlated with each other. Method (3) is more accurate than method (2) because this calculation looks at the [NOx]/[CO2] ratio which will become large during fuel cut-off phase but does not in reality contribute to the total mass emissions over the trip.

Fuel Enrichment Screening for Gasoline Vehicles

As commonly known, the stoichiometric mixture for a gasoline engine is about 14.7. Based on this, the actual Air to Fuel Ratio (AFR) can be calculated from the measured O2 concentration (see Appendix 6). Direct measurements of the actual AFR of a gasoline vehicle, particularly when in closed loop control, can be used to verify the fuel enrichment strategy applied by the manufacturer does not exceed what is allowed by regulation. The maximum enrichment level with tolerance is defined by the Lean Best Torque plus four percent enrichment per Federal US EPA regulation (US EPA, 2014), as stated below:

> "*… the nominal air-to-fuel ratio cannot be richer at any time than the leanest air-to-fuel ratio required to obtain maximum torque (lean best torque or LBT). An air-to-fuel ratio of LBT plus a tolerance of 4 percent additional enrichment will be allowed in actual vehicle testing to protect for any in-use variance in the air-to-fuel ratio from the nominal LBT air-to-fuel determination, for such reasons as air or fuel distribution differences from production variances or aging."*

However, enrichment outside of the LBT plus 4 percent can be allowed if approved as an Engine protection AECD ((US EPA CFR 40 Subpart S 86.1811-17 (d)(2))):

> *(d) Special provisions for Otto-cycle engines.*
>
> *(2) Engine protection. AECDs that use commanded enrichment to protect the engine or emission control hardware must not use enrichment more frequently or to a greater degree than is needed for this purpose. For purposes of this section, commanded enrichment includes intended engine operation at air-fuel ratios rich of stoichiometry, except the following:*
>
> *(i) Cycling back and forth in a narrow window between rich and lean operation as a result of feedback controls targeted to maintain overall engine operation at stoichiometry.*
> *(ii) Small changes in the target air-fuel ratio to optimize vehicle emissions or drivability. This may be called "closed-loop biasing."*
> *(iii) Temporary enrichment in response to rapid throttle motion.*
> *(iv) Enrichment during cold-start and warm-up conditions.*
> (v) *Temporary enrichment for running OBD checks to comply with § 86.1806.*

For instance, if the LBT AFR is 12.8, the LBT AFR minus 4% = 12.8/1.04 = 12.3. Of course, knowledge of the approved LBT AFR level would be necessary to check compliance, but screening data that shows unexpectedly low AFR values during close loop control would be a potential indicator that enrichment is outside of compliance limits unless it related to a "special provision" as indicated above (e.g., temporary enrichment for running OBD monitor or rapid throttle motion). As an exercise, the actual AFR is plotted for the Volkswagen EOS over the 23.5-mile drive cycle as well as the closed loop control status of the fuel system. See Figure 2 below.

