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Evaluation of a FTIR Emission Measurement System for Legislated Emissions Using a SI Car

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ABSTRACT

A series of chassis dynamometer test trials were conducted to assess the performance of a Fourier Transform Infra Red (FTIR) system developed for on-road vehicle exhaust emissions measurements. Trials used a EURO 1 emission compliant SI passenger car which, alongside the FTIR, was instrumented to allow the routine logging of engine speed, road speed, throttle position, air-fuel ratio, air flow and fuel flow in addition to engine, exhaust and catalyst temperatures. The chassis dynamometer facility incorporated an 'industry standard' measurement system comprising MEXA7400 gas analyzer and CVS bag sampling which was the 'benchmark' for the evaluation of FTIR legislated gas-phase emissions (CO, NO_x, THC and CO₂) measurements.

Initial steady state measurements demonstrated strong correlations for CO, NO_x and THC (R^2 of 0.99, 0.97, 0.99, respectively) and a good correlation for CO₂ ($R^2 = 0.92$). Subsequent transient and total mass emissions measurements from replicate samplings of four different driving cycles (two standard cycles, FTP75 and NEDC, and two novel cycles based on real-world data collected in Leeds) also show good response of FTIR and satisfied agreement between the FTIR and CVS bag sampling measurements.

In general, the trial results demonstrate that the on-board FTIR emission measurement system provides reliable in-journey emissions data.

INTRODUCTION

Current methods for evaluating exhaust emissions from road transport are mainly based on measurements from rolling road/ constant volume sampling facilities using standard drive cycles. Emissions are typically described as a function of average speed, distance traveled or fuel consumed for the complete cycle. The average values are subsequently used to estimate transport emissions.

However, various research studies have demonstrated that many other parameters such as individual driver behavior, vehicle operating conditions, traffic conditions (free-flow, congested, etc), topography and road geometry strongly influence real world emissions (1-5). Real world emission studies provide direct measures of the uncertainty associated with emission trends estimated using standard dynamometer methods. However, such methods need vigorous validation if they are to be most useful.

As part of an on-going research project investigating real world vehicle emissions, University of Leeds researchers are using two vehicle exhaust emission measurement systems, the FTIR and a Horiba series 1000 On-Board emission measurement System (OBS1300), to collect on-road data. The FTIR (Fourier Transform Infrared) spectrometer is a portable instrument that is capable of measuring 51 species including legislated CO, NO_x, THC and CO₂ emissions as well as water, ammonia, N₂O, and many other hydrocarbon species. OBS1300 is a specially designed on board emission measurement system for monitoring CO, NO_x, THC and CO₂ emissions. These systems have been evaluated in a series of trials. This paper reports the findings of a chassis dynamometer evaluation of the FTIR system. The OBS1300 has deployed alongside the FTIR during these trials and the results of that evaluation will be reported in the future.

the on-board measurement system also included a MAX710 fuel consumption measurement system, a DC-AC converter and two batteries, and weighed approximately 180kg. The FTIR is capable of measuring concentrations as low as 0.5~3 ppm, depending on the application. It has an estimated accuracy of approximately 2% of the measurement range (8).

The FTIR monitored both legislated emissions (CO, NO_x, THC and CO₂) and selected non-legislated emissions (ammonia and speciated VOCs and nitrogen oxides) during the evaluation trials. Table 2 listed the 51 species measured by the FTIR, including 39 hydrocarbons.

However, only legislative emissions are discussed here. FTIR THC measurements are not directly equivalent to the values measured by legislated FID instruments. The FTIR tended to underestimate THCs by comparison to FID (8). Therefore, one of the objectives of this research was to determine the correction factors for FTIR and FID measurements.

The FTIR software can log additional analog inputs and here engine manifold pressure was logged as one of these inputs and used to time align emission measurements with vehicle and thermal parameters (including engine manifold pressure) logged to a second laptop.

MASS EMISSION CALCULATION

Volumetric FTIR emission measurements were converted into mass measurements using a conventional emission index (EI: g/kg fuel) conversion:

$$EI = K * C * (1 + A/F) * 1000 \text{ g/kg fuel}$$

Where:

- K is the conversion coefficient (the ratio of molecular weight the monitored species to the molecular weight of the whole sample gas). The molecular weight of exhaust gas is similar to that of air and typically does not vary more than 1% for gasoline H/C ratios (about 2), irrespective of the air/fuel ratio. Therefore, K is typically treated as a constant when calculating gasoline exhaust emissions.
- C is concentration of the monitored species, ppm or %. The equation has to be multiplied by 10⁻⁶ (ppm) or 10⁻² (%) respectively.
- A/F is the air/fuel ratio on a mass basis determined by wet based carbon balance or measured directly using lambda sensor.

For transient and total test cycle measurements, the EI was converted into emission units of g/sec or g/km using

fuel consumptions and distance simulated. Then the cycle total emissions (g) were obtained by the integration of whole cycle period. The fuel consumption could be measured directly using on-board MAX710 fuel consumption measurement system. Unfortunately, this system was broken down during the tests. So the fuel consumption was obtained by carbon balance method.

