

Modelling Vehicle Emissions from an Urban Air- Quality Perspective: Testing Vehicle Emissions Interdependencies

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Statement of Original Authorship

“I hereby declare that this submission is my own work and, to the best of my knowledge and belief, it contains no material previously published or written by another person, except where due reference is made in the thesis. Nor it contains material that to a substantial extent has been accepted for the award of any other degree or diploma at USYD or any other educational institution, except where due acknowledgment is made in the thesis”

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Abstract

This thesis employs a statistical regression method to estimate models for testing the hypothesis of the thesis of vehicle emissions interdependencies. The thesis at the beginnings, reviews critically the formation of emissions in gasoline-fuelled engines, and also reviews existing and emerging models of automotive emissions. The thesis then, presents the relationships between the urban transport system and vehicle emissions. Particularly, it summarises different types of emissions and the contributory factors of the urban transport system to such emissions. Subsequently, the thesis presents the theory of vehicle emissions interdependencies and the empirical framework for testing the hypothesis of the thesis. The scope of testing the hypothesis of the thesis is only limited to gasoline-fuelled conventional vehicles in the urban transport environment.

We use already available laboratory-based testing dataset of 542 passenger vehicles, to investigate the hypothesis of the thesis of vehicle emissions interdependencies. HC, CO, and NO_x emissions were collected under six test drive-cycles, for each vehicle before and after vehicles were tuned. Prior to using any application, we transform the raw dataset into actionable information. We use three steps, namely conversion, cleaning, and screening, to process the data. We use classification and regression trees (CART) to narrow down the input number of variables in the models formulated for investigating the hypothesis of the thesis. We then, utilise initial results of the analysis to fix any remaining problems in the data. We employ three stage least squares (3SLS) regression to test the hypothesis of the thesis, and to estimate the maximum likelihood of vehicle variables and other emissions to influence HC, CO, and NO_x emissions simultaneously. We estimate twelve models, each of which consists of a system of three simultaneous equations that accounts for the endogenous relations between HC, CO and NO_x emissions when estimating vehicle emissions simultaneously under each test drive-cycle.

The major contribution of the thesis is to investigate the inter-correlations between vehicle emissions within a well controlled data set, and to test the hypothesis of vehicle emissions interdependencies. We find that HC, CO, and NO_x are endogenously or jointly dependent in a system of simultaneous-equations. The

results of the analysis demonstrate that there is strong evidence against the null hypothesis (H_0) in favour of the alternative hypothesis (H_1) that HC, CO, and NO_x are statistically significantly interdependent. We find, for the thesis sample, that NO_x and CO are negatively related, whereas HC and CO emissions are positively related, and HC and NO_x are positively related.

The results of the thesis yield new insights. They bridge a very important gap in the current knowledge on vehicle emissions. They advance not only our current knowledge that HC, CO, and NO_x should be predicted jointly since they are produced jointly, but also acknowledge the appropriateness of using 3SLS regression for estimating vehicle emissions simultaneously.

The thesis measures the responses of emissions to changes with respect to changes in the other emissions. We investigate emission responses to a one percent increase in an emission with respect to the other emissions. We find the relationship between CO and NO_x is of special interest. After vehicles were tuned, we find those vehicles that exhibit a one percent increase in NO_x exhibit simultaneously a 0.35 percent average decrease in CO. Similarly, we find that vehicles which exhibit a one percent increase in CO exhibit simultaneously a 0.22 percent average decrease in NO_x .

We find that the responses of emission to changes with respect to other emissions vary with various test drive-cycles. Nonetheless, a band of upper and lower limits contains these variations. After vehicle tuning, a one percent increase in HC is associated with an increase in NO_x between 0.5 percent and 0.8 percent, and an increase in CO between 0.5 percent and one percent. Also, for post-tuning vehicles, a one percent increase in CO is associated with an increase in HC between 0.4 percent and 0.9 percent, and a decrease in NO_x between 0.07 percent and 0.32 percent. Moreover, a one percent increase in NO_x is associated with increase in HC between 0.8 percent and 1.3 percent, and a decrease in CO between 0.02 percent and 0.7 percent. These measures of the responses are very important derivatives of the hypothesis investigated in the thesis. They estimate the impacts of traffic management schemes and vehicle operations that target reducing one emission, on the other non-targeted emissions.

However, we must be cautious in extending the results of the thesis to the modern vehicles fleet. The modern fleet differs significantly in technology from the dataset that we use in this thesis. The dataset consists of measurements of HC, CO, and NO_x emissions for 542 gasoline-fuelled passenger vehicles, under six test drive-cycles, before and after the vehicles were tuned. Nevertheless, the dataset has a number of limitations such as limited model year range, limited representations of modal operations, and limitations of the measurements of emissions based only on averages of test drive-cycles, in addition to the exclusion of high-emitter emission measurements from the dataset.

The dataset has a limited model year range, i.e., between 1980 and 1991. We highlight the age of the dataset, and acknowledge that the present vehicle fleet varies technologically from the vehicles in the dataset used in this thesis. Furthermore, the dataset has a limited number of makes - Holden, Ford, Toyota, Nissan, and Mitsubishi. There are also a limited number of modal operations. The model operations presented in the dataset are cold start, warming-up, and hot stabilised driving conditions. However, enrichment episodes are not adequately presented in the test-drive cycles of the dataset. Moreover, the dataset does not take into account driving behaviour influences, and all measurements are cycle-based averages. The emission measurements of laboratory-based testings are aggregated over a test drive cycle, and the test drive-cycle represents an average trip over an average speed. The exclusion of the measurements of high emitting vehicles from the dataset introduces further limitations. Remote sensing studies show that 20 percent of the on-road vehicle fleet is responsible for 80 percent of HC and CO emissions.

The findings of the thesis assist in the identification of the best strategies to mitigate the most adverse effects of air-pollution, such as the most severe pollution that have the most undesirable pollution effects. Also, they provide decision-makers with valuable information on how changes in the operation of the transport system influence the urban air-quality. Moreover, the thesis provides information on how vehicle emissions affect the chemistry of the atmosphere and degrade the urban air-quality.

List of Abbreviations

ARRB	Australian Road Research Board
ARFCOM	Australian Road Fuel Consumption Model
bmep	brake mean effective pressure (N/m ²): it is the work output of an engine, as measured by a brake or dynamometer
CART	Classification and Regression Trees
CARB	California Air Resources Board
CO ₂	Carbon dioxides
CO	Carbon monoxide
CMEM	Comprehensive Modal Emissions Model
CH ₄	Methane
C ₈ H ₁₈	Iso-octane
CVS	Constant Volume Sampling
EGR	Exhaust Gas Re-circulation
EPA V	Environment Protection Authority of Victoria
EMFAC	Emissions Modelling for Air Conformity
g	Grams
GDP	Gross Domestic Product
GNP	Gross National Product
HC	Hydrocarbons
H ₂ O	Water
IQR	Interquartile range
kg	Kilograms
km	Kilometres
km/h	Kilometres per hour
L	Liters
MBT	Minimum (ignition) advance for best torque (degrees)
Mt	Million tonnes
m/sec ²	Meters per second squared
MOBILE	Mobile source emission factor
N	Nitrogen
NISE	National In-Service Emissions
NO ₂	Nitrogen dioxides
NO	Nitric oxide
NO _x	Nitrogen oxides
NMVOC	Non-methane volatile organic compound
NSW	New South Wales
NSW EPA	New South Wales Environmental Protection Authority
NSW RTA	New South Wales Roads and Traffic Authority
O ₂	Oxygen
O ₃	Ozone
OBD	On-board diagnostics
OECD	Organisation for Economic Cooperation and Development
OLS	Ordinary least-squares
P	Pressure
Pb	Lead
ppm	Parts per million (gaseous concentrations) = mole fractions x 10 ⁶
PM	Solid particulate matter

PM ₁₀	Particulate matter less than or equal 10 micro millimetres in diameter
PSIA	Pressure / Square Inches Area
ROC	Reactive organic compound
rpm	Revolutions per minute
RVP	Reid vapour pressure
SO ₂	Sulphur dioxide
Std	Standard deviation
3SLS	Three stage least-squares
TSP	Total suspended particulates
USYD	University of Sydney
US	United States
USA	United States of America
US EPA	United Sates Environmental Protection Agency
V	Volume
Vol %	Volume percentage (gaseous concentrations) = mole fractions x 10 ²
VT	Virginia Tech
VKT	Vehicle kilometres travelled
VOC	Volatile organic compound
WOT	Wide-open throttle

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Chapter One

Introduction

Urban air-quality plays an important role in the ecological system, and also it is an essential asset to human lives (Section 1.1). Evaluation of the urban air-quality requires a thorough understanding of the causes and effects of air pollution, such as: (i) emissions modelling, (ii) pollutant dispersions, and (iii) pollutant concentrations (Appendix IV).

Emissions are produced by a large number of sectors. However, transport is a major contributor to emissions, and hence air pollution (Section 1.2). Petrol-fuelled vehicles with conventional engines that are common to passenger vehicles comprise a significant share of transport (Section 1.3). Many interacting operating vehicle conditions and other confounding physical and chemical in-engine factors work together to influence vehicle emissions simultaneously (Section 1.5.2).

Many research initiatives have been undertaken to model and predict the complexity of vehicle emissions in order to control air-pollution of vehicles (Section 1.4 and Section 1.5.3). However, the mechanisms by which they affect the atmosphere and degrade the urban air-quality are not completely identified (Section 1.5.1).

Consequently, additional investigation of vehicle emissions is essential to safeguard the urban air quality, to recognise any potential changes in the climate, and to justify imposing new regulations. It is vital to increase the ability of policymakers to reach sound and reasoned decisions about vehicle emissions and air quality in order to support research interpretations and conclusions.

1.1 The Urban Air-Quality

The urban air-quality is a prime environmental concern at all times. Over the next decade, it is anticipated that the levels of nitrogen oxides (NO_x) and particulate matter (PM) will be critical determinants for the urban air-quality, in addition to CO_2 (Joumard *et al.*, 1996; ECMT, 2001). Over the past decade in the Sydney Region, the concentrations of nitrogen dioxide (NO_2) and ambient ozone (O_3), the latter of which is formed by the reactions between NO_x and HC in the presence of strong sunlight, have several times exceeded the standards of the National Health and Medical Research Council (NSW, 1994).

The urban air-quality is an essential asset to human lives. The elevation in the concentrations of PM_{10} and the ambient ozone have caused between 21 percent and 38 percent of the total deaths in England and Wales during the heat wave in August 2003 (Stedman, 2004). The deterioration of the urban air-quality has significant impacts on the welfare of a large number of peoples. Künzli *et al.* (2000) estimated that on average about 6 percent of the total annual mortality in three European countries, namely Austria, France, and Switzerland, were attributed to air pollution. They mentioned that more than 40,000 cases of death were related to air pollution, i.e., twice as many deaths were related to air pollution as to traffic accidents.

Air pollution generates large economic costs to the society. Air pollution is estimated to cost the European Union approximately €37 billion per annum, equivalent to 0.6 percent of gross domestic product (GDP), of which 90 percent is attributed to road transport (DG VII, cited in Marsden *et al.*, 2001). The local pollution in a number of European countries is estimated between 0.03 and 1.05 percent of gross national product (GNP) in terms of impacts on human health, material damage, and vegetation (Kageson, cited in Quinet, 1997).

The health costs of air-pollution are substantial, particularly for aged population. Air pollution increases significantly the use of medical care by the elderly in the US (Fuchs and Frank, cited in VTPI, 2002). Transport air-pollution incurs large costs of medical treatment. In Australia, the costs of medical treatment are

estimated AU\$34 million for CO, AU\$4.5 million for NO₂, and between AU\$95 and AU\$285 million for O₃ (McGregor *et al.*, 2001). Similarly, in the US the costs of medical treatment are estimated between US\$656 and US\$5,696 million for CO, between US\$640 and US\$3,308 million for NO₂, and between US\$129 and US\$1,094 million for O₃ (Table 1-1).

Table 1-1 Medical Treatment Costs Resulting from Vehicular Pollution

Emissions	Ambient pollutant	Health effects	Lower bound*	Upper bound*
CO	CO	mortality	302	3,743
		hospitalisation	48	148
		headaches	306	1,805
NO _x	NO ₂	sore throat	341	1,749
		excess phlegm	157	817
		eye irritation	142	742
NO _x , HC	O ₃	asthma attacks	13	231
		lower resp. illness	52	446
		upper resp. illness	16	136
		eye irritation	48	281

Source: McCubbin and Delucchi (1996)

*in the US, expressed in millions 1990 US\$

1.2 Transport Air-Pollution

Transport air-pollution contributes to worsening the urban air-quality. Transport uses mainly fossil fuels as energy sources, and thereby produces pollution.