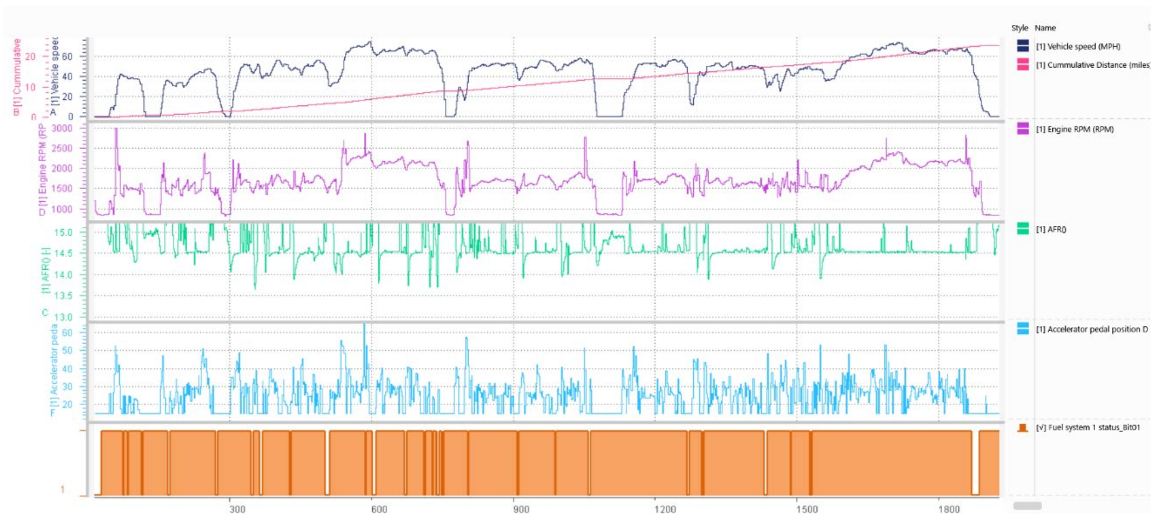

Figure 2 : Actual AFR plotted along with closed-loop control status for the for Volkswagen EOS over a 23.5-mile mixed cycle in the Real World

The average AFR appears to be about 14.5 when closed loop is active with temporary enrichment associated with rapid throttle motion for this particular cycle, and therefore, the level of enrichment is as expected (i.e., not lower than 12 AFR). If the screening data showed an actual AFR less than 12 while closed loop control was active, this would be flagged for additional investigation.

Cold Start Testing Cases and Sample Results

Measurement of cold start emissions were taken for various soak periods on a similar 6-mile route. The same set of soak time and routes were tested for both vehicles. Test conditions are given below in Table 2. Vehicle speed and NOx concentration data is plotted as a function of time and distance in Figure 3 and 4 respectively.

		Engine coolant start temperature (degC)		Ambient Temperature (degC)	
Test #	Soak Time	Volkswagen EOS (gasoline)	Mercedes S350 (diesel)	Volkswagen EOS (gasoline)	Mercedes S350 (diesel)
1	20 hours	6	3	12	3
2	90 min	59	62	22	3
3	50 min	76	72	21	3
4	20 min	90	78	16	3
5	5 min	96	81	25	2

Table 2 : Cold Start Cases

Figure 3 : Results of NOx emissions for fully soaked vehicle conditions (>20 hours) compared over similar driving route. Data is plotted against time (top) and distance (bottom). Over the first 180 seconds, the average NOx concentration for diesel vehicle during this route was 295 ppm while average NOx concentration for the gasoline vehicle is 70 ppm. Emission data is uncorrected.

Figure 4 : Test 3 results of NOx emissions for 20-minute soak compared over a very similar driving route. Data is plotted against time (top) and distance (bottom). For the first 180 seconds following cold start event, the average NOx concentration for the diesel vehicle is 185 ppm while the average NOx concentration for the gasoline vehicle is 98 ppm. Emission data is uncorrected.

Examining the data as a function of distance can be used to determine how closely the driving routes were followed, as shown. Ideally, for a pure A-B comparison, the total mileage should be equal. In the data generated, one can see that the diesel vehicle route, although minor, is slightly different; with differences noted at the 3.5-mile mark.

The time resolved data of parameters that are typically used to control cold start emissions were captured for each test in Table 2. In Figure 5, the first 200 seconds are plotted for vehicle speed, catalyst temperature, and estimated cumulative NOx mass (grams) for the Volkswagen EOS. Figure 6 shows the key elements which are used to reduce cold start emissions for this vehicle, namely engine idle speed, intake throttle position, spark ignition timing, and fuel mass flow.