STEADY STATE AND DRIVING CYCLE TRIALS

Steady state emission measurements were collected using a step change procedure: The test car was first run in the neutral gear position at different RPM and then driven at a range of different speeds in different gears. Figure 2 shows typical speed and rpm time-series profiles for this sampling procedure. Emissions were measured by the FTIR and MEXA7400 systems. Comparisons of emissions between two measurement systems were then carried out using regression analysis. Thus the correlation between the FTIR and MEXA7400 measurements were determined. The model for FTIR correction was developed if appropriate.

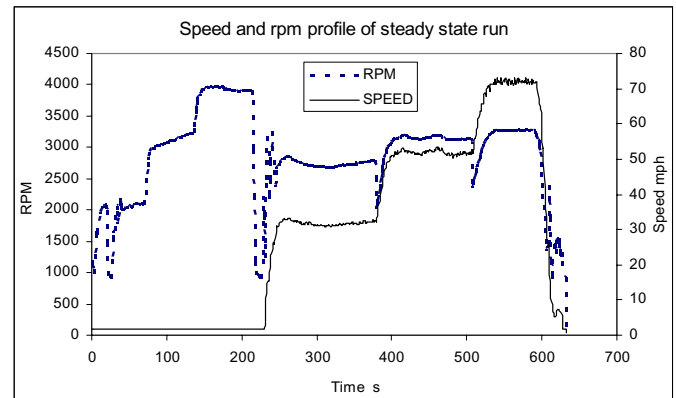


Figure 2 Vehicle speed and engine RPM profiles of steady state sampling.

Emission measurements were also taken by the FTIR and CVS bags on five test cycles, typically run in the order: FTP75, NEDC, LEEDS-BS, LEEDS-HEDLY, KETCH, with FTP75 run from a cold start and all other test cycles started warm/hot. FTP75 and NEDC are US and EU regulatory standard test cycles. LEEDS-BS and LEEDS-HEDLY are two test cycles developed at University of Leeds using real world driver behavior data. KETCH is a standard cycle (based on the extra urban component of NEDC) that PVRC use to prepare the test vehicle for the next days operation. The cycle total mass emissions were compared between the FTIR measurements and CVS bag samplings.

Figure 3 shows the driving profiles of two Leeds real world test cycles: LEEDS-BS and LEEDS-HEDLY. LEEDS-BS is a typical urban driving cycle with free flow driving patterns. LEEDS-HEDLY cycle is a combination of congested and high speed cruising patterns.

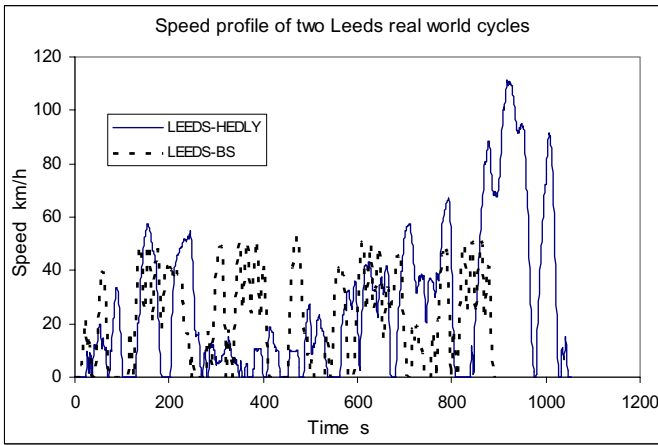


Figure 3 Driving profiles of two real world test cycles developed by Leeds University

STEADY STATE MEASURES: CORRELATION AND CALIBRATION

GENERAL METHODS

Raw FTIR data was linear regressed against the 'benchmark' MEXA7400 data and the regression assessed by analyzing the regression residues in their standardized form:

$$\text{Residue } (e_i) = [n]\text{FTIR} - [n]\text{fitted}$$

$$\text{Standardized residue } (d_i) = e_i / (\text{MSres})^{1/2} = \text{SSres} / (N-p)$$

Where:

- $[n]\text{FTIR}$ is the raw FTIR measurement of species n .
- $[n]\text{MEXA, fitted}$ is the linear regression ($y = \text{FTIR}$, $x = \text{MEXA7400}$) fitted FTIR measurement of species n .
- SSres is the sum of squared residues for the regression fit, i.e. FTIR data Vs regression fitted MEXA7400 data.
- N is the number of residues.
- p is the number of parameters.

The linearity of FTIR/MEXA7400 relationships were then determined using residue time-series analysis and appropriate data fitting (linear or weighed linear) selected for calibration. A small amount of measurements (typically < 0.5% of data), standardized residues were larger than 3. Here, this data appears to be associated with sampling during non-equilibrium periods where the engine was not at steady state. So, as elsewhere (6,7), these were considered outliers and dismissed from the data sets used for the final calibration. The outlier-excluded data sets were then re-

regressed by setting the FTIR data as an independent variable (FTIR data as X and MEXA data as Y). Thus the corrected/calibrated FTIR data (model fitted FTIR data) was obtained.