Transport emits volatile organic compounds (VOC), such as HC – the reactive organic compound (ROC) –, carbon monoxide (CO), nitrogen oxides (NO_x), carbon dioxides (CO₂), solid carbon particulate matter (PM), sulphur dioxide (SO₂), and lead (Pb). These contribute to global warming, ozone depletion, forest decline, and smog. Also, they reduce visibility and cause respiratory and other health problems (Table 1-2).

Table 1-2 The Effects of Transport Air-Pollution

	Perceived pollution	Health impact	Smog	Forest decline	Ozone depletion	Enhanced greenhouse gases
HC	+	++	++	+	+	+
CO		+	+			+
NO_x		+	++	++	+	+
CO₂						++
PM	++	++				
SO₂		+		++		+
Pb		+				

Source: Joumard *et al.* (1996)

“+” indicates the degree of contribution; “++” > “+”.

Transport air-pollution was first recognised in the 1940s in the Los Angeles basin in the US (Heywood, 1988). Transport air pollution is a significant share of the total air-pollution, despite that industrial air-pollution is substantial. The transport sector in New South Wales accounts for 40 percent of total HC emitted and 35 percent of the total NO_x. Similarly in the UK, transport accounts for 16 percent of HC and 45 percent of NO_x. Likewise, in the US transport accounts for 35 percent of total HC emitted, for 47 percent of total NO_x emitted, as shown in Table 1-3.

Table 1-3 Transport Emissions as Percentages of Total Emissions

Emission	Emissions from transport as % of total emissions		
	Australia*	UK**	USA***
VOC	40	16	35
CO	45	59	66
NO_x	35	45	47
PM-10	25	19	5
SO₂	2	0	4

* in 2003 for NSW GMR, from on and off road transport: source: DEC (2006)

** in 2002 from road transport source: Dore *et al.* (2004)

*** in 2001 source: BTS (2002)

1.3 Emissions of Gasoline-Fuelled Vehicles

Gasoline-fuelled vehicles with conventional engines common to passenger vehicles are still major air-quality concerns, despite that technological advance

according to MacLean *et al.* (2003) have reduced more than 90 percent of their emissions. Passenger vehicles comprise a significant share of transport modes in many countries. They are the main mode in all cities in Australia. They account for two-thirds of the energy consumed by road transport, which consumed 78 percent of the total transport energy, between 1998 and 1999 (ABS, 2002).

Although that certified emissions of new vehicles on test drive-cycles have declined 96 percent for HC, 97 percent for CO, and 87 percent for NO_x (Pickrell, 1999), emissions of on-road vehicles have achieved lower levels. The average emissions per mile for the on-road fleet in the US have declined 79 percent for HC, 73 percent for CO, and 58 percent for NO_x. The real-world on-road vehicles emit on average, between one and half and two times higher than at the time of certification, and some vehicles emit 50 times higher (Ramsden, cited in Bin, 2003). Several factors are responsible for not achieving fully the potential improvements of real-world emissions (BTS, 1997), such as:

- (1) ***Emissions testing procedures:*** testing procedures of emissions do not represent the actual on-road driving conditions. They do not represent enrichment events, such as accelerating and starting (Skabardonis, 1997). Also, they do not account for various driving behaviours.
- (2) ***On-road driving conditions:*** new on-road vehicles give, sometimes, unanticipated higher levels of emissions. In this regard, control emission systems play an important role. Control emission systems under real world emissions do not function as well as under laboratory-controlled conditions (Pickrell, 1999). Laboratory conditions better control the fuel quality and the temperatures under testing.
- (3) ***Exhaust after-treatment systems:*** exhaust after-treatment systems become less effective as vehicles age.
- (4) ***Tampering with exhaust after-treatment systems:*** Guenther *et al.* (1994) demonstrated that the majority of gross polluting vehicles in the US are tampered with their exhaust after-treatment systems, despite laws to the contrary.

1.4 Controlling Air-Pollution of Vehicles

Efforts to control vehicles air-pollution are continuing. Many countries have used several measures to controlling air-pollution of vehicles, such as: (i) regulatory instruments, e.g., regulations and standards of emissions (1.4.1); (ii) technological options (1.4.2); and (iii) inspection and maintenance programmes (1.4.3), in addition to (iv) restricting vehicle kilometre travelled (1.4.4). For example, the US has undertaken several measures over the years to control air-pollution of vehicles, as shown in Table 1- 4.

Table 1-4 Milestones in Reducing Vehicles Air-pollution in the US

Year	Milestone
1970	New Clean Air Act sets auto emissions standards
1971	To meet evaporative standards, charcoal canisters appear
1973	To meet NO _x standards, emission gas recycle (EGR) valves appear
1974	Fuel economy standards are set
1975	The first catalytic converters appear for hydrocarbon and CO. Unleaded gas appears for use in catalyst-equipped cars
1981	Three-way catalysts with onboard computers and O ₂ sensors appear.
1983	Inspection and maintenance programs (I/M) programs are established in 64 cities.
1989	Fuel volatility limits are set for Reid Vapor Pressure (RVP)
1990	The 1990 Amendments set new tailpipe standards
1992	Oxyfuel introduced in cities with high CO levels
1993	Limits set on sulfur content of diesel fuel
1994	Phase-in begins of new vehicle standards and technologies.
1995	Onboard diagnostic systems in 1996 model-year cars.
1995	Phase I Federal Reformulated Gasoline sales begin in worst ozone non-attainment areas
1998	Sales of 1999 model-year California emissions-equipped vehicles begin in the Northeast

Source: (U.S. EPA, 2005)

1.4.1 Regulatory Instrument

The regulatory instruments are important factors to control air-pollution of vehicles. Nevertheless, some regulations eliminate some vehicle emissions, and tend to increase other emissions. For example, the regulation to ban the use of lead as a gasoline additive, despite having important health implications, tends to increase HC in old engines. Lead treats the metal walls of the engine and reduces the capacity of the walls to absorb un-burnt particles of HC, and hence reduces the build-up of deposits (Schäfer and Basshuysen, 1995; Pulkrabek, 1997). Also, the regulation to equip vehicles with three-way catalyst converters have reduced HC,

CO, and NO_x emissions, but increased CO₂ emissions, because catalyst-equipped vehicles consume more fuel (Bielli *et al.*, 1998).

Additionally, the progressive tightened emission standards in many countries assists controlling air-pollution of vehicles. In Australia, the Australian Design Rules “ADR 27A” were introduced in July 1976 through until 1978, and then updated to “ADR 27C” and remained in effect till December 1985. Afterwards in January 1986, the Rules were tightened to “ADR 37/00” through until 1997, and then were updated to “ADR 37/01” (DOTARS, 2001; FORS, 1996). In 2003, the Australian standards were tightened to “ADR 79/00” through to 2004, and in 2005 were updated to “ADR 79/01” (DEC, 2003). Similarly, in 2004 the US standards of emissions were updated to “Tier 2”, in 2005 the European standards were updated to “Euro 4”, and in 2005 the Japanese standards were updated to “long-term regulation” (OECD, 2004).

1.4.2 Technological Innovations

Technological innovations are another factor that plays an important role in controlling air-pollution of vehicles. Examples, of technological innovations are alternative design options of the engine, emission after-treatment systems, and fuel-efficient vehicles. Nevertheless, more fuel-efficient vehicles use more fuel in transport according to the Vancouver Conference on Sustainable Transportation (OECD, 1997b). The Conference concurs with the 19th century principle of Jevons that suggests the more efficient coal burning becomes, the more coal is used (OECD, 1997b).

Likewise regulations, some technologies tend to improve one aspect of emissions at the expense of another. For example, lean burn technology improves fuel consumption considerably, and thereby reduces CO₂. Also, it decreases HC and CO, but tends to increase NO_x significantly (DEH, 2003).

1.4.3 Inspection and Maintenance Programmes

Inspection and maintenance (I/M) programmes, in addition to the other two factors assist to control air-pollution of vehicles. I/M programmes achieve good results in reducing air-pollution of on-road vehicles in many countries. In Sweden, I/M

programmes reduced CO by 20 percent and HC by 7 percent (Faiz *et al.*, 1998). Also, in Switzerland I/M programmes reduced CO by 30 percent and HC by 20 percent (Faiz *et al.*, 1998).

Some inspection programmes that are designed to reduce both HC and CO often increase NO_x, such as engine tuning-up (Hickman, 1994; Faiz *et al.*, 1998). Servicing vehicles decrease both CO and HC, but increase NO_x. A study by Potter and Savage (cited in Hickman, 1994) illustrated that both CO and HC decreased after vehicles were serviced, but NO_x increased. Another study by the French Institute National de Recherche sur les Transports et Leur Sécurité (INRETS) (cited in Faiz *et al.*, 1998), tested vehicles before and after being tuned to manufactures' specifications, and found that both CO and HC decreased significantly after vehicles were tuned, but NO_x increased.

1.4.4 Vehicle Kilometres Travelled

In addition to the other three factors, restricting the growth in vehicle kilometres travelled (VKT) is equally important in controlling air-pollution of vehicles, and in achieving tangible improvements. The increase in demand on transport and mobility made both regulatory instruments and technological contributions insufficient to controlling air-pollution of vehicles (Bielli *et al.*, 1998). The growth in vehicle kilometres travelled (VKT) aggravates air-pollution of vehicles, despite that vehicles have achieved lower rates of emissions per kilometre.

Three main forces drive the increase in total vehicle kilometres travelled in many countries (ECMT, 2001): (i) population growth, (ii) increased urbanization, and (iii) economic development. Total vehicle kilometres travelled grow annually on average by approximately 2 percent in OECD countries, and around 4.7 percent in the rest of the world (OECD, 1995). Total vehicle kilometres travelled is directly correlated with the vehicle fleet size (Figure 1-2). The total VKT in Australia for example, increased by 23.5 percent between 1990 and 2000, and the vehicle fleet size grew by 27 percent (DEC, 2003). Total vehicle kilometres travelled are sometimes outstripping the growth in population. The total VKT in NSW for example, increased by 44 percent, between 1976 and 1995 (NSW EPA, 1997), whereas the population grew by 24 percent (ABS, 2004).

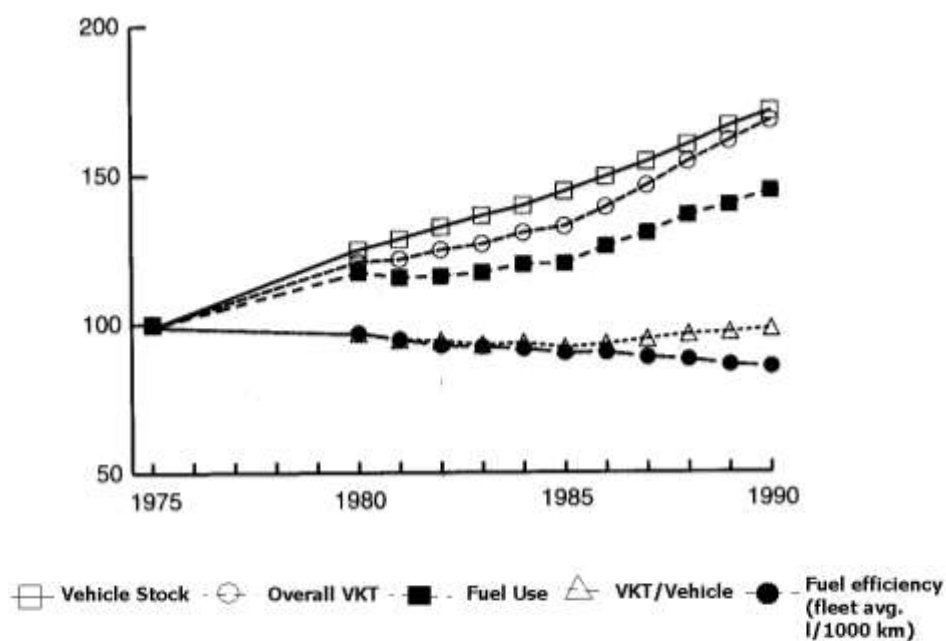


Figure 1-1 Trends of VKT and Fleet Size in OECD - Europe

Source: (OECD/IEA, cited in OECD, 1995): *data normalised between 1975 and 1990.