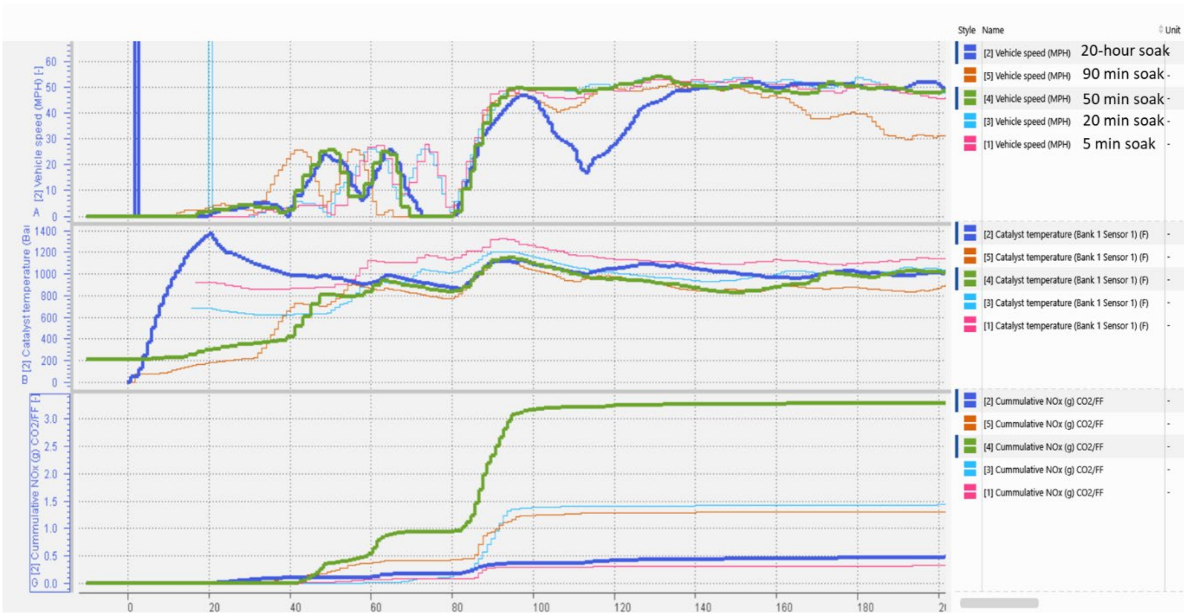

Figure 5 : Time resolved data for cold start test cases for the Volkswagen EOS gasoline vehicle; Vehicle speed, cumulated NOx mass (uncorrected), and catalyst temperature

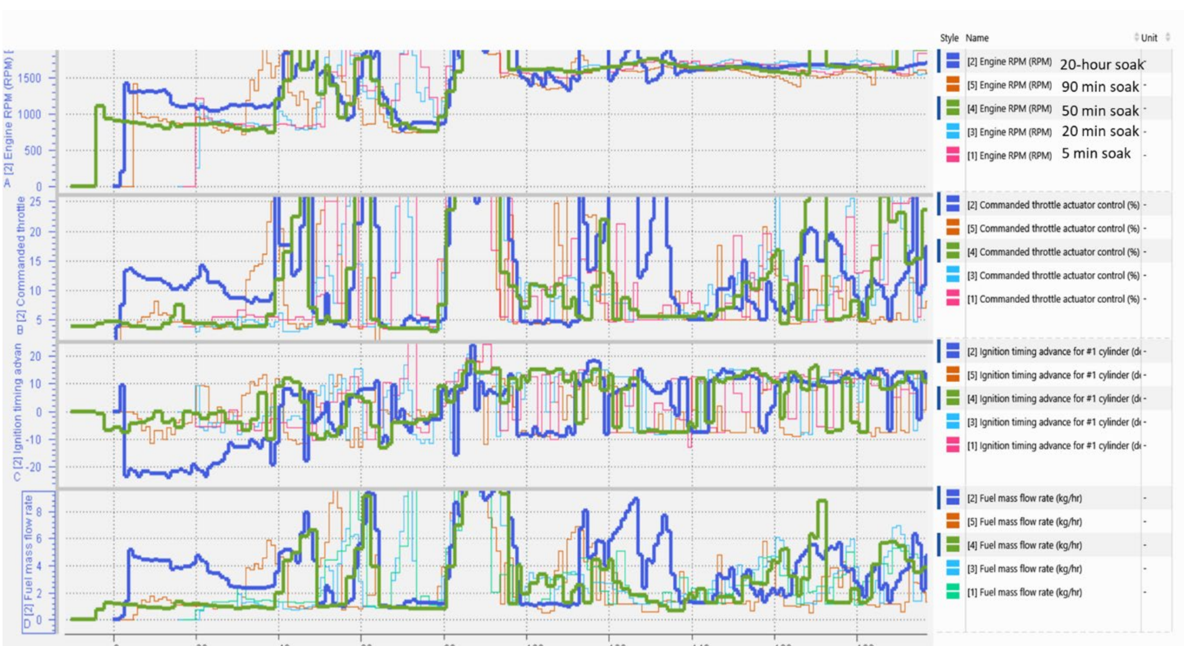

Figure 6 : Time resolved data for cold start test cases for the Volkswagen EOS gasoline vehicle; cold start related parameters

From the data in Figures 5 and 6, the cold start emission control system is active for the fully soaked condition (20-hour). By implementing a strategy that aggressively increases the catalyst temperature which peaks at nearly 1400 degF (760 degC) at about 20 seconds after the start event, the estimated NOx emissions are controlled to nearly the same rate as the 5-minute soak case. The data shows that to accomplish this, the idle speed is elevated, the intake is throttled, spark timing is retarded, and the relative fueling is increased (or enriched). These are obviously all CSERS elements. It is also noted how poorly cold start emissions are controlled for the intermediate soak time (e.g., 50-minute soak time) when the strategy is not implemented.