CO EMISSIONS

Both calibration and outlier data from the analysis of FTIR and MEXA7400 CO steady state emissions measurements are presented in Figure 4. The FTIR data exhibited a linear correlation with MEXA7400 data over the measured range ($R^2=0.9897$). The residues and standardized residues were calculated to identify outliers and justify the regressed model by assuring that the residues were contained in the horizontal band. The final outlier-excluded regression equation is shown below. The standard deviation of the FTIR CO measurements against MEXA7400 was 96ppm.

$$\text{Corrected CO (model fitted) (ppm)} = 1.1473x \text{ FTIR raw CO(ppm)} - 20$$

$$R^2 = 0.9959 \quad (1)$$

The above equation was obtained for hot engine conditions. The engine could produce much high CO emissions during cold starts. To examine the correlation in high CO concentrations, a rich steady state run was conducted and results are shown in Figure 5. In general, the FTIR data showed an approximately linear relationship with MEXA7400 data below 40000 ppm and deviated away from linearity above 40000 ppm. The highest CO emissions during cold start for this test car was at 40000~50000 ppm, which was just in linear correlation range. So the linear regressed equation was used for all tests including cold start.

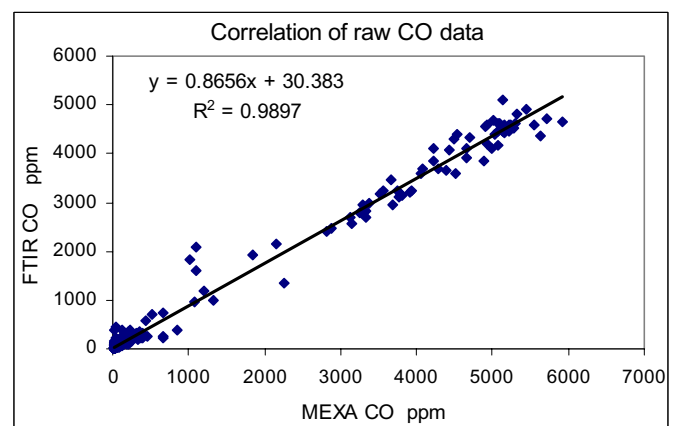


Figure 4 Raw FTIR CO data Vs MEXA CO data

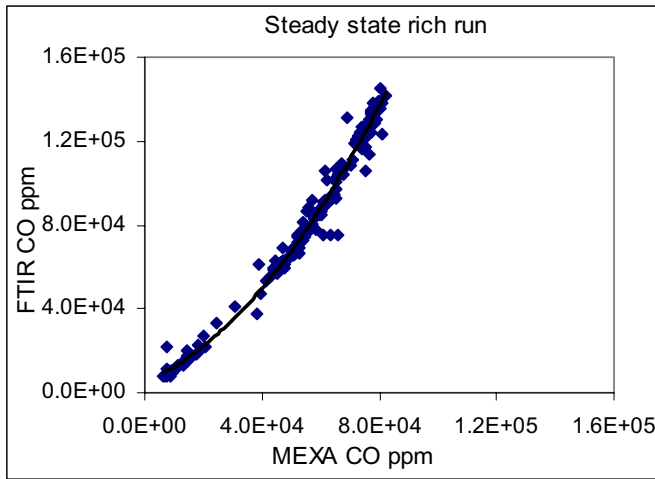


Figure 5 Comparison of CO emissions for a rich steady state run

NO_x EMISSIONS

Both calibration and outlier data from the analysis of FTIR and MEXA7400 NO_x steady state emissions measurements are presented in Figure 6. In general, the FTIR data exhibited an approximately linear correlation with MEXA7400 data over the entire concentration range observed during the steady state trials (approximately 0-800 ppm; R² ≈ 0.94). The residues and standardized residues were calculated to identify outliers and justify the regressed model by assuring that the residues were contained in the horizontal band. The final outlier-excluded regression equation is shown below. The standard deviation of the FTIR NO_x measurements against MEXA7400 was 26 ppm.

$$\text{Corrected NO}_x \text{ (model fitted) (ppm)} = 1.09 \times \text{FTIR raw NO}_x \text{ (ppm)} - 26.5$$

$$R^2 = 0.9697 \quad (2)$$

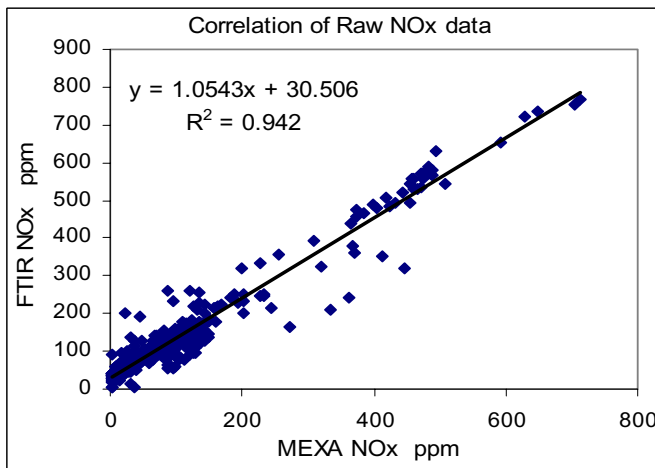


Figure 6 Raw FTIR NO_x Vs MEXA NO_x emissions

TOTAL HYDROCARBONS (THC) EMISSIONS

A significant proportion of observed THC measurements exceeded 50 ppm, the 'top end' calibration point of the MEXA7400 THC analyzer on Line 2. However, the agreement between this data set and that collected using the Line 1 THC analyzer (which was calibrated up 2000 ppm) was excellent ($y=0.99x$; $R^2 > 0.99$), indicating that the Line 2 MEXA7400 THC data could be used with reasonable confidence over this extended range. Figure 7 shows the correlation between line 1 and 2 THC data.