1.4.5 Looking Forward

In the future, it is likely that there will be several technological options to reduce further the pollution of vehicles, such as the use of alternative technologies for both the engine and fuel. However, vehicles have relatively long life cycle of about 20 years, of which 7 years are in the production line and 13 years are actual operating life (Schäfer and Basshuysen, 1995). Thus, the technological improvements will take many years before they will have visible effects on existing fleets (Stopher, 2004; Dabbas and Hensher, 2002). Existing fleets consist of new, aging, and out-of-state unregistered vehicles. A study by Younglove *et al.* (2004) demonstrated that between zero percent and 6.45 percent of the vehicles in several counties in the US were unregistered.

Additionally, more tightened emission standards will also take many years to affect existing vehicle fleets significantly. This will be especially true in countries, where there is a low vehicle turnover and scrappage rate, such as Australia. The Australian national in-service emissions study by the Federal Office of Road Safety (FORS) estimated that if every on-road vehicle in 1997 was tuned-up, then

HC emissions would be reduced by ten times greater than it would be achieved if every new vehicle added to the fleet was zero-emitting (NISE, 1996).

To accommodate a period of transition to new technologies, progressive tightened emission standards, and reinforced measures to controlling vehicles air-pollution. Continued efforts to investigating vehicle emissions are still vital. We need to learn more about the mechanisms by which vehicles pollute the air and, therefore, to target reducing the most adverse impacts of vehicles pollution on the urban air-quality.

1.5 The Thesis Key Issues

HC, CO, and NO_x are three key vehicle emissions that affect the urban air-quality. The three emissions are mainly produced from vehicles with gasoline-fuelled conventional engines that are common to passenger vehicles. The three emissions are primarily produced by the internal combustion processes in the engine and are simultaneously emitted by the exhaust to the atmosphere. HC, CO, and NO_x once emitted create air-pollution at three levels, namely global, regional, and local levels. Globally, the main effects of vehicles air-pollution are climate change caused by enhanced greenhouse gases, and depletion of ozone layer in the upper atmosphere. Regionally, the main effects of vehicles air-pollution are photochemical smog and ground level ozone caused by HC and NO_x in the presence of strong sunlight, in addition to the health effects of NO₂. Locally, the main effects of vehicles air-pollution are the immediate localised health effects of CO emissions; CO disperses rapidly into the atmosphere (NSW, 1996).

1.5.1 Vehicles Air-Pollution

Primary and Secondary Vehicle Pollutants: emissions of vehicles once present in the atmosphere are pollutants. Pollutants of vehicles are classified into primary and secondary (NSW, 1994; DEFRA, 2004). Primary pollutants are simultaneously produced and directly emitted into the atmosphere, such as HC, CO, and NO_x. While, secondary pollutants are formed by physio-chemical changes in the atmosphere, such as ozone (O₃) and PAN – peroxyacetyl nitrate – (H₃C-CO-

OONO₂). Moreover, some vehicles pollutants are both primary and secondary pollutants (Glassman, 1977), such as NO₂, CO, and Aldehydes (H-C-O). NO₂ is photochemically produced in the atmosphere by NO (between 90 percent and 98 percent of NO_x emissions), in addition to being emitted directly by the exhaust. Also, CO and Aldehydes (H-C-O) are formed in the atmosphere by the atmospheric oxidation of hydrocarbons, in addition to being emitted directly by the exhaust (Glassman, 1977).

The relationships between primary pollutants and secondary pollutants are very complex. Ambient secondary pollutants can reduce the concentrations of primary pollutants that were emitted in large quantities, whereas reducing the emissions of primary pollutants does not always lead to corresponding reductions in the concentrations of ambient secondary pollutants. Additionally, the relationship between NO_x emissions and ambient concentrations of nitrogen dioxides (NO₂) is not very clear, since the urban atmosphere has a limited capacity to convert NO into NO₂ (Schäfer and Basshuysen, 1995).

Vehicle Pollutants and Enhanced Greenhouse Gases: HC, CO, and NO_x emissions can act as indirect enhanced greenhouse gases through affecting the atmospheric chemistry (Prather *et al.*, 2001). They form ozone (O₃) an enhanced greenhouse gas, and change the lifetime of methane (CH₄) another enhanced greenhouse gas. Ozone is the third most important enhanced greenhouse gas after CO₂ and CH₄ (Prather *et al.*, 2001).

NO_x and HC in the presence of the sunlight react chemically and give tropospheric ozone, as follows:



When NO_x increases in the atmosphere, it would increase, on the one hand, ozone (O₃), and it would decrease, on the other hand, methane (CH₄) (Prather *et al.*, 2001). Thus, we want to target decreasing the levels of NO_x in the atmosphere. For, methane is reduced when oxidised with OH in the atmosphere (Hobbs, 2000; Jacob, 1999).

CO affects the oxidising capacity of the troposphere. By adding CO to the atmosphere the OH-CH₄-O₃ chemistry is agitated. When CO increases in the atmosphere, on the one hand it would increase CH₄, and on the other hand it would decrease OH. Calculations of atmospheric model indicate that 100 Mt (10⁶ tonne) of CO emissions stimulate perturbation of the atmospheric chemistry equivalent to 5 Mt of CH₄ emitted directly into the atmosphere (Prather *et al.*, 2001). When the concentrations of OH are decreased, atmospheric concentrations of CH₄ and CO would be increased. Both CH₄ and CO are oxidised by OH; OH is a principle sink for both of them (Hobbs, 2000; Jacob, 1999).

1.5.2 The Research Questions

The literature on conventional engines discusses the theoretical principles that underlie Gasoline-Fuelled Engines. It indicates that several physical, chemical, and kinetic combustion processes occur internally within conventional engines. All these processes occur almost instantaneously in a very short time of the engine cycle. The air-fuel mixture flows into the engine during the first stroke of the cycle – induction –. Then, the mixture is compressed during the second stroke – compression – that raises the pressure in the cylinder. The mixture is combusted at the end of the second stroke and lasts into the third stroke – expansion-. The gaseous molecules of the air-fuel mixture, such as O₂, N₂, and HC, react chemically under high levels of pressure and temperature, and cause the flame resulting from the reactions to propagate. The propagation of the flame and the combustion reactions that take place in the engine produce CO, HC, and NO_x emissions. The emissions, then, exist during the fourth stroke – exhaust –.

Air-fuel mixtures with various fuel equivalence ratios, i.e., strengths of the mixture, produce various levels of HC, CO, and NO_x emissions. Various combustion processes contribute variably to every emission. CO and NO_x are principally produced by chemical and kinetic mechanisms of the engine; while HC is produced by the physical processes of the engine and the physics of combustion in the chamber (Fomunung *et al.*, 1999; Patterson and Henein, 1972). The physical, chemical, and kinetic processes in the engine occur almost simultaneously in a very short time. Also, these processes contribute in several various ways to

produce simultaneously HC, CO, and NO_x emissions. Therefore, questions are raised on whether the internal processes of the engine that produce HC, CO, and NO_x emissions are interdependent.

Additionally, it is not possible to eliminate HC, CO, and NO_x emissions simultaneously. A change in one engine design variable that normally reduces one emission may increase the other emissions (Schäfer and Basshuysen, 1995). CO depends almost exclusively on the air/fuel ratio, whereas NO_x and HC depend on several other influences, such as the chamber area, cylinder displacement, spark plugs, and ignition timing. Moreover, the maintenance of vehicles, particularly when altered from manufacturers' procedures and specifications increase some emissions. For example, NO_x is increased when vehicles are tuned more finely (NSW Parliament, 1994). Also, several studies, e.g., Hickman, 1994; Faiz *et al.*, 1998, INRETS, cited in Faiz *et al.*, 1998, illustrate that both HC and CO increase after servicing vehicles, but NO_x decrease. Therefore, once again questions are raised on whether HC, CO, and NO_x emissions are interdependent.

Both vehicle design variables and operation conditions determine the levels of vehicle emissions, in addition to the maintenance status. Vehicle design variables are interrelated and affect collectively vehicle emissions. Thus, it is difficult to isolate the effects of one single variable on emissions (Schäfer and Basshuysen, 1995; Heywood, 1982). Engine-operating conditions are interrelated, and all together influence vehicle emissions. Both rich and lean conditions produce higher HC and lower NO_x (NSW Parliament, 1994). Moreover, the design variables have significant impacts on the operating conditions, such as the engine speed, the engine load, and thermal conditions of both the engine and catalyst, in addition to driving behaviours. Driving behaviours, in turn, affect the operating conditions. CO is almost unaffected by driving modes except under hard accelerations, while HC and NO (between 90 and 98 percent of NO_x) are greatly affected by engine loads and driving behaviours (LeBlanc *et al.*, 1993).

We argue that, if all variables work together to produce a flow in the exhaust pipe that consists of HC, CO, and NO_x emissions simultaneously. Therefore, questions are raised whether HC, CO, and NO_x emissions should be estimated

interdependently when modelling traffic pollution. We also argue that if the interactions between vehicle emissions were significant, then it is inaccurate to estimate HC, CO, NO_x emissions separately, but rather they must be estimated simultaneously.

1.5.3 The Research Approach

This thesis addresses the degree of interactions between three key vehicle emissions namely, HC, CO, and NO_x. Although the literature on internal combustion engines supports that vehicle emissions are interdependent, a very few advances have accounted for quantifying vehicle emissions interdependencies, except for Washburn *et al.* (2001), who modelled simultaneously CO, HC, and CO₂. Conversely, Wenzel and Ross (2003) debated fiercely the proposed models, and consequently Washburn and Mannering (2003) initiated a big storm of discussions.

The mainstream literature on modelling vehicle emissions uses ordinary least squares (OLS) regression to estimate HC, CO, and NO_x emissions separately and independently of the other two emissions. Examples are, COPERT developed for the European Union, MEASURE developed by Georgia Institute of Technology, DGV from Graz in Austria, MOBILE developed by the US Environmental Protection Agency and EMFAC developed by the US State of California. Although, the data orientation tends to differ somewhat in these models, they are based on using OLS to fit a relationship between one of three main emissions, i.e., HC, CO, and NO_x and data on vehicle characteristics and operations, but independent of the other emissions. An alternative to OLS regression is three stage least squares (3SLS) regression (Washburn *et al.*, 2001). Three stage least squares regression accounts for the endogenous relations between HC, CO, and NO_x emissions.

In this thesis, we focus on three key vehicle emissions HC, CO and NO_x emissions and investigate the significance of vehicle emissions interdependencies using already available laboratory-based emission measurements. Specifically, this thesis addresses the following themes:

- (1) Identifying in an empirical context, a set of characteristics of vehicles and the driving environment that potentially influence vehicle emissions.
- (2) Establishing simultaneous relationships between the three main vehicle emissions, namely, HC, CO, and NO_x.
- (3) Estimating the influences of vehicle and traffic conditions on vehicle emissions interdependencies.
- (4) Testing vehicle emissions interdependencies for laboratory-based emission measurements of 542 passenger vehicles.
- (5) Deriving indicators to measure emission responses to changes in the other two emissions under several standardised test drive-cycles.

1.6 Organisation of the Thesis

This thesis is organised into ten chapters; Chapter 1 introduces the thesis. Chapter 2 provides a critical review of the existing literature on modelling vehicle emissions, and presents an overview on existing and emerging models particularly in terms of modelling approaches and algorithms. Chapter 2 also identifies a gap in the current knowledge on vehicle emissions. Chapter 3 is concerned with establishing relationships between the urban transport system and vehicle emissions, particularly contributory factors, such as traffic flow conditions, operational variables, driving behaviour and vehicle technology. Chapter 4 presents the theory of the thesis, and demonstrates interdependencies of the combustion processes in the engine. Chapter 5 illustrates the empirical framework to test the hypothesis of the thesis for vehicle emissions interdependencies. It identifies a set of potential variables that influence vehicle emissions. Also, it defines contextual variables that capture other road-driving variables. The chapter proposes statistical regression method to estimate models formulated to account for emissions interdependencies, and suggests parameters to test the models formulated on emissions interdependencies.

Chapter 6 explores and examines already available data on laboratory-based measurements of vehicle emissions for testing the thesis hypothesis. It presents data sourcing and the vehicle sample of observations. It also provides preliminary

quality assessment of the data, and describes various test drive-cycles that are employed in measuring the sample emissions. Chapter 7 presents statistical issues that complicate analysing vehicle emissions, such as vehicle emissions inter-variability and intra-variability. It also outlines different emission measuring methods. Chapter 8 presents data coding scheme, data processing, and data descriptive analyses. Chapter 9 presents exploratory analyses, using classification and regression trees, to investigate the relative importance of the variables in influencing each of HC, CO, and NO_x emissions.