Similar data for the cold start test cases for the Mercedes diesel passenger vehicle is shown in Figure 7 and 8. Figure 7 plots vehicle speed, cumulative NOx, catalyst temperature, EGR duty cycle, and commanded boost pressure for the full cycle.

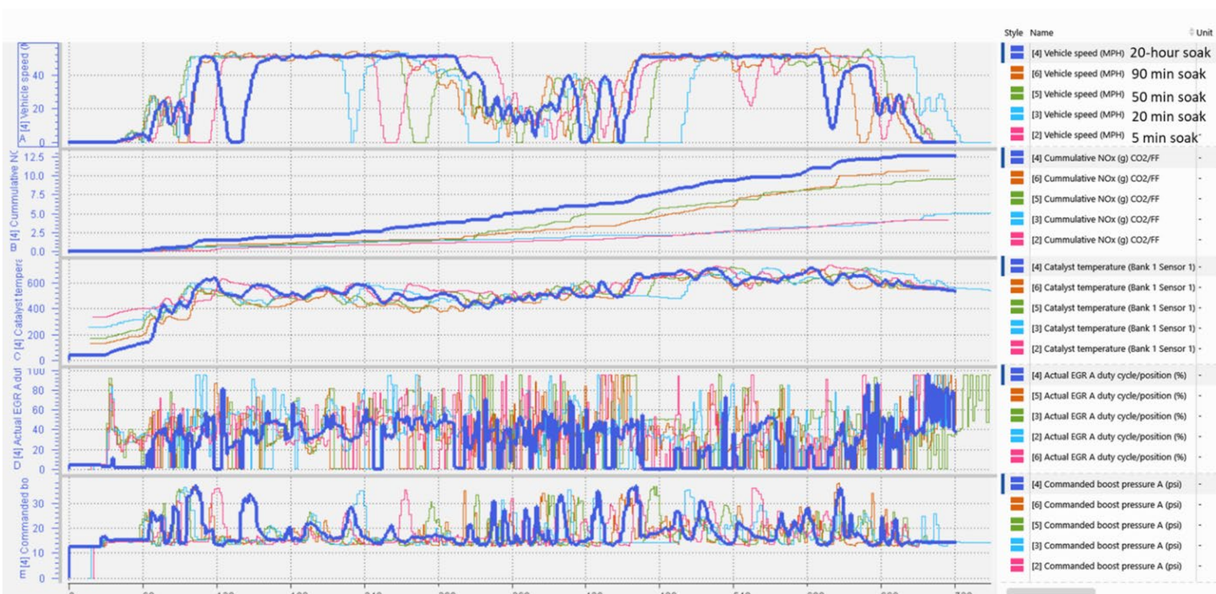

Figure 7 : Time resolved data for cold start test cases for the Mercedes S350 diesel vehicle; Vehicle speed, cumulative NOx mass (uncorrected), catalyst temperature, actual EGR rate, commanded boost pressure

Figure 8 shows other related elements that can be used to control cold start emissions; namely, fuel rail pressure, intake throttle position, EGR valve duty cycle, commanded boost pressure, and EGR VGT position.