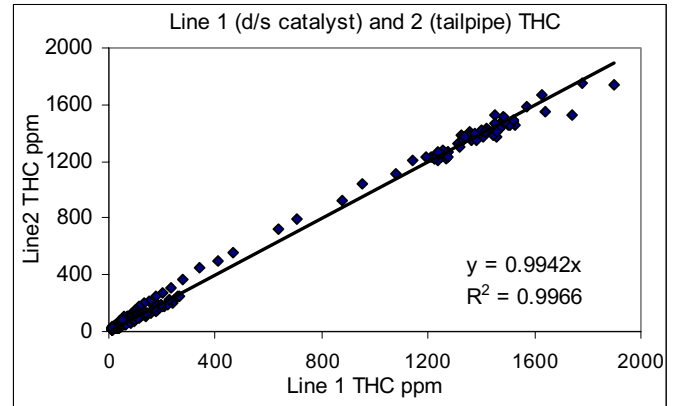


Figure 7 Correlation of line 1 and 2 THC measurement

Both calibration and outlier data from the analysis of FTIR and MEXA7400 THC steady state emissions measurements are presented in Figure 8. In general, the FTIR data exhibited a linear correlation with MEXA7400 data over the entire concentration range observed during the steady state trials ($R^2 \approx 0.99$). Analysis of the residue and standardized residue plots indicated that variance increased significantly with measurement concentration (i.e., the residue data tended towards an outward-opening funnel shape) and therefore that weighted regression was most appropriate. Weighing was applied inversely proportional to the residue variance, so that data about the top end of measurements (i.e. about 1500 ppm by MEXA7400) was weighed 0.5 by comparison to data in the main cluster of measurements (i.e., about 20~200 ppm by MEXA7400). Outlier-excluded THC measurements indicate that, consistent with previous observations (8), the FTIR underestimated THC by comparison to the MEXA7400. This discrepancy is not unexpected because the two analyzer systems measure different properties of hydrocarbons: The FTIR uses infrared absorbance to measure the concentrations of 39 individual hydrocarbons then sums these as an estimate of THC emissions. The FID (the analyzer in the MEXA7400) measures carbon combustion and reports this as methane equivalent THC. Accepting the FID measurement of THC as a 'benchmark' for legislative emissions reporting, a correction factor of approximately 2.4 ($1/0.42$. 0.42 was the gradient after outlier-excluded regression) was estimated for FTIR THC measurements. The final outlier-excluded regression equation is shown below. The standard deviation of the FTIR THC measurements against MEXA7400 was 14 ppm.

$$\text{Corrected THC (model fitted) (ppm)} = 2.4 \times \text{FTIR raw THC(ppm)} - 42$$

$$R^2 = 0.9935 \quad (3)$$

It is worth stating that vehicle exhaust gases are complicated mixtures comprising more than a hundred species. The HC species in the exhaust gases are related to driving conditions. To get more precise THC measurement for the FTIR, more quantification (instrument calibration for each HC) is needed. In addition, this correlation is determined based on SI vehicles; it may not be suitable for diesel vehicles.