Chapter 10 tests the thesis hypothesis and presents the estimation results of twelve models under six test drive-cycles for each of before and after vehicles were tuned. Each model consists of a system of three jointly estimated equations. Variables that statistically significantly influence each of the three equations in every model of the twelve models are identified. Based on the estimation results, indicators of an emission response to changes in the levels of the other two emissions are also derived. Chapter 11 provides a summary of the thesis conclusions, contributions, and recommendations for further considerations.

Appendix I illustrates initial coding used of the raw data. Appendix II presents detailed tables of the estimation results of twelve models formulated for testing the hypothesis of the thesis. Appendix III presents a brief summary on the theoretical and physical principles that underlie the formation of exhaust emissions in gasoline-fuelled engines. Appendix IV demonstrates a framework that relates transport planning to the air-pollution of vehicle emissions.

Chapter Two

Modelling Vehicle Emissions: A Review of the Literature

2.1 Introduction

A review of the existing literature on vehicle emissions interdependencies indicates this to be a new topic of inquiry. The interdependencies among vehicle emissions have been consistently ignored in almost all models of vehicle emissions. Almost all models use algorithms that ignore that vehicle emissions are jointly dependent in addition to being functions of vehicle characteristics.

Existing traditional models have used ordinary least-squares (OLS) regressions to estimate vehicle emissions, but independently from one another. These models leave a vacuum in our knowledge about the relationships among vehicle emissions themselves and the role that transport variables play to influencing simultaneously vehicle emissions. Also, our current knowledge about the impacts of changes in one emission on the other emissions is still very limited. The literature does not elaborate on the degree of associations among vehicle emissions. More importantly, the literature falls short on establishing relationships among various vehicle emissions, with very rare exceptions.

Researchers with a wide range of expertise contribute to the development of the existing literature, with two main foci. The first focuses on engine technology and investigates vehicle emissions with regards to engine quality, and the second focuses on modelling vehicle emissions with regards to the urban air quality. At the beginning, we review briefly emissions of gasoline-fuelled vehicles. This topic is treated with more details in Chapter 4 and Appendix III. Then, we review the existing literature on modelling automotive emissions, especially existing classical models and a number of emerging models. The emphasis of the review is placed on whether the simultaneous effects of emissions were taken into considerations when estimating emissions.

2.2 Emissions of Gasoline-Fuelled Vehicles

Gasoline-fuelled vehicles, common to passenger vehicles, emit significantly three key emissions, carbon monoxide (CO), hydrocarbons (HC), and nitrogen oxides (NO_x) mainly as nitric oxide (NO) – between 90 and 98 percent of NO_x–. Vehicle emissions are primarily produced by the engine, and simultaneously emitted by the exhaust (Houghton, 1995). Vehicle emissions are generally emitted by three sources (Horowitz, 1982; NSW Pollution Control Commission, 1980): (i) by the crankcase vent that produces hydrocarbons, (ii) by both the tank and carburettor vents that produce hydrocarbons, and (iii) by the exhaust that emits CO, HC, NO_x emissions simultaneously.

Vehicle design variables are interrelated and affect collectively vehicle emissions (Stone, 1999; Pulkrabek, 1997; Schäfer and Basshuysen, 1995; Heywood, 1988; and Patterson and Henein, 1972). The main design variables of conventional vehicles are (MacLean and Lave, 2003): (i) a tank to store the fuel; (ii) a fuel pump to distribute the fuel; (iii) an activated carbon canister to absorb the vapours of fuel; (iv) an internal combustion engine, e.g., a spark-ignited engine for gasoline-fuelled vehicles or compression-ignited engine for diesel-fuelled vehicles; (v) a transmission system to transfer the power in the engine to the wheels; and (vi) an exhaust after treatment system to minimise vehicle emissions.

Additionally, engine-operating conditions influence vehicle emissions. Both rich and lean conditions produce higher HC and lower NO_x emissions (NSW Parliament, 1994). Operational factors, such as engine speed, engine load, thermal conditions of both the engine and catalyst, and driving behaviour, determine the vehicle operating conditions, and in turn affect emissions. The effects of these together with other operational factors and design variables are discussed in Chapter 3 and Appendix III respectively.

Both vehicle design variables and operational factors act together to determine the levels of emissions. Moreover, the maintenance status of a vehicle plays an important role in the determination of emissions. The maintenance status, particularly when altered from manufacturers' procedures and specifications

increase some emissions (Section 3.7 in Chapter 3). For example, NSW RTA demonstrated that NO_x increased when vehicles are tuned more finely (NSW Parliament, 1994).

2.3 The Effects of Design Variables on Vehicle Emissions

The literature on theoretical and physical principles that underlie gasoline-fuelled vehicles, e.g., Stone, 1999; Schäfer and Basshuysen, 1995; and Heywood, 1988, has clearly and on a scientific basis established that it is difficult to study the effects of a single design variable on emissions in isolation from the other variables. Various engine processes produce various vehicle emissions. Both CO and NO_x are principally produced by chemical and kinetic mechanisms of the engine, and HC is produced by the physical processes of the engine and the physics of combustion in the chamber (Fomunung *et al.*, 1999; Patterson and Henein, 1972). Also, various operational factors affect various emissions variably. CO is almost unaffected by driving modes except under hard accelerations, while HC and NO are greatly affected by engine loads and driving behaviour (LeBlanc *et al.*, 1993).

Additionally, it is not possible to eliminate simultaneously all emissions. A change in one of the variables that normally reduces one vehicle emission may increase one or more of the other emissions (Schäfer and Basshuysen, 1995). CO depends almost exclusively on the air/fuel ratio, whereas NO_x and HC depend on several other influences, such as the chamber area, cylinder displacement, and ignition timing. More details on this topic are in Chapter 4.

The effects of several design and operating variables on HC, CO, and NO emissions for non catalyst-equipped vehicles for example, are shown in Table 2-1. The table shows that a stoichiometric air-fuel ratio produces minimal both HC and CO, and maximal NO_x . Also, the table shows that the more ignition is retarded, both HC and NO_x will be reduced, but will have relatively small effects on CO. Moreover, the table shows that the more fuel is injected, both CO and HC will be reduced, and NO_x will be increased.

Table 2-1 The Effects of Design and Operational Variables on Emissions

Variable increased	HC (conc)	CO (conc)	NO* (conc)	Intake air mass flow under a constant load
Air-fuel ratio				↑
Engine Load	—	—	↑	↑
Engine Speed	↓	—	↓ ↑	↑↑
Spark retard	↓	—	↓	↑
Exhaust back pressure	↓	—	↓	↑
Valve overlap	↓	—	↓	↑
Intake manifold pressure	—	—	↑	↑
Combustion chamber deposits	↑	—	↑	—
Surface to volume ratio	↑	—	—	—
Combustion chamber area	↑	—	—	—
Stroke to bore ratio	↓	—	—	↑
Displacement per cylinder	↓	—	—	↑
Compression ratio	↑	—	↑	—
Air injection	↓	↓	— ↑	↓
Fuel injection	↓	↓	↑	↑
Coolant temperature	↓	— ↓	↑	—

Source: Patterson and Henein (1972);

* NO accounts for between 90 and 98 percent of NO_x;

An arrow indicates a major change; an upward arrow means an increase and a downward arrow means a decrease;

A dash “—” indicates a relatively small change;

An arrow and a dash indicate either a major change or a relatively small change;

Two arrows indicate major changes in two directions, either an increase or a decrease.

We argue that, if variables of the engine operate all together to produce a flow in the exhaust pipe that consists simultaneously of HC, CO, and NO_x emissions. Then for modelling traffic pollution, it would not be accurate to estimate an emission separately from the other two emissions. Rather vehicle emissions must be estimated simultaneously if the interactions between the emissions are significant.

2.4 Classification of Studies on Vehicle Emissions

To date, researchers have developed several algorithms for modelling automotive emissions with various approaches and spatial scales. Nevertheless, the interdependencies of vehicle emissions have been consistently ignored in almost all algorithms, except in very rare examples, such as Washburn *et al.* (2001). A wide range of studies in the literature review modelling automotive emissions from many perspective, e.g., Rakha *et al.*, 2004; Sharma and Khare, 2001; Latham *et al.*, 2000; Sturm *et al.*, 1998; Boulter *et al.*, 1997; Zachariadis and Samaras, 1997; Abbott *et al.*, 1995. The studies vary from just simple measurements to more elaborate models. Reviewing these suggests classifying the studies in the literature on modelling automotive emissions in terms of: (i) modelling objectives, (ii) spatial scale (resolution in time and space), (iii) research strategy, and (iv) modelling algorithms.

2.4.1 Modelling Objectives

Automotive emissions are modelled for several purposes, such as air quality studies, pollution control strategies, planning transport projects, and environmental impacts studies. When the objective is to evaluate urban air quality then both automotive emissions and dispersion of emissions are modelled. When the objective is to collect emissions inventories then studies at the regional levels that use average vehicle speeds are sufficient (Zachariadis and Samaras, 1997). If the focus is on traffic planning and environmental impact assessments, then local studies at the operational levels of roads are required. Examples on pollution control studies are SMART, STEP, and OFFNET, which were developed in the nineties to forecast vehicle emissions for transport control management (TCM) schemes (Herzerg *et al.*, 2002).

2.4.2 Spatial Scale – Resolution in Time and Space –

Models of automotive emissions use primarily two scales, namely macroscopic and microscopic. The scale of the models should match the spatial details of the transport system under consideration (Sturm *et al.*, 1996). However, several studies argued against using more detailed models, e.g., Zachariadis and Samaras,

1997, because: (i) detailed models need large databases; and (ii) they are not necessarily much more accurate, despite being better theoretically to describe real-world on-road vehicle emissions. Moreover, discussions are carried out in the US on whether modelling vehicle emissions should be trip-based or link-based. In this regard, Ito *et al.* (2000) highlighted three points of interest: (i) it is not well established which details of computational-level is theoretically correct for modelling urban air quality, (ii) trip-based models are not formulated to use the data of four-step travel demand models, and (iii) trip-based models require cumbersome computations.

An *et al.* (1997) categorised vehicle emissions models into strategic, regional, and local, as shown in Figure 2-1:

- (a) **Strategic models:** are established at the macroscopic level, and are based on macroscopic parameters, such as average trip speed and average driving profile. Examples are KEMIS and COPERT that are used for forecasting regional emissions and for assessing the environmental impacts of enhanced greenhouse gases (Sturm *et al.*, 1996).
- (b) **Regional models:** are developed at the mesoscopic level, and are based on the transport networks, e.g., MOBILE and EMFAC. Both models are capable of estimating large-scale inventories, but they are not capable of estimating emissions at the operational-levels of roads (Rakha *et al.*, 2004).
- (c) **Local models:** are established at the microscopic level, and are based on trip, street, and junction levels. Local models are useful for studying the impacts of driving behaviour and speed limits on vehicle emissions. Local models estimate vehicle emissions in second-by-second resolution and by either using data on the engine-load or the vehicle speed/acceleration. Both Rakha *et al.* (2004) and Venigalla *et al.* (2002) described two emerging microscopic models, namely the comprehensive modal emissions model (CMEM) and the Virginia Tech microscopic energy and emissions model (VT-Micro model). They also reported other microscopic models, such as the Mobile

Emissions Assessment System for Urban and Regional Evaluation model (MEASURE) by Georgia Institute of Technology.