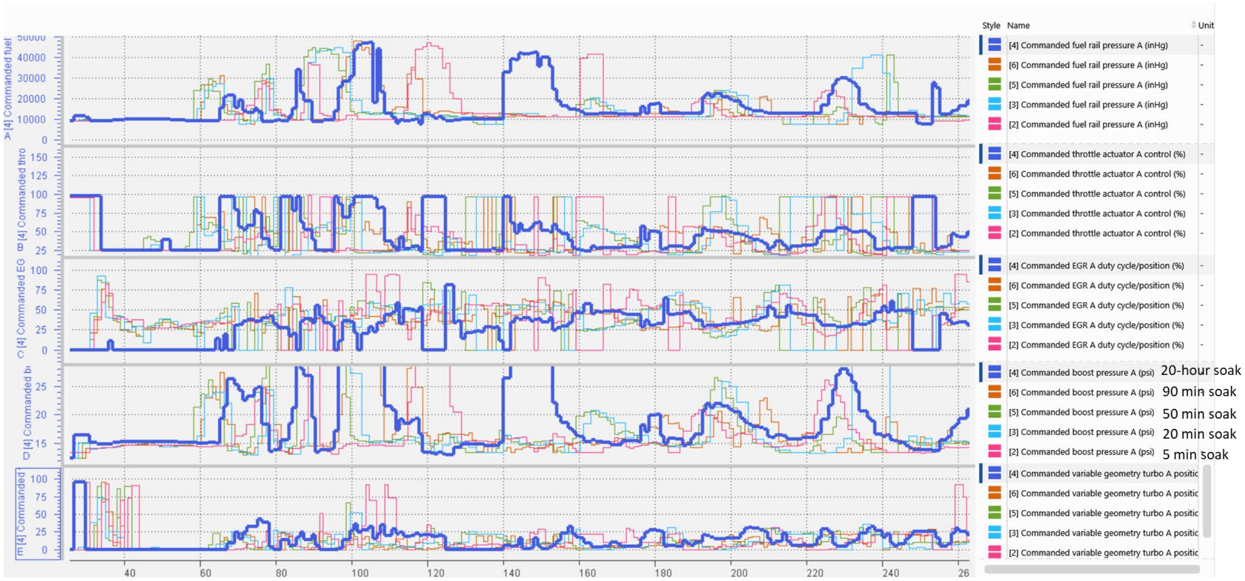

Figure 8 : Time resolved data for cold start test cases for the Mercedes S350 diesel vehicle; cold start related parameters

In the diesel vehicle data, the estimated cumulative NOx emissions are proportional to the catalyst start temperature with the highest NOx mass emission aligned to the lowest starting catalyst temperature. In the data measured from the supported PIDs, the EGR rate (e.g., actual EGR duty cycle, commanded EGR duty cycle, commanded VGT position) is the only parameter that seems to be significantly different from the fully soaked 20-hour cases in comparison to the others. Most likely due to concerns of the ability to start the vehicle or water condensation. EGR is not applied in the first 60 seconds of the 20-hour soak case when engine coolant start temperature was at 3 degC, as compared to all other cases. Without EGR, the engine out NOx emissions as well as post SCR NOx emissions will be higher. This data could be compared to the expected cold start performance listed in the AECD documentation to verify the accuracy of the documentation. Additional parameters such as the commanded DEF dosing would be useful, but this would require the software description file (A2L), calibration file (HEX/S19), software documentation, and CAN-based tool (ETAS INCA) to read extended controller specific parameters that are not supported with a J1979 defined PID.

To get an idea of the differences between the NOx emissions over the cold soak cases tested for each vehicle, the estimated cumulative NOx mass (grams) is compared at the 180 second mark for each case tested and for each vehicle, per Figure 9.