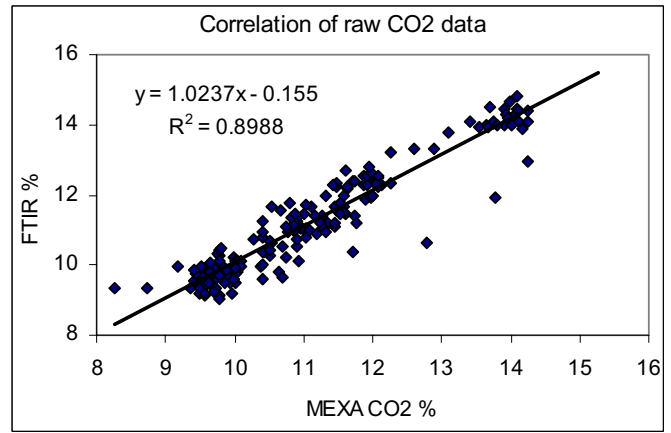


Figure 9 Raw FTIR CO₂ Vs MEXA CO₂ emissions

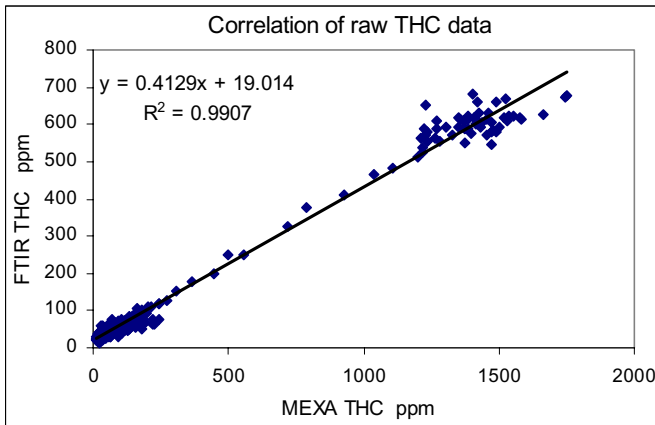


Figure 8 Raw FTIR THC data Vs MEXA THC data

CO₂ EMISSIONS

Both calibration and outlier data from the analysis of FTIR and MEXA7400 CO₂ steady state emissions measurements are presented in Figure 9. In general, the FTIR data exhibited an approximately linear correlation with MEXA7400 data over the entire concentration range observed during the steady state trials. The raw and outlier-excluded CO₂ correlations ($[R^2 \approx 0.90$ and 0.92 , respectively]) were slightly lower than these observed for other evaluated species (all $R^2 > 0.97$). This reflected the limited measurement range available for calibration (approximately 8-15%; less than an order of magnitude) rather than a deficiency in instrument performance. The residues and standardized residues were calculated to identify outliers and justify the regressed model by assuring that the residues were contained in the horizontal band. The final outlier-excluded regression equation is shown below. The standard deviation of the FTIR CO₂ measurements against MEXA7400 was 0.26%.

$$\text{Corrected CO}_2(\text{model fitted}) (\%) = 0.99 \times \text{FTIR raw CO}_2(\%) + 0.6$$

$$R^2 = 0.92 \quad (4)$$

TRANSIENT EMISSIONS MEASUREMENTS

MEXA7400 data was logged at 1 Hz. However, the FTIR, which simultaneously sampled and Fourier transformed infrared data, logged measurements at a rate of approximately 0.5 Hz (~1 measurement every 2 seconds, although the interval was not consistent). The FTIR and MEXA7400 had different length of sampling pipes. Plus instrument response time was different. So it was difficult to achieve a good time alignment between two measurements, which made regression analysis less reliable (lower R^2). Therefore direct regression comparisons were not made for transient emissions measurements collected during the different driving cycles. However, time-series comparisons of MEXA7400 and calibrated FTIR data were made and some examples (FTP75 test data) were shown in Figures 11-15. Figure 10 shows the speed profile of FTP75 cycle. In general, FTIR measurements were in good agreement with MEXA7400 measurements. However, figure 13 shows that FTIR underestimated THC measurement during cold start significantly by comparison to the MEXA7400. This is most likely due to different THC measurement techniques for FTIR and MEXA7400. Nevertheless, results demonstrated that the on-board FTIR emission measurement system had good response to transient events and provided reliable in-journey (transient) emissions data.