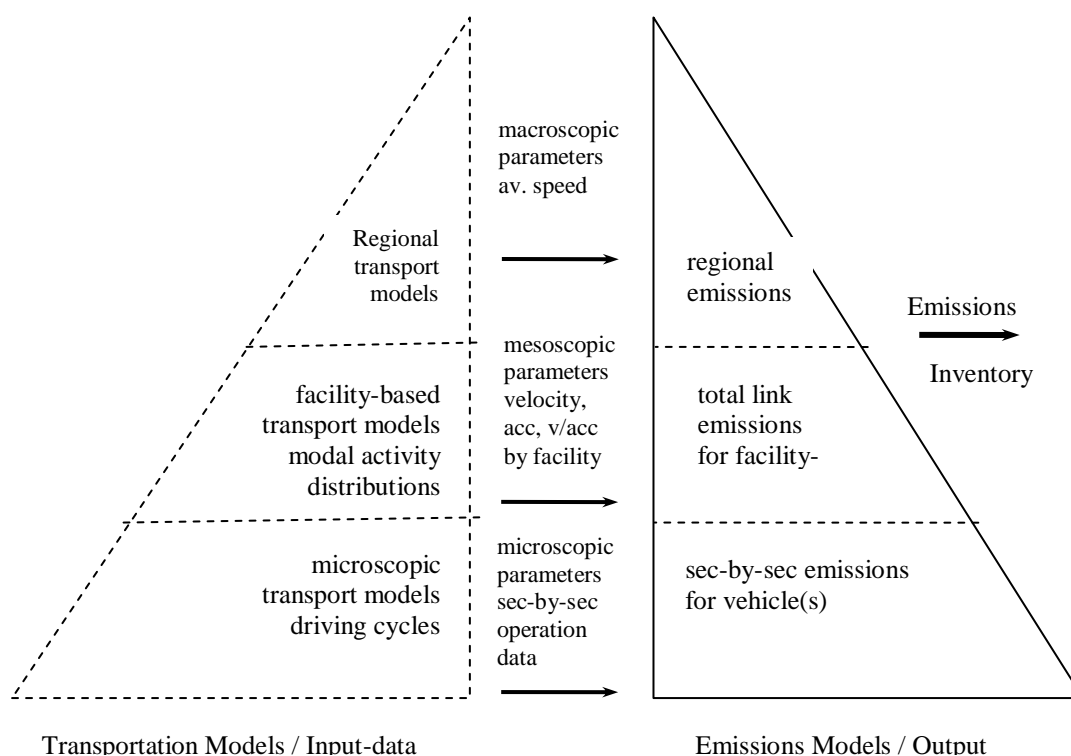


Figure 2-1 Transportation / Emissions Model Interface

Source: An *et al.* (1997)

2.4.3 Research Strategy

Automotive emissions models are processed either in a bottom-up or a top-down manner. Sturm *et al.* (1996) considered neither approach is capable of meeting the requirements for every spatial scale simultaneously. In the bottom-up approach, the input is a vehicle operating at the level of the road and on a fine time unit, such as second-by-second, and the output is aggregated to predict emissions for the average mix of vehicles in several seconds (Sturm *et al.*, 1996). For example, CMEM is a bottom-up approach model (An *et al.*, 1997). It considers both temporal and vehicular aggregation. Initially, it focuses on a high temporal resolution, such as a few seconds, and then it aggregates upward. Models that are processed in a less aggregated manner are top-down or kilometre-based models

(Sturm *et al.*, 1996). These models are used for collecting national or global inventories of emissions, and when the available data is inadequate for estimating emissions at the level of roads.

2.4.4 Modelling Algorithms

Although existing automotive emissions models are important milestones in the formulation of algorithms for estimating automotive emissions, they do not account for vehicle emissions interdependencies. Existing models in general employ ordinary least-squares (OLS) regression to estimate vehicle emissions, but independently from each other.

Several algorithms developed over the past two decades, for modelling the dispersion of vehicular emissions in street canyons, such as empirical, box, and Gaussian models (Sharma and Khare, 2001). Likewise, for modelling traffic pollution and estimating vehicle emissions, several algorithms are utilised. The earlier models used primarily velocity, whilst more recent models drew upon velocity and the interaction between velocity and acceleration (Sturm *et al.*, 1998). The Austrian Digitalized Graz method (DGV) uses average speeds to estimate factors of emissions (Zachariadis and Samaras, 1997). Both the Swiss/German Handbook of Emission Factors (HBEFA) and the Drive-Model (MODEM) use instantaneous vehicle speeds and accelerations to estimate such factors. Other examples are the mobile source emission factor (MOBILE) model developed by the US Environmental Protection Agency (US EPA) and EMFAC developed by California Air Resources Board (CARB). Both models use ordinary least-squares (OLS) regression to estimate the parameters of the models. Both models use several variables, such as average travel speeds and mileage (Sharma and Khare, 2001; Barth *et al.*, 1997). Nonetheless, the use of average travel speeds could lead to large errors in the prediction of vehicle emissions (Section 3.3.2.1).

Additionally, several researchers use various algorithms to predict vehicle emissions. Comrie and Diem (cited in Sharma and Khare, 2001) used multivariate regression models to predict CO. Fomunung *et al.* (1999) used OLS regression to estimate NO_x. Washington *et al.* (1997) used hierarchical tree-based regression

(HTBR) to estimate emissions, in order to avoid problems encountered in classical OLS regression, such as multi-level categorical variables and multi-collinearity. Ericsson (2001) used vehicle speed, engine speed, and actual gear level to estimate vehicle emissions. Washburn *et al.* (2001) used three-stage least squares regression to estimate a simultaneous equations model for CO, HC, and CO₂. Bin (2003) estimated logit regression, on I/M – inspection and maintenance— testing data to estimate the likelihood that CO and HC emissions will exceed the standards. Rahka *et al.* (2004) employed a log-transformed third order polynomial model to predict fuel consumption and emissions. Teng *et al.* (2005) used three-stage least squares (3SLS) to estimate a simultaneous equations model of both CO and HC under hot-stabilised conditions only. Beydoun and Guldman (2006) estimated logit regression models of the test failures for I/M testing data.

2.5 Trends in Existing Emissions Models

To date, existing literature reports three major long-established methods for modelling vehicle emissions. These methods vary mainly in the manner which they treat the interactions between vehicle operations and emissions (EC, 1999). Nevertheless, none of these methods accounts for the simultaneous effects on emissions. These methods are described very briefly, as follows (EC, 1999):

- (1) The first generation uses average speed over a trip as the only independent variable to predict average emissions.
- (2) The second generation uses a non-numerical parameter to describe traffic flow conditions together with the average trip speed. The non-numerical parameter describes traffic flow conditions and variations in trip speeds.
- (3) The third generation uses a second numerical variable, together with the average trip speed to describe traffic operations more accurately. The second numerical variable is acceleration or the product of speed and acceleration. Unlike the first two generations, average emissions are not considered, but rather factors are assigned to a combination of two instantaneous variables measured every second.

2.6 Emerging Vehicle Emissions Models

The most recent models account for microscopic road emissions. They use instantaneous measurements of speeds and accelerations, and in some cases consider events of enrichment, but still do not acknowledge emissions interdependencies.

Rakha *et al.* (2004) described two emerging emissions models, namely comprehensive modal emissions model (CMEM), and Virginia Tech microscopic energy and emissions model (VT-Micro Model version 2.0). CMEM, developed by the University of California is a modal power demand-based emissions model that uses a physical approach to relate the production of emissions to the corresponding physical operating phenomena. The Virginia Tech microscopic energy and emissions model (VT-Micro Model version 2.0) uses a non-linear polynomial model to relate one dependant variable, such as instantaneous emissions measurements, to a set of independent variables, such as instantaneous speeds and accelerations.

2.7 Available Vehicle Emissions Models: Overview

Drawing on the available modelling studies, such as Latham *et al.*, 2000; Schulz, 2000; Fomunung, 1999; Herzog *et al.*, 2002; EC, 1999, this section tabulates very briefly several current vehicle emissions models across the world. These models have used various test drive-cycles to represent real-world on-road driving conditions, and have used either laboratory-based testing or real-world measurements to compile the necessary databases for modelling emissions. We tabulate available information on the models, in order to reveal whether emissions interdependencies were recognised when estimating the available models (see Table 2-2).

Table 2-2 Available Vehicle Emissions Models

Model Name	Name	Developers	Emissions	
			Addressed	Modelled
Mobile Source Emissions Factor Model	MOBILE ¹	US-EPA	HC,CO,NO _X	Separately
The Mobile Emissions Assessment System for Urban and Regional Evaluation Model	MEASURE ²	Georgia Institute of Technology	HC,CO,NO _X	Separately
Comprehensive Modal Emissions Model	CMEM ³	University of California, Riverside & Michigan University	HC,CO,NO _X , CO ₂	Separately
Design manual for Road and Bridges	UK DMRB ⁴	UK Department of Roads and Bridges	HC,CO,NO _X , PM	Separately
Modelling of Emissions and Fuel Consumption in Urban Areas	MODEM ⁴	INRETS (France), TRL (UK), TÜV Rheinland (Denmark)	HC,CO,NO _X , CO ₂	Separately
The Computer programme for Estimating Emissions from Road Transport	COPERT II ⁵	CORINAIR and European Environmental Agency	CO,NO _X ,N ₂ O, SO ₂ ,NMVOC, CH ₄ ,CO ₂ , NH ₃ ,PM,Pb	Separately
Workbook on Emissions Factors for Road Transport	HBEFA ⁵	German Federal Environmental Agency & Swiss Federal Ministry for the Environmental Forestry & Agriculture	HC,CO,NO _X , CO ₂ ,PM, SO ₂	Separately
The Digitalised Graz Model	DGV ⁵	Graz University /Austria	HC,CO,NO _X , CO ₂ ,PM	Separately

Sources : 1 Latham *et al.* (2000); Herzog *et al.* (2002)

2 Fomunung (2000)

3 Schulz *et al.* (2000)

4 Latham *et al.* (2000)

5Latham *et al.* (2000); EC (1999)

2.8 Framework to Investigate Emissions Interdependencies

We develop a framework to investigate the inquiry into vehicle emissions interdependencies (Figure 2-2). The framework has three main components, namely the research context, empirical work, and the thesis contributions. We review existing vehicle emissions models, and also we review types of vehicle emissions. Moreover, we review factors of the urban transport system that contribute to vehicle emissions.

Additionally, we use for testing the hypothesis of the thesis, measurements of six test drive-cycles, for each of before and after vehicles were tuned. We undertake three principle steps to transform the raw data into actionable information. Firstly, we carry out exploratory analysis to find variables for estimating twelve models, each of which consists of three-equations, and each of which represents one emission under investigation, i.e., HC or CO or NO_x. Then, we use three stage least squares (3SLS) to estimate models of vehicle emissions interdependencies.

The major contribution of the thesis is to investigate the inter-correlations between vehicle emissions within a well controlled data set, and to test the hypothesis for vehicle emissions interdependencies. The thesis tests the hypothesis of the thesis that CO, HC, and NO_x emissions are statistically significantly interdependent. The findings of testing the hypothesis of the thesis yield new insights. They bridge a very important gap in the current knowledge on vehicle emissions. They advance not only our current knowledge that HC, CO, and NO_x should be predicted jointly since they are produced jointly, but also acknowledge the appropriateness of using 3SLS regression for estimating and modelling vehicle emissions simultaneously.

The thesis measures the responses of emissions to changes with respect to changes in the other emissions. We investigate emission responses to changes with respect to other emissions for twelve test drive-cycles. These measures of the responses are very important derivatives of testing the hypothesis of the thesis. They estimate the impacts of traffic management strategies and vehicle operations that target reducing one emission on the other non-targeted emissions.