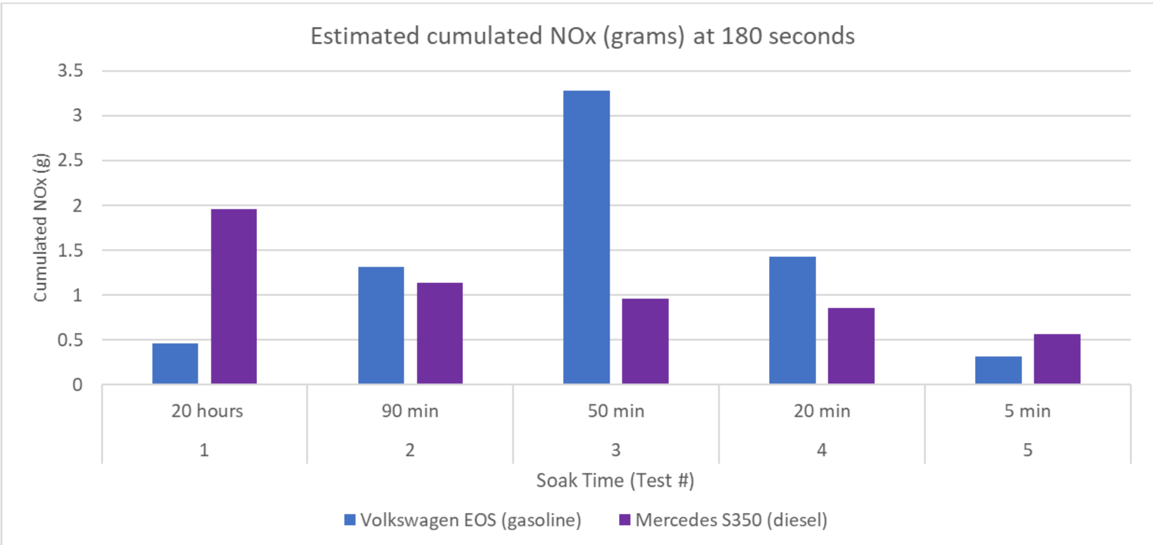

Figure 9 : Estimated cumulative NOx mass (grams, uncorrected) at the 180 second time point based on soak time for both vehicles

Trends in the NOx mass can be seen for the cases tested. The diesel performance is best for short soak period (Test #5) and poorest for fully soaked case (Test #1) for the start temperatures tested (Table 2). The gasoline vehicle has the lowest cold start emission for both fully soaked (Test #1) and short soak (Test #5) with relatively poor intermediate soak performance (Case 3).

Screening Plan

To optimize work efficiency, a good plan should be prepared. For example, screening could be conducted over specific driving routes while controlling the following parameters:

- Air conditioning (ON / OFF)
- Driver select mode (ECO / SPORT)
- Engine Start/Stop (ON/OFF)
- Safety related modes that latch across key cycles (e.g., Lane departure detection ON / OFF)
- Vehicle load / weight (max / min rating)
- Indoor soak time with controlled ambient conditions (e.g., 68 degF to 86 degF)
- Ambient temperature during test
- Route variation to adjust transient driving
- Route variation to adjust high load operation (e.g., hill climbing)
- Route variation to screen for impacts due to altitude (e.g., testing routes in Colorado)
- Route variation to screen for impacts due to timer related features

For each test, variables relating to the test conditions should be controlled independently. Ideally, the screening plan should be considered following a review of the AECD documentation and be tailored to verify performance (e.g., fuel enrichment level for gasoline operation) under real-world conditions.

Conclusions

The data generated from a NOx/O2 concentration sensor can be used to estimate real-world NOx emissions, screen for operating modes with high NOx emissions or significant enrichment, verify expected cold start emission performance strategies, and check these conditions against AECD documentation to verify in-use compliance. Although this work was done using only the supported Mode $02 PIDs with inexpensive generic OBD diagnostic tools, ideally this work should be done with the access to the engine controller software description file (A2L), calibration file (HEX/S19), software documentation, and a CAN based tool that can read and measure software labels (INCA).

Any unexpected results determined from this type of screening effort could be very useful to identify and address emission control system software or calibrations that create unintentional effects. For example, with the limited study conducted, it was identified that the CSERS strategy for the gasoline vehicle was only applied following fully soaked start conditions. These results could be compared to the AECD documentation to verify the results are as expected.

Cold start factors such as soak time, idle time prior to drive-away, and high-power demands following cold starts are all conditions that are known to have high real-world emissions for many current light-duty vehicles. The California Air Resources Board's (CARB's) Advanced Clean Car II (ACC II) program has identified a clear objective to legislate rule-making in the near future to address these gaps in the current emission regulation and the NOx/O2 sensor method can be a useful tool to assess the robustness of the cold start strategy to these factors.

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Appendix 1: Test Vehicle Specifics

Vehicle Type	**Gasoline Passenger Car**	**Diesel Passenger Car**
Manufacture	Volkswagen	Mercedes-Benz
Modal Year	2014	2012
Modal	EOS TSI	S350 Blue-Tech
Vehicle Odometer (~miles)	45,000	125,000
Engine Displacement/Type	2.0L I4 Turbo	3.0L V6 Turbo?
Power Level	200 hp @ 5100 rpm	240 hp @ 3600 rpm
Transmission	Dual-clutch 6-speed automatic	4-MATIC 7-speed automatic
Aftertreatment	3-way catalyst	DOC/DPF + SCR
Emission Standard	Tier2 Bin5 / LEVII (ULEV)	Tier2 Bin5 / LEVII (ULEV)
NOx Standard (g/mile)	0.07	0.07

Figure 10 : Test Vehicle Specifications

Appendix 2: Vehicle Preparation

The NOx/O2 concentration sensor is required to be mounted in the tailpipe. Rather than make any modification to the vehicle being tested, a custom tailpipe fixture to mount the sensor was fabricated. Placing the sensor in the tailpipe also ensures that it is non-intrusive with respect to the emission control system. The sensor is mounted on the top of the pipe to avoid any risk of coming into contact with water. The sensor should be placed at least 6 inches upstream of the outlet of the pipe to prevent back flow air being measured from the sensor; the further the better. Examples of the fixtures made for this work are shown in Figure 11.