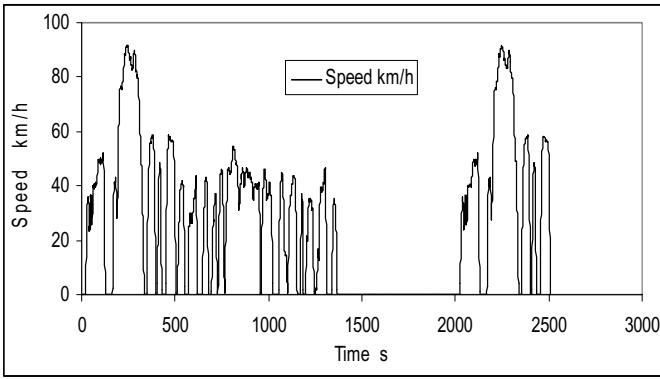


Figure 10 Speed profile of FTP75 cycle

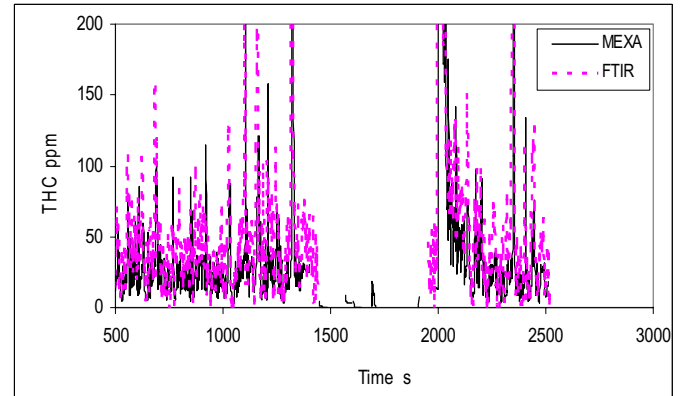


Figure 14 Comparison of THC emissions after warm up

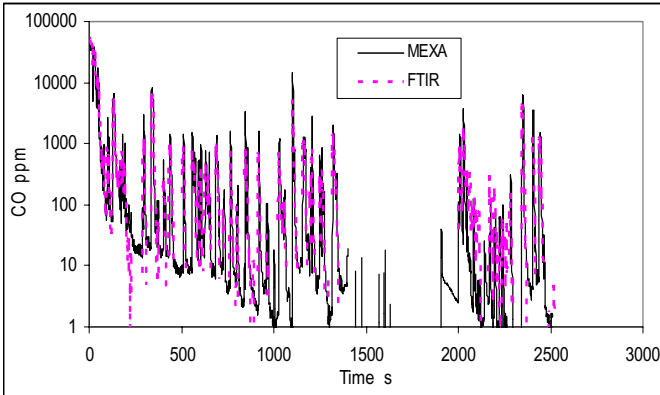


Figure 11 Comparison of CO emission profile

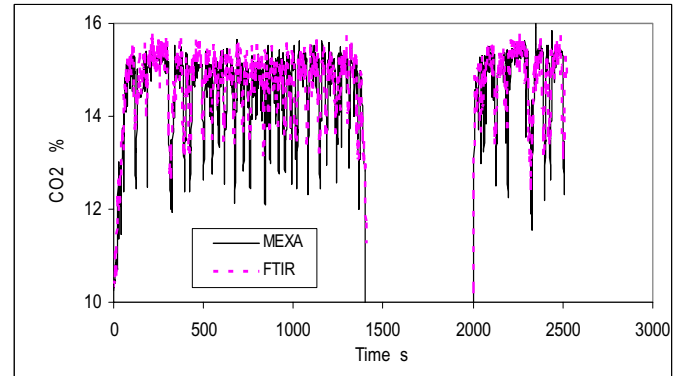


Figure 15 Comparison of CO₂ emission profile

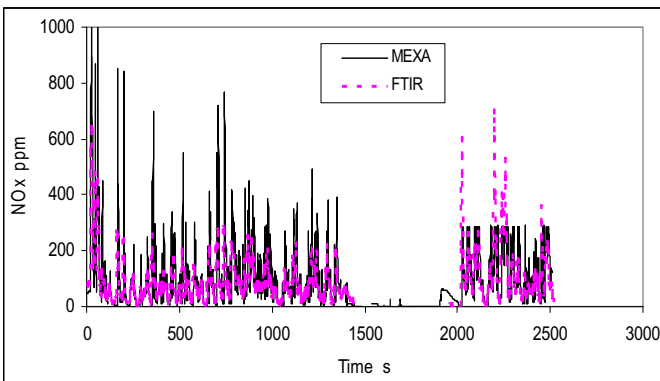


Figure 12 Comparison of NO_x emission profile

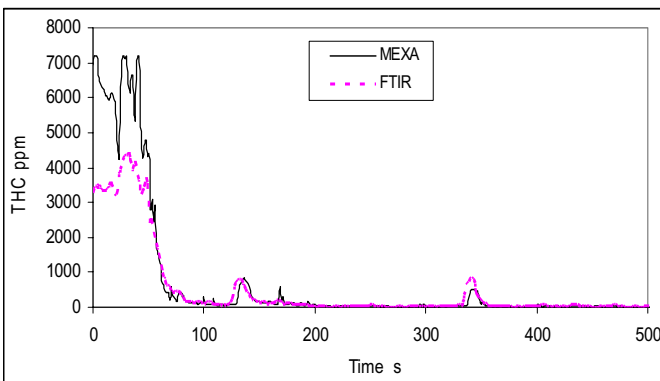


Figure 13 Comparison of THC emissions during cold start

DRIVING CYCLE TOTAL MASS EMISSIONS: CVS BAG SAMPLING AND FTIR

Tables 3 and 4 present CVS bag sampling and FTIR integrated total mass emissions for CO, NO_x, and CO₂. These measurements were obtained from replicate tests of FTP75, NEDC, LEEDS-BS and LEEDS-HEDLY cycles. THC mass emissions were calculated from integration of MEXA data as the THC measurement involves localized combustion and has to be measured on a second by second basis.

These four driving cycles represented a wide range of urban and suburban driving conditions including cold starts. Therefore, this provided a representative range of total mass emissions of CO, THC and CO₂ for evaluation purposes.

FTIR and CVS measurement differences are summarized in Table 5. The agreement between techniques for CO, NO_x and THC was improved significantly after calibration (i.e., CO 92% to 99.9%; NO_x 72% to 97% and THC 45% to 95%). Agreement for CO₂ was good and satisfied for both FTIR raw data and model fitted data (approximately 97.2% and 97.7%, respectively), indicating that the basic FTIR quantification method provided good measurements for CO₂. The poor agreement for FTIR raw NO_x and THC data most likely reflected the measurement techniques used and the nature of the monitored species: (1) The FTIR uses Fourier transform infrared to measure all

species. The MEXA7400 uses conventional infrared absorption to measure both CO and CO₂. Both methods basically measure the same properties in the measured species. However, by contrast the MEXA7400 uses chemiluminescence absorption and flame ionization to measure NO_x and THC, respectively. These different techniques most likely have different response characteristics to Fourier transform infrared. (2) Both CO and CO₂ are discrete chemical species for which calibrations sets can be easily prepared. NO_x and THC are composite species, comprising more than one discrete species each most likely exhibiting difference response characteristics. In addition, FTIR only measured limited hydrocarbon species (39 species). The accuracy of FTIR THC measurement can also probably be improved if more calibrations for other hydrocarbon species are carried out and included in the THC calculation.