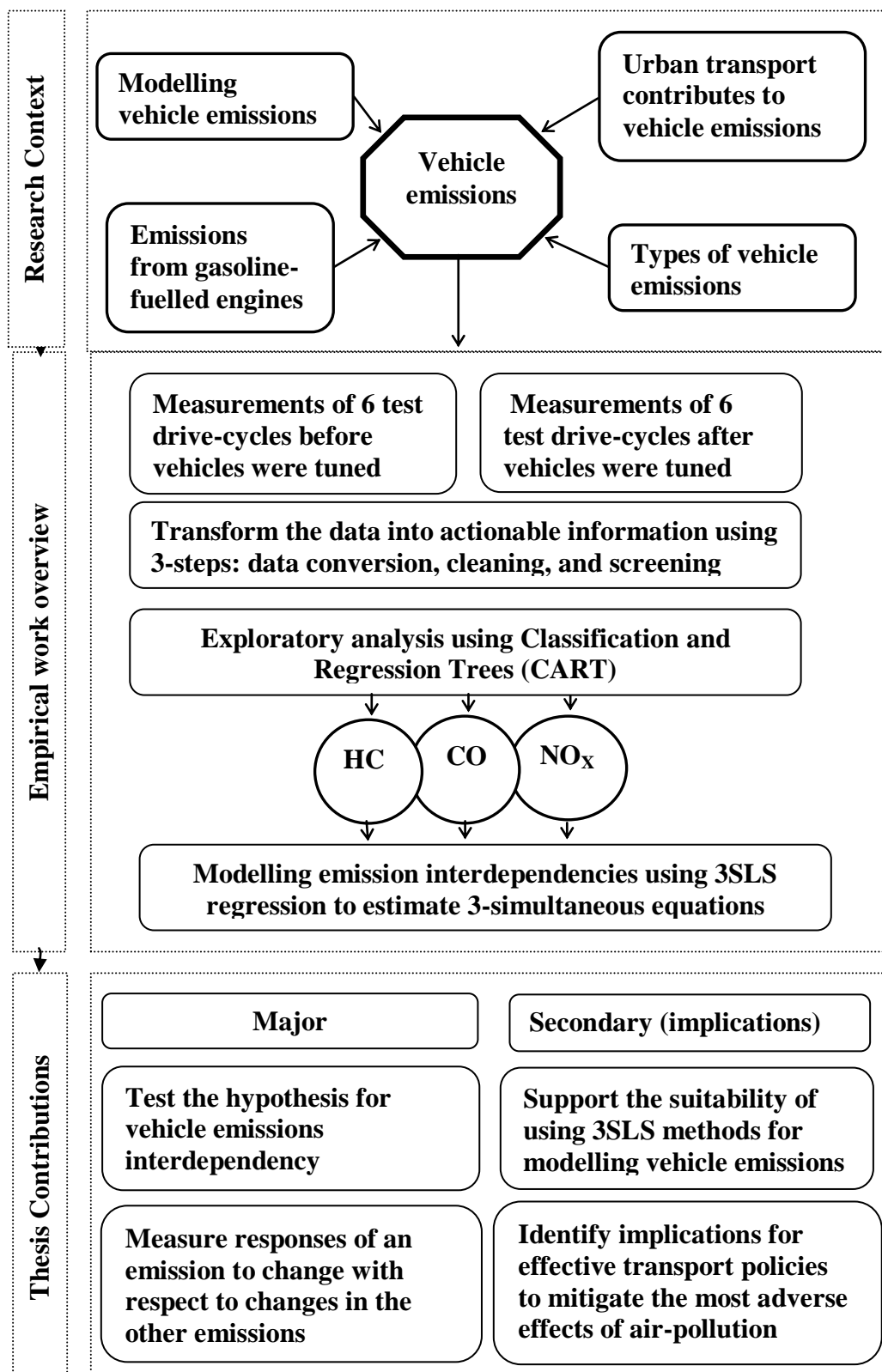


Figure 2-2 Framework of the Thesis

The findings of this thesis assist to identify the best strategies to mitigate the most adverse effects of air-pollution, such as the most undesirable health effects. Also, they provide decision-makers with valuable information on how changes in the operation of the transport system influence the urban air-quality. Moreover, they provide more information on how vehicle emissions will affect the chemistry of the atmosphere and degrade the urban air-quality. Particularly, the findings shed more lights on how vehicle emissions influence enhanced greenhouse gases and thereby degrade air-quality.

2.9 Conclusions

Almost all existing models treat vehicle emissions in isolation of one another and largely ignore the interdependencies of emissions. The models predict primarily vehicle emissions using one of three long-established methods. These methods vary in the way they treat the interactions between vehicle operations and emissions. Although that existing models were important milestones in the formulation of several algorithms for the estimations of vehicle emissions, they do not account for vehicle emissions interdependencies, except for Washburn *et al.* (2001).

Researchers predict mainly vehicle emissions in isolations of one another. Also, they estimate primarily parameters of models of vehicle emissions by ordinary least-squares regression (OLS). The researchers use various algorithms to estimate vehicle emissions, such as multivariate regression and hierarchical tree-based regression, but separately from one other. Moreover, although recent models account for microscopic road emissions, such as VT and CMEM, they do not account for the interdependencies between vehicle emissions.

Nonetheless, a very few advances have accounted for quantifying the interdependencies of vehicle emissions, such as Washburn *et al.* (2001), who modelled simultaneously CO, HC, and CO₂. Conversely, Wenzel and Ross (2003) debated fiercely the proposed models, and Washburn and Mannering (2003) initiated consequently a big storm of discussions. These debates and discussions,

after all, were not conclusive, which supports the contributions of this thesis to science.

This chapter develops a framework to investigate empirically the hypothesis that vehicle emissions are interdependent. Also, the framework assists to find indicators of measures of emissions responses to changes of emission levels with respect to other emissions. We propose three stage least-squares (3SLS) regression to test the hypothesis for vehicle emissions interdependencies. Chapter 3 looks critically at the relationships between the urban transport system and vehicle emissions. It identifies potential variables to estimate models proposed to test the hypothesis of the thesis.

Chapter Three

Relationships between the Urban Transport System and Vehicle Emissions

3.1 Introduction

The relationships between the urban transport system and vehicle emissions are approached from different perspectives, by different expertise, and using various details of measurement. Various studies investigated different combinations of vehicle emissions, some studies have investigated CO, HC, and NO_x, others only HC and CO, and a few others analysed HC, CO, in addition to fuel consumption. The results of various studies are not comparable, especially because conditions of testing vary in different regions, and also due to the lack of a common vocabulary used by specialists in various disciplines to describe some influences. Also, according to Beydoun and Guldmann (2006) measurement units of emissions create further uncertainty. Some studies use g/mile or g, and others use concentrations, such as vol % or ppm.

While Chapter 2 reviews models of vehicle emissions, this chapter gives an overview on transport contributory factors to such emissions from an empirical perspective.

3.2 Types of Vehicle Emissions

Road transport emissions are categorised into three main types, cold start, hot stabilised, and evaporative emissions (Abbott *et al.*, 1995; CEC, 1991). Vehicle emissions vary with the operating states of the engine, of which there are two main states, namely stabilised and transient operations (Patterson and Henein, 1972). Reviewing the theoretical and physical principles of gasoline-fuelled engines suggests classifying vehicle emissions into cold start, warming-up, hot stabilised, and high power, as follows:

3.2.1 Cold Start Emissions

Cold start emissions are most likely to arise under urban driving conditions, such as starting and frequent stop-start conditions. About one quarter of all journeys in Great Britain, are cold starts over less than 3 km (Stead, 1999). Gasoline-fuelled engines become hot in about 8 minutes or over between 3 km and 6 km (Boutler *et al.*, 1997). Under laboratory conditions, Joumard *et al.* (cited in Kyriakis and André, 1998) found that gasoline-fuelled engines became hot over between 4.6 km and 8.1 km. After which, the water temperature in the engine was between 70 °C and 90 °C, and the oil temperature in the engine was between 60 °C and 100 °C (Joumard *et al.*, cited in Kyriakis and André, 1998).

The US EPA defines cold starts, for non catalyst-equipped vehicles, as any start that occurs 4 hours or later following the end of the preceding trip, and for catalyst-equipped vehicles, 1 hour or later following the end of the preceding trip (Venigalla *et al.*, 1995a; 1995b). In comparison, Bendtsen and Thorsen (1994) defined cold starts more precisely. A cold start occurs when a vehicle has been running for less than 2.5 minutes after being stationary with the engine turned-off for more than two hours around ambient temperature that is equal to 7° C (Bendtsen and Thorsen, 1994).

A cold start is responsible for large percentages of total vehicle emissions. Emissions from cold engines are double that from hot engines (Stead, 1999). Cold start from catalyst-equipped vehicles over less than 6 km contributed to 34 percent of the total vehicle emissions, of which 27 percent were from cold engines and 7 percent were from hot engines (Bendtsen and Thorsen, 1995).

CO and HC emissions from cold engines are higher than the levels of NO_x emissions. NO_x are elevated with high temperatures in the engine. Kyriakis and André (1998) demonstrated that cold emissions, in 1993 in Germany, were between 33 percent and 42 percent of the total CO and HC, and between 4 percent and 7 percent of the total NO_x. Also they demonstrated that cold emissions, in 1993 in Greece, were between 22 percent and 34 percent of the total CO and HC, and between 1 percent and 5 percent of the total NO_x.

Several studies investigated the effects of ambient temperatures on HC, CO, and NO_x, in addition to the effects on fuel consumption, and found that low ambient temperatures when starting vehicles, increase fuel consumption and both HC and CO emissions, but have no significant effects on NO_x. A study by Quader (cited in Laurikko, 1997) observed that starting a vehicle below +20 °C ambient temperature, consumes between 5 and 6 times more fuel than starting above +20 °C ambient temperature. Another study by Laurikko (1995) demonstrated that the average CO for a fleet of vehicles was 20.6 g and 96.9 g for +22 °C and -7 °C of normal and low ambient temperatures, respectively – approximately five times –. Also, he found that the average HC for the fleet was 2.3 g and 10.4 g for +22 °C and -7 °C, respectively –approximately five times –. Additionally, he found that NO_x is almost unaffected by ambient temperatures, where the average NO_x for the fleet was 1.26 g and 1.32 g around +22 °C and -7 °C, respectively –almost identical –.

3.2.2 Warming-up Emissions

Warming-up conditions are transient operations that produce higher emissions than hot stabilised emissions from steady-state operations. Warming-up conditions elevate sharply the levels of HC and CO emissions. Warming-up conditions are strongly affected by the time needed by the engine and the catalytic converter to reach stabilised thermal conditions. Controlling warming-up emissions is critical to reduce traffic pollution. Nonetheless, current strategies control hot stabilised emissions better (Skabardonis, 1997).

The time needed by a vehicle to warm-up depend on several factors, such as the temperature of the intake pipes and walls, air-fuel mixture, and the catalytic converter, of which the latter two are the most critical factors (Schäfer and Basshuysen, 1995). During warming-up conditions, the fuel-injection and ignition timing must be well coordinated to ignite well the air-fuel mixtures. Also, the temperature of the catalyst converter must be around 300 °C to attain stabilised thermal conditions and convert emissions effectively. Laurikko (1997) observed that the catalytic converter lights off, i.e., become capable to convert 50 percent of the exhaust emissions (Appendix III), between 200 seconds and 260 seconds, and over between 1.5 km and 3 km.

3.2.3 Hot Stabilised Emissions

Hot stabilised emissions result from steady-state operations. These operations occur under normal engine temperatures between 80 °C and 90 °C (Boulter *et al.*, 1997). A hot start is any start that occurs either within less than 4 hours after the end of the preceding trip, for non catalyst-equipped vehicles, or within less than 1 hour after the end of the preceding trip for catalyst-equipped vehicles (Venigalla *et al.*, 1995a; 1995b). Hot stabilised emissions are affected by a wide range of variables, such as vehicle age, engine size, vehicle speed, and maintenance status, in addition to infrastructure designs and climate conditions (Sections 3.3.1 to 3.3.5). Nonetheless, ambient temperatures, under hot stabilised operations, do not influence the normal operations of both the engine and the catalytic converter (Laurikko, 1997).

3.2.4 High Power Emissions

Both events of accelerating and going upgrades produce higher emissions. When vehicles accelerate onto a freeway or go uphill, they are under wide-open throttle (WOT) conditions, and therefore under enrichment conditions. Kelly and Groblicki (1993) demonstrated that enrichment of a 3.8 litre V-6 engine, occur at throttle openings larger than 40 percent of WOT, and engine speeds more than 2000 revolutions per minute (rpm).

Enrichment events produce higher levels of CO emissions than a cold start (Laurikko, 1995; Kelly and Groblicki, 1993). Despite the significance of enrichment events on the levels of emissions, the current test drive-cycles failed to represent enrichment events well. The US California Air Resources Board (CARB) noted that enrichment events are not accounted for in the present emissions models (Skabardonis, 1997).

More importantly, is commanded enrichment (Williams *et al.*, 1998; Kelly and Groblicki, 1993). Commanded enrichment is the enrichment of the air-fuel mixture in response to high engine loads (Kelly and Groblicki, 1993). Commanded enrichments for 451 seconds –1.2 percent of the time for the study – contribute to 88 percent of the CO emitted over 352 miles in 10.6 hours (Kelly and Groblicki,

1993). Kelly and Groblicki (1993) found that commanded enrichments affect CO 60 times more than HC, but do not affect NO.

3.3 The Urban Transport System and Vehicle Emissions

According to Nicolas (2000), three combined traffic factors contribute to road traffic pollution, namely traffic mix, traffic volume, and traffic flow conditions. We classify, in the context of this thesis, the urban transport system that interfaces with vehicle emissions into four groups: (i) traffic flow conditions, (ii) vehicle operational variables, (iii) driving behaviour, and (iv) vehicle technology. These four categories are elements in the urban transport system that influence vehicle emissions, and hence the urban air-quality (Figure 3-1).