Figure 11 : Example images of custom tailpipe fixtures used to mount NOx/O2 concentration sensor

Appendix 3: NOx/O2 Concentration Sensor & OBD2 PID Hardware/Software

This testing utilized a NOx/O2 concentration sensor with pressure compensation from ECM (Figure 12), model type NOxCANt.

Figure 12 : ECM NOxCANt Model which measure NOx and O2 concentration simultaneously

http://www.ecm-co.com/product.asp?ncant

The sensor can output NOx concentration, O2 concentration, and calculated AFR simultaneously. NOx/O2 concentration sensor with pressure compensation, software, external display, CAN-USB adapter, and CAN extension cables can be procured for under $7k USD.

OBDII Mode$01 PID data was captured by installing a blue-tooth OBDII scanner. We chose ELM 327 Mini Bluetooth device (Figure 12) which supports a wide range of OBDII communication protocols. This hardware is very inexpensive and can be procured for under $15 USD.

Figure 13 : Mini Bluetooth OBD2 Scanner OBDATOR ELM327

https://www.amazon.com/obdator-Bluetooth-Scanner-AutomotiveDiagnostic/dp/B08NWZQKZJ

To capture real-time PID Mode $01 data, Touch Scan software was used. The software also reads Mode $02 to Mode $0A. This software is also very inexpensive, at around $30 USD.

Figure 14 : TouchScan software used to view and record real-time OBDII Mode data

https://www.obdsoftware.net/software/touchscan

Appendix 4: Determining Mass Flow of Emissions Components Using Exhaust Mass Flow

$$\dot{m}_i = CF \cdot m_i \cdot \frac{M_i}{M_{exhaust\ gas}} \cdot \dot{m}_{exhaust\ gas}$$

i = specific exhaust gas component (i.e., NOx, HC, O2, CO, or CO2)

$\dot{m}_i$ = mass flow rate of specific exhaust gas component i

M_i = molecular weight of the specific exhaust gas component i

$M_{exhaust\ gas}$ = Molecular weight of the exhaust gas

$\dot{m}_{exhaust\ gas}$ = mass flow rate of the exhaust gas =

m_i= Volume fraction of the specific exhaust gas component i

CF = Correction factor for Intake air temperature and humidity

Additional notes regarding NOx emission estimation

- The instantaneous exhaust mass flow ($\dot{m}_{exhaust\ gas}$) is estimated from the summation of the intake air mass flow rate plus engine fuel rate PIDS

- **Estimated** Molecular weight of exhaust:

    a. gasoline exhaust ~ 28.9 g/mole;
    0.71 N2 + 0.14 CO2 + 0.13 H20 + 0.02 CO

    b. diesel exhaust ~ 27.6 g/mole
    0.67 N2 + 0.12 CO2 + 0.11 H20 + 0.1 O2

- **Estimated** Molecular weight of NOx

    a. For gasoline engine (stoichiometric spark-ignited) assume all NOx is NO:
        i. $M_{NOx\_gasoline} \sim M_{NO} = 30$ g/mol

    b. For engine out diesel engine (compression ignition) with NOx storage assume molar concentration of NOx is 25% NO and 75% NO2
        i. $M_{NOx\_tailpipe\ diesel} \sim 0.25\ M_{NO} + 0.75\ M_{NO2} = 42$ g/mol

- The corrected NOx mass flow rate can be corrected (CF) based on the intake air conditions, namely the intake air temperature and humidity as given in 40 CFR 89.418.