CONCLUSION

The chassis dynamometer evaluation of the on-board FTIR exhaust emissions monitoring system demonstrated that the on-board FTIR provides reliable in-journey emissions data. The main findings can be summarized as follows:

1. Under steady state conditions FTIR and 'benchmark' MEXA7400 exhaust gas measurements (CO, NO_x THC and CO₂) were found to exhibit excellent correlations, R² of 0.99, 0.97, 0.99 and 0.92 respectively.
2. FTIR demonstrated good response in transient conditions and was generally comparable with MEXA7400.
3. CO, NO_x and THC were found to be in good to excellent agreement with CVS bag results (99.9%, 97% and 95% respectively) after calibration.
4. Direct FTIR CO₂ measurement has good agreement with CVS bag results (97.2%) and can be used without calibration.

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REFERENCES

1. Samuel S., Morrey D., et al; The Most Significant Vehicle Operating Parameter for Real-World Emission Levels, SAE technical paper 2004-01-0636.
2. Takada Y., Miyazaki T. AND Lida N.; Study on Local Air Pollution Caused by NO_x from Diesel Freight Vehicle. SAE technical paper 2002-01-0651.
3. Dembski N., Guezennec Y. and Soliman A.; Analysis and Experimental Refinement of Real-World Driving Cycle. SAE technical paper 2002-01-0069.
4. The Role the Highways Agency in Local Air Quality Management. Annex2. Department for Environment, Food & Rural Affairs, UK.
5. Hans Peter and Christian Cozzarini: Emissions and Air Quality. SAE Reference book R-237.2000.
6. Montgomery D C., Peck E A. and Vining G.G; Introduction to Linear Regression Analysis. Third edition, 2001.
7. Johnson R A. and Bhattacharyya G K.; Statics principles and methods. Fourth edition, 2001.
8. Daham B., Andrews G.E., Li H., Bellesteros R., Bell M., Tate J. and Ropkins K.; Application of a Portable FTIR for Measuring on road Emissions. SAE technical paper 2005-01-0676.

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ABBREVIATIONS

CVS: Constant Volume sampling

FID: Flame Ionization Detector

FTIR: Fourier Transform Infra Red

FTP: Federal Test Procedure

HC: Hydrocarbon

NEDC: New European Driving Cycle

OBS: On-Board emission measurement System

SD: Standard Deviation

SI: Spark Ignition

THC: Total Hydrocarbon

TWC: Three Way Catalyst

VOC: Volatile Organic Compounds

APPENDIX

Table 1 MEXA system specifications

	Model	Sampling	Line 1 range	Line1 Span	Line 2 Range	Line2 Span
	7400DETR DETR = Diesel, Egr, TRacer					
NO _x	Chemiluminescence CLA-720MA	Hot/Dry	2000 ppm	1320 ppm	200 ppm	199 ppm
THC	FID FIA-725A	Hot/Wet	2000 ppmC ₁	1530 ppmC ₁	50 ppmC ₁	45 ppmC ₁
CO(H)/CO ₂	NDIR AIA-722	CO Cool/Dry CO ₂ Cool/Dry	0-12 v% 0-20 %	10.3% 12.1%	12% 20%	2.97% 4.2%
CO(L)	NDIR AIA-721	Cool/Dry			2500 ppm	149 ppm

Table 2 FTIR measurement components and their ranges

Species	Calibrated range	unit	Species	Calibrated range	unit
Water vapor	50	%	1,3-Butadiene	100	ppm
CO ₂	30.1	%	Benzene	500	ppm
CO	9960	ppm	Toluene	500	ppm
N ₂ O	500	ppm	m-xylene	500	ppm
NO	2008	ppm	o-xylene	500	ppm
NO ₂	4885	ppm	p-xylene	500	ppm
SO ₂	1000	ppm	1,2,3-trimethylbenzene	500	ppm
COS	200	ppm	1,2,4-trimethylbenzene	500	ppm
NH ₃	503	ppm	1,3,5-trimethylbenzene	500	ppm
HCN	500	ppm	Ethylbenzene	*	ppm
HCl	489	ppm	Indene	*	ppm
HF	91	ppm	Methanol	500	ppm
Methane	995	ppm	Ethanol	500	ppm
Ethane C ₂ H ₆	506	ppm	Propanol	500	ppm
Propane C ₃ H ₈	500	ppm	Butanol	*	ppm
Butane C ₄ H ₁₀	500	ppm	MTBE	500	ppm
Pentane C ₅ H ₁₂	500	ppm	Dimethyl Ether	*	ppm
Iso-pentane C ₅ H ₁₂	*	ppm	Formaldehyde	96	ppm
Hexane C ₆ H ₁₄	500	ppm	Acetaldehyde	200	ppm
Heptane C ₇ H ₁₆	500	ppm	Formic acid	500	ppm
Octane C ₈ H ₁₈	*	ppm	Acetic acid	500	ppm
Iso-octane C ₈ H ₁₈	500*	ppm	Acrolein	500	ppm
Cetane C ₁₆ H ₃₄	*	ppm	Naphthalene	305	ppm
Acetylene C ₂ H ₂	98.8	ppm	1-ethylnaphthalene	500	ppm
Ethylene C ₂ H ₄	493	ppm	Sulfur hexafluoride	49.4	ppm
Propene C ₃ H ₆	500	ppm			