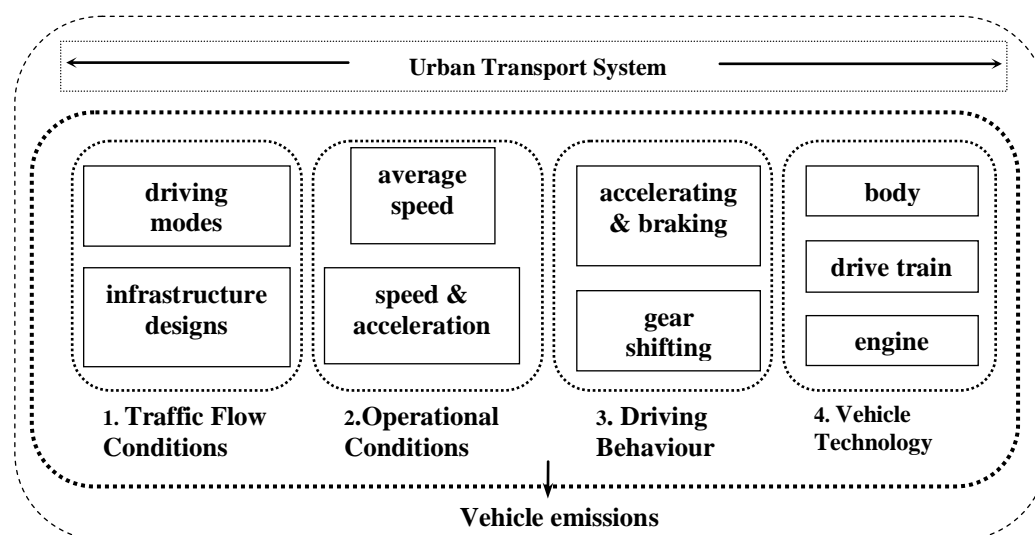


Figure 3-1 Transport and Vehicle Emissions: the Interfaces

3.3.1 Traffic Flow Conditions

Vehicle emissions depend on the traffic flow conditions of a traffic stream. Despite the importance of the effects of traffic on the levels of emissions, the current test drive-cycles failed to represent daily variations in traffic flow conditions. Lin and Niemeier (2003) observed that the current test drive-cycles do not represent daily variations in traffic flow conditions. Traffic flow conditions are linked to several driving modes and operational conditions. Two main variables describe best the

influence of traffic flow conditions on vehicle emissions, namely driving modes and infrastructure designs, as follows:

3.3.1.1 Vehicle driving modes

Traditionally, vehicle emissions are described by the modal approach that uses several driving modes, such as idle emissions, cruising emissions, acceleration emissions, and deceleration emissions. Driving modes are represented by test drive-cycles, and test-drive cycles measure vehicle emissions of the average traffic flow conditions (see Section 3.3.5). We discuss driving modes, as follows (Pulkrabek, 1997):

- **Idle mode** – under very low engine speeds, idling closes the throttle, creates a high vacuum in the intake system, and induces fuel-rich mixtures that emit higher HC and CO. During idle speeds, misfires and poor combustion are common. A misfire of two percent will increase the levels of emissions between 100 percent and 200 percent.
- **Cruising mode** – the engine is in a steady-state condition, under cruising mode, which requires less power and consumes less fuel.
- **Acceleration mode** – acceleration requires more fuel, and therefore fuel injectors supply richer air-fuel mixtures.
- **Deceleration mode** –rapid deceleration, under high engine speeds, requires more air. However, the closed throttle restricts the airflow, and therefore the vacuum induces larger flows of fuel. Deceleration modes produce misfires and higher levels of both HC and CO.

Recently, An *et al.* (cited in Marsden *et al.*, 2001) adopted a new approach to describe vehicle emissions. Instead of using driving modes in the modal approach, they used four states of the engine, such as stoichiometric emissions, cold /warm-start emissions, enrichment emissions, and lean-burn emissions. They also identified the relationships between the emissions of engine states and the emissions of driving modes, as shown in Table 3-1. The table illustrates that both cold/warm start and enrichment emissions are strongly correlated with start emissions. Also, it shows that stoichiometric emissions are significantly correlated with idle, cruise and acceleration emissions.

Table 3-1 Correlation between Emissions of Driving Modes and Engine States

	Idle	Start	Cruise	Acceleration	Deceleration
Stoichiometric	++		++	++	+
Cold/warm start		+++			
Enrichment		+++	+	++	+
Lean-burn	++		++		+++

Source: An *et al.* (cited in Marsden *et al.*, 2001)

Almost all existing models use the modal approach to describe vehicle emissions. The modal approach splits a driving profile into several driving modes that correlate vehicle emissions with different traffic activities. A study by Hallmark *et al.* (2002) found that the most significant traffic activities to describe emissions were: (i) queue position, (ii) grade, (iii) upstream and downstream volume per lane per hour, (iv) distance to the nearest downstream signalised intersection, (v) percent of heavy vehicles, and (vi) posted link speed limit. Also, they used hierarchical tree-based regression analysis (HTBR) to identify the proportions of different driving modes in various traffic activities.

3.3.1.2 Infrastructure designs

Infrastructure Class: vehicle emissions are affected by the class of the road infrastructure that in turn influence significantly traffic flow conditions, such as free and congested flows, and stop-start conditions. Emissions of congested flows are generally five times those of free flows (Nicolas, 2000). The impacts of road infrastructure on emissions have been investigated by several studies, e.g., Várhelyi, 2002; El-Fadel *et al.*, 2000; Al-Suleiman and Al-Khateeb, 1996; Robertson *et al.*, 1996. On the one hand, HC and CO tend to decrease with the increases in average speeds of traffic and with reductions in frequencies of idling and accelerating, while on the other hand NO_x tends to increase. In contrast, Watson and Lu (1993) claimed that stop-start conditions produce five times more NO_x, three times more CO and HC, and require 100 percent more fuel.

Infrastructure Gradients: vehicle emissions are affected by the road gradients. The gradients of roads affect the quantity of air that flows into the combustion chamber, and also affect the aerodynamic forces on the vehicle (Sturm *et al.*, 1996). This is illustrated in the Australian research on models for fuel consumption and emissions, such as the power model (ARFCOM) developed by (ARRB)

Australian Road Research Board (Biggs, 1988; Greenwood and Bennett, 1996) and Watsons's positive kinetic energy model, (Watson, cited in Jourmard *et al.*, 1999; Watson *et al.*, 1985). A few models consider road gradients when investigating vehicle emissions (Latham *et al.*, 2000). Nevertheless, when models take into consideration altitudes and gradients, HC differ by 21 percent, CO by 40 percent, and NO_x by 15 percent (Sturm *et al.*, 1996). Vehicle emissions are double when travelling uphill (Cicero-Fernández *et al.*, cited in Fomunung *et al.*, 2000). Travelling uphill produce consistently more NO_x, whilst travelling downhill produce less NO_x (Potter and Savage, cited in Cloke *et al.*, 1998). Pierson *et al.* (1996) summarised automotive emissions from mountain tunnels in the US and found that, in most cases, NO_x increased from zero at slopes of -3.76 percent to five times the level-road NO_x at +3.76 percent. They also showed that CO and HC in some cases were maximal uphill, and in other cases were maximal downhill. The highest observed HC was downhill, and the lowest observed HC was on a level road.

Infrastructure altitudes: the road altitude affects vehicle emissions of non-catalytic convertor vehicles. The altitude of the road affects the quantity of air that flows into the combustion chamber (Sturm *et al.*, 1996). For non catalyst-equipped vehicles, it has been found that HC and CO at an altitude of 3000 metres were twice as much as at sea level, and NO_x was half as much as at sea level (Cloke *et al.*, 1998). For catalyst-equipped vehicles, altitude has only a nominal effect on emissions (Cloke *et al.*, 1998). Because almost all on-road vehicle fleets are catalyst-equipped vehicles, altitude is not considered as a factor affecting vehicle emissions, except when converters are malfunctioning, tampered with, or under abnormal thermal operating conditions (See Section 1.3 in Chapter 1 and Section 7.1 in Chapter 7).

3.3.2 Vehicle Operational Variables

Vehicle emissions are affected by operational variables, in addition to the ambient climate, and thermal conditions of the engine and catalytic converter. Operational variables are described by several common parameters (André, cited in Ericson, 2001), such as:

- (i) duration,
- (ii) average speed,
- (iii) acceleration standard deviation,
- (iv) positive kinetic energy,
- (v) idle period,
- (vi) number of stops per kilometre,
- (vii) running speed (excluding stops),
- (viii) average speeds,
- (ix) acceleration and deceleration,
- (x) average running periods,
- (xi) number of acceleration and deceleration periods,
- (xii) relative and joint distribution of speed, and
- (xiii) relative and joint distribution of accelerations and decelerations.

Nevertheless, the mainstream literature uses either average speeds or products of instantaneous speeds and accelerations, for investigating the effects of operational variables on vehicle emissions. Several studies questioned which one is more accurate. A study by Jourmard *et al.* (cited in Ericsson, 2001) argued in favour of average speeds. Another study, by Guensler (cited in Ericsson, 2001) in addition to other researchers argued in favour of instantaneous speeds (Section 3.3.2.2). We discuss both average speeds and instantaneous speeds and acceleration, as follows:

3.3.2.1 Average speed

Many studies use average speed, because it is the only practical measurement of the traffic on roads (Negrenti *et al.*, 2001). Emissions in general are triple when average speeds are between 10 km/h and 15 km/h (OECD, 2004), while most emissions are minimal at average speeds between 40 km/h and 60 km/h (OECD, 2004; The Royal Commission on Environmental Pollution, 1995). Both CO and HC are minimal at average speeds and tend to increase at very high speeds, whereas NO_x increases with high speeds and high engine loads.

Ward *et al.* (cited in OECD, 2004) found that NO_x is low at speeds between 35 km/h and 40 km/h, while HC is low at speeds between 55 km/h and 65 km/h, as

shown in Figure 3-2. On the one hand, NO_x tends to increase with high speeds, on the other hand both HC and CO tend to increase with lower speeds typical of heavily congested conditions.

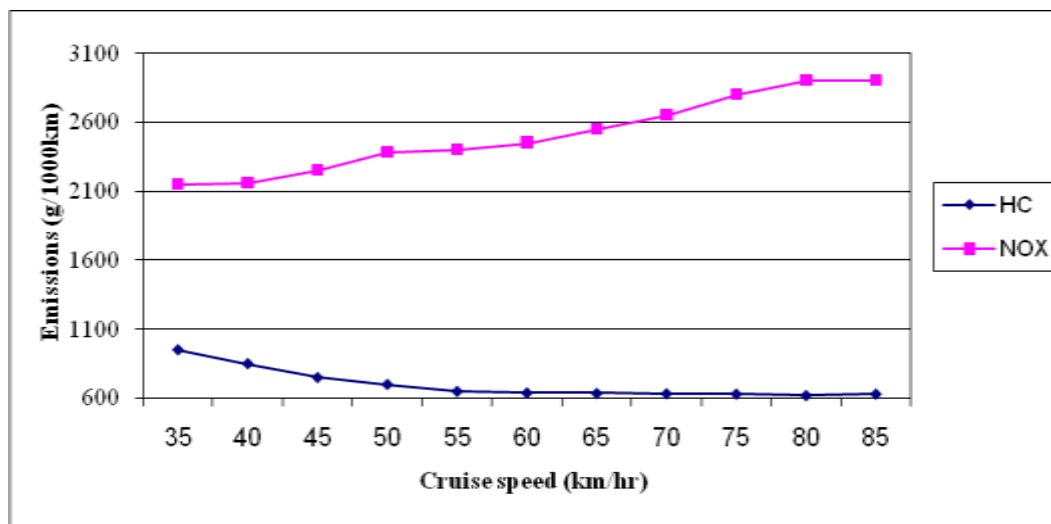


Figure 3-2 The Effects of Travel speeds on HC and NO_x

Source: Ward *et al.* (cited in OECD, 2004); approximate plot

Sturm *et al.* (1994) illustrated that reducing the speed limit on the secondary network in Graz, from 50 km/h to 30 km/h, reduced NO_x by 24 percent and increased CO by 4 percent, and have no effects on HC and fuel economy. For non-catalyst vehicles, André and Pronello (1997) found that when the average speed is increased from 20 km/h to 40 km/h at 0.5 m/s², CO is decreased by 30 percent and HC by 34 percent, but NO_x is increased by 14 percent. Also, for catalyst-equipped vehicles they found that when the average speed is increased from 20 km/h to 40 km/h at 0.5 m/s², CO is decreased by 20 percent, HC by 21 percent, and NO_x by 3 percent, as shown in Table 3-2.