Appendix 5: Determining NOx mass flow Using CO2 Concentration and Mass Fuel Flow

If the exhaust mass flow rate is not measured, the NOx mass emission per distance unit can be estimated based on the CO2 concentration as the following (Bernard, Y., German, J., Kentroti, A., Muncrief, R., 2019);

$$\frac{\boldsymbol{NOx\ mass}}{\boldsymbol{distance}} = \frac{\boldsymbol{M_{NOx}}}{\boldsymbol{M_{CO2}}} \cdot \frac{[\boldsymbol{NOx}\,]}{[\boldsymbol{CO2}]} \cdot \left(\frac{\boldsymbol{CO2\ emissions\ of\ fuel}}{\boldsymbol{mass\ of\ fuel}}\right) \cdot \frac{\boldsymbol{mass\ of\ fuel\ consumed}}{\boldsymbol{distance}}$$

where,

M_{NOx} = Molecular weight of NOx

M_{CO2} = Molecular weight of CO2

$[NOx\,]$ = NOx concentration in the exhaust gas

$[CO2]$ = CO2 concentration in the exhaust gas

The CO2 concentration in the exhaust, $[CO2]$, as can be determine from the measured O2 concentration based on the relationship between O2 and CO2 during combustion (TSI Incorporated (2004)).

$$\%\boldsymbol{CO_2} = \%\boldsymbol{CO_2}\ (\boldsymbol{maximum}) \cdot \frac{(\boldsymbol{20.9} - \boldsymbol{O_2}\%\ \boldsymbol{measured})}{\boldsymbol{20.9}}$$

The maximum possible CO2 exhaust concentration, $\%\boldsymbol{CO_2}\ (\boldsymbol{maximum})$, is a unique property determined from chemical analysis which depends on the carbon content of the fuel and for diesel fuel, this value is roughly 13.5% (Vermeulen, Ligterink, Vonk, & Baarbé, 2012).

Because of the fuel consumption and the amount of mass of CO2 emitted on a volume basis for a specific fuel type are specifically linked, the ratio of the CO2 emissions of fuel per mass of fuel term, $\left(\frac{\boldsymbol{CO2\ emissions\ of\ fuel}}{\boldsymbol{mass\ of\ fuel}}\right)$, can be approximated as a constant. The US EPA uses the following average carbon content values used to estimate CO2 emissions from gasoline and diesel fuels (US EPA Q&A, 2014), as:

CO2 emissions from gasoline: 8,887 grams of CO2 / gallon = 3.14 g of CO2 / g of gasoline fuel

CO2 emissions from diesel: 10,180 grams of CO2 / gallon = 3.16 g of CO2 / g of diesel fuel

This can be used to determine the amount of CO2 emissions per mass of fuel combusted based on the density of the fuels (diesel = 3.22 kg/gal and gasoline = 2.83 kg/gal):

<u>For Gasoline Fuel:</u>

$\left(\frac{\boldsymbol{CO2\ emissions\ of\ fuel}}{\boldsymbol{mass\ of\ fuel}}\right)$ **= 3.14 mass units of CO2 / mass units of gasoline fuel combusted**

<u>For Diesel Fuel:</u>

$\left(\frac{\boldsymbol{CO2\ emissions\ of\ fuel}}{\boldsymbol{mass\ of\ fuel}}\right)$ **= 3.16 mass units of CO2 / mass units of diesel fuel combusted**

Using the difference in the amount of mass of CO2 produced per mass unit of diesel verses gasoline, the maximum % CO2 for gasoline was estimated at 13.4 (= 13.5*(3.14/3.16)).

The estimated NOx mass / distance will be most accurate if measured over the entire trip, or cycle, by using the mean NOX concentration, mean CO2 concentration, total mass of fuel consumed over the trip, and the total distance over the trip. The total mass of fuel consumed, and distance traveled could be determined from measuring refueling, odometer measurements, or from associated PIDs available (supported by OBDII J1979 communication). Also, the estimation technique can be applied to calculate the instantaneous NOx mass rate per distance, but will have errors; since during fuel cut-off phases, the CO2 concentration will become close to zero thereby creating a high [NOx]/[CO2] concentration ratio that does not contribute to the total mass emissions over the trip.

Appendix 6: Determining Actual AFR from O2 Concentration

$$\boldsymbol{AFR_{actual} = \frac{20.9}{(20.9 - [O_2])} \cdot AFR_{stoich}}$$

$[O_2]$ = Oxygen Concentration

AFR_{stioch} = Stoichiometric Air to Fuel ratio (fuel specific, 14.7 for gasoline)