- The component was not uniquely calibrated for this particular instrument and thus generic libraries were used in the software for any quantitative analysis.

Table 3 CO and NO_x emissions for CVS bags, FTIR raw and model fitted values in terms of cycle total emissions (g)

Test cycles	CO g			NO _x g		
	CVS bags	FTIR	Model fit	CVS bags	FTIR	Model fit
NEDC-1	5.54	5.61	5.68	3.07	4.08	3.30
NEDC-2	6.54	6.07	6.77	3.00	3.93	3.15
NEDC-3	7.39	6.28	7.11	3.03	3.07	2.73
FTP75-1	20.02	17.39	19.59	3.85	5.39	4.17
FTP75-2	20.96	17.33	18.70	3.63	5.05	3.86
FTP75-3	20.32	16.54	18.74	3.51	4.46	3.36
LEEDS-BS-1	7.08	6.06	6.80	3.72	4.57	3.78
LEEDS-BS-2	6.52	6.04	6.77	3.69	4.57	3.78
LEEDS-HEDLY-1	11.53	11.31	11.30	3.56	4.90	3.96
LEEDS-HEDLY-2	8.18	8.06	8.25	3.63	4.63	3.79
LEEDS-HEDLY-3	11.55	10.56	11.93	3.76	4.77	3.92

Table 4 THC and CO₂ emissions for CVS bags, FTIR raw and model fitted values in terms of cycle total emissions (g)

Test cycles	THC g			CO ₂ g		
	CVS bags	FTIR raw data	Model fit	CVS bags	FTIR raw data	Model fit
NEDC-1	1.81	0.85	1.81	2008.91	1904.36	1911.78
NEDC-2	1.75	0.84	1.79	2014.43	1982.98	1991.45
NEDC-3	1.91	0.80	1.68	2068.49	1993.45	2003.15
FTP75-1	2.97	1.19	2.41	3925.49	3754.52	3768.94
FTP75-2	2.91	1.29	2.63	3877.87	3795.50	3813.15
FTP75-3				3819.98	3672.63	3690.66
LEEDS-BS-1	1.67	0.73	1.57	1568.00	1576.35	1587.02
LEEDS-BS-2	1.39	0.73	1.57	1633.90	1570.91	1581.56
LEEDS-HEDLY-1	1.80	0.82	1.66	1843.00	1840.92	1818.94
LEEDS-HEDLY-2	1.65	0.73	1.54	1857.90	1831.54	1840.87
LEEDS-HEDLY-3	2.04	0.93	2.00	1851.70	1818.94	1828.88

Table 5 Comparison of deviations of FTIR measurement Vs CVS measurement in terms of total cycle emissions (g)

Test cycles	% Difference							
	CO		NO _x		THC		CO ₂	
	FTIR vs MEXA	model vs MEXA	FTIR vs MEXA	model vs MEXA	FTIR vs MEXA	model vs MEXA	FTIR vs MEXA	model vs MEXA
NEDC-1	1.42	2.68	33.04	7.69	-53.12	0.04	-5.20	-4.84
NEDC-2	-7.14	3.55	30.92	5.16	-51.73	2.32	-1.56	-1.14
NEDC-3	-15.01	-3.72	1.38	-9.79	-58.21	-12.09	-3.63	-3.16
FTP75-1	-13.12	-2.15	39.98	8.22	-59.90	-18.78	-4.36	-3.99
FTP75-2	-17.30	-10.81	39.21	6.47	-55.80	-9.56	-2.12	-1.67
FTP75-3	-18.61	-7.77	27.06	-4.29			-3.86	-3.39
LEEDS-BS-1	-14.34	-3.97	22.97	1.60	-55.99	-5.98	0.53	1.21
LEEDS-BS-2	-7.42	3.77	23.84	2.33	-47.22	12.78	-3.86	-3.20
LEEDS-HEDLY-1	10.29	12.77	33.98	10.14	-54.23	-7.84	-3.15	-2.70
LEEDS-HEDLY-2	-1.43	0.90	27.57	4.54	-55.56	-6.72	-1.42	-0.92
LEEDS-HEDLY-3	-8.56	3.26	26.95	4.28	-54.65	-1.95	-1.77	-1.23
Mean %	-8.29	-0.13	27.90	3.30	-55.17	-4.78	-2.76	-2.27
SD %	8.84	6.48	10.45	5.82	3.76	8.67	1.65	1.71