Table 3-2 The Effects of the Increase in Average Speed on CO, HC, and NO_x

Acceleration	0.3 m/s ²			0.5 m/s ²		
Vehicle type	CO	HC	NO _x	CO	HC	NO _x
ECE 1503	-30%	-31%	+2%	-30%	-32%	+14%
ECE 1504	-30%	-34%	+1%	-29%	-34%	+14%
Catalyst vehicles	-26%	-29%	-11%	-20%	-21%	-3%

Source: Andre and Pronello (1997)

3.3.2.2 Instantaneous speeds and accelerations

Although many studies considered that average speed is the main operational influence on emissions, Le Blanc *et al.* (1995) suggest that the manner in which the average speed is reached is equally important, because vehicle emissions may vary under various test drive-cycles with similar average speeds. André and Hammarström (2000) concur with Le Blanc *et al.* (1995) and argued against using average speeds for estimating emissions, particularly because of high spatial and temporal variations in emissions. They suggested that several combined driving modes could give the same average speed. Likewise, Negrenti *et al.* (2001) illustrated that emissions based on the vehicle kinetics, such as instantaneous speeds, give higher and more realistic results than emissions based on average speeds. They demonstrated that emissions under test drive-cycles with similar average speeds but different speed distributions vary by 300 percent.

Notwithstanding Section 3.2.2, we point out that the relative contributions of various operating conditions, such as, acceleration, deceleration, cruising and idling, to both fuel consumption and vehicle emissions are established. Strategic Transport planning models use average speed by necessity. However, any more detailed models would account for the variations in speed over a journey, and for other effects such as road gradients.

3.3.3 Driving Behaviour

Driving behaviour represents the interactions between the driver and the vehicle. Driving behaviour is defined by the way the driver handles the accelerator, the brake pedal, and the gear stick (Guensler, cited in Ericsson, 2001). Variations in driving behaviours are restricted by the physical structure of the vehicle. Johansson *et al.* (cited in Ericsson, 2001) found that various vehicle makes were differently affected by various driving behaviours.

A few studies measured the effects of driving behaviour on emissions. A study by Shih *et al.* (cited in Fomunung *et al.*, 2000) used throttle openings to model driving behaviour. Another study by Gense (cited in OECD, 2004) investigated driving behaviour by observing changes in emissions of various behaviours (Table 3-3).

Table 3-3 The Effects of Driving Behaviour on HC, CO, and NO_x

Driving behaviour	Aggressive* (% change)	New** (% change)	Egg *** (% change)
HC	+ 280	+31	+22
CO	+ 750	+78	+4
NO _x	+ 91	+7	-18

Source: Gense (cited in OECD, 2004)

* aggressive: 80% more acceleration and 20% more average engine revolutions

** new: it combines defensive driving with special way of accelerating and shifting gears, it is the newest Dutch version of the Swiss "ECO_DRIVE".

*** egg: very slow acceleration

3.3.3.1 Accelerating and Braking

On the one hand, aggressive driving, such as hard acceleration and deceleration, produce higher emissions and may alter the emitting status of vehicles from being low emitters to being high emitters (LeBlanc *et al.*, 1995). Gense (cited in OECD, 2004) found that aggressive driving increased CO by 750 percent, whereas very slow acceleration reduced NO_x by 18 percent (Table 3-3). De Vlieger (1997) found that sporty driving styles – sudden and high acceleration and heavy braking – emit four times more HC and CO than moderate acceleration and braking for both urban and rural traffic conditions (De Vlieger, 1997).

On the other hand, calm driving emits significantly lower CO and HC than normal driving – moderate acceleration and braking –, and also emits equal or even higher NO_x. De Vlieger (1997) found that calm driving –smooth driving using the highest gear – in some cases, emits ten times lower emissions than a sporty driving style.

3.3.3.2 Gear-shifting

A few studies have investigated the effects of gear shifting on vehicle emissions. Ericsson (2001) adapted the levels of the gear among other variables, for studying emissions. He found that late shifting between the second and the third increased both HC and NO_x. Cloke *et al.* (1998) noted that emissions under steady state operations vary inconsistently with the selected gear. They also noted that they do not differ greatly when the third or fifth gear is selected between 50 km/h and 70 km/h.

3.3.4 Vehicle Technology

Vehicle technology has been technically developed to achieve several targets, such as fuel-efficient, less polluting, lighter and safer vehicles that have more comfort features. However, the process of developing new models is complex, and is often a compromise between several conflicting targets. Saarialho (1993) combine the main factors that influence the development of vehicle technology, as follows:

$$\text{FDAT} = f (3\text{C} + 2\text{L} + \text{E}_{(3\text{E}+2\text{E})} + 2\text{P} + 2\text{M})$$

FDAT	Future development of automotive technology
3C:	Consumer demands, Co-operation with the component industry, and Competition
2L:	Legislation, and Laws of the nature
3E:	Emissions, Energy, and Economy
2E:	Engine technology, and Electronics technology
2P:	Power transmission technology, and Packaging layout
2M:	Materials technology, and Manufacturing technology

The impacts of vehicle technology on vehicle emissions have been investigated by many studies, such as Burgess and Choi, 2003; OECD, 1996; Wong, 2001; Van den Brink and Van Wee, 2001; DeCicco and Ross, 1996; OECD 1991. Van den Brink and Van Wee (2001) identified three elements in vehicle technology that affect fuel consumption, such as engine technology, transmission system, and aerodynamic properties. We adopt these to illustrate the effects of vehicle technology on emissions, as shown in Figure 3-3.

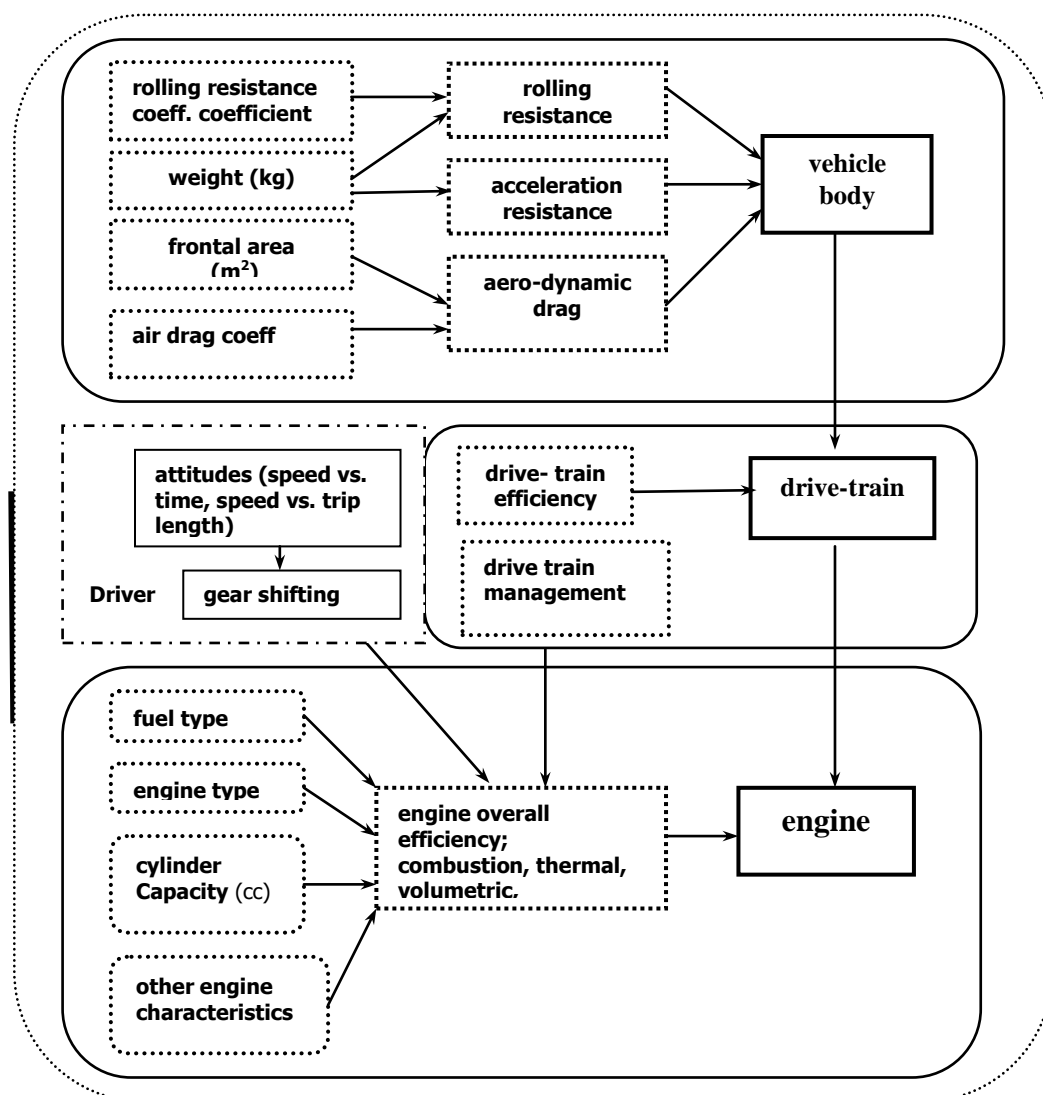


Figure 3-3 Vehicle Technology

Adapted with modifications from Van den Brink and Van Wee (2001)

Vehicle makes and models are not comparable, because they use different technologies that employ various components, such as various cycle and cylinder types (Table 3-4).

Table 3-4 Vehicle Technology

Parameters	Attributes
Ignition type	Spark ignition, compression ignition
The cycle in the engine	4-stroke cycle, 2-stroke cycle
Shapes of cylinders	Single cylinder, V-engine, others
Fuel input system	Carburetted, multiple port fuel injection, throttle body Fuel injection
Cooling type	Air cooled, water cooled
Air intake system	Naturally aspirated, supercharged, turbocharged, Crankcase compressed
Locations of intake & exhaust valves	

Source (Pulkrabek, 1997)

Many studies, e.g., Schäfer and Basshuysen, 1995, investigated the effects of vehicle technology on vehicle emissions and the impacts of its main design features (Table 3-5).

Table 3-5 Vehicle Design Variables

Item	Attributes
Engine displacement (litres)	
Engine management system	Electronic ignition, mechanical timing
Fuel delivery system	Carburettor, Fuel injection system
Exhaust Gas Re-circulation (EGR)	
Exhaust after-treatment systems	Three-way catalyst converter
Transmission type	Automatic, manual
Gear speeds	3,4,5
Maintenance level	Engine oil, battery condition, battery (level of water), fuel filter, air filter, radiator, vacuum hoses, spark plugs, etc.

Adapted from Schäfer and Basshuysen (1995)

This section discusses the impact of main factors in the technology of conventional vehicles, i.e., internal combustion. Other factors are treated in Appendix III.

3.3.4.1 Engine capacity

Large engines consume and burn more fuel normally. On the one hand, they produce at least 50 percent more NO_x than small engines under similar driving conditions (Gover *et al.*, cited in Stead, 1999). On the other hand, large engines under low speeds consume less fuel than small engines under full engine power (Van den Brink and Van Wee, 2001). For catalyst-equipped vehicles, on the one hand, engine capacity affects CO and HC at lower engine speeds (Cloke *et al.*, 1998). On the other hand, engine capacity affects NO_x at higher engine speeds (Cloke *et al.*, 1998). For non-catalyst vehicles, engine capacity correlates well with CO and HC at higher engine speeds. It also correlates well with NO_x at a wide range of speeds (Cloke *et al.*, 1998).

3.3.4.2 Vehicle weight

Vehicle weight is an important determinant of energy, and thereby emissions. Computer-aided techniques advance the use of lightweight materials in the manufacturing of vehicles, such as composites, high-strength low alloy steel, plastics, aluminium, and metal-plastic laminates, (DeCicco and Ross, 1996). Despite that vehicles are heavier in recent years. Factors like improved safety, pollution control features, and comfort related equipment, such as air conditioning, electric windows, seats, and mirrors, has increased the weights of vehicles (Van den Brink and Van Wee, 2001). Burgess and Choi (2003) demonstrated that the average weight of passenger vehicles has increased by 190 kg. Additionally, updating of emission standards in some countries has contributed to the increases in the average weight of vehicles. For example, the application of Tier 1 and Tier 2 emission standards respectively is estimated to cause the average weight of American vehicles to increase 5 lb (2.3 kg) and 15 lb (6.80 kg) (Duleep, cited in, Decicco and Ross, 1996).

3.3.4.3 Vehicle age / odometer reading

Emissions are elevated as vehicles age. Vehicle age affects emissions in three ways:

- (i) Age is a surrogate for maintenance status of the vehicle; the older is the vehicle the less likely it is maintained (Anable *et al.*, cited in Stead, 1999).

However, the status of maintenance might mask the expected relation with age (Beaton *et al.*, cited in Washburn *et al.*, 2001). The differences between emissions of inadequate and emissions of well-maintained vehicles with similar age are significantly greater than the differences between emissions of well-maintained vehicles across various age cohorts.

- (ii) Age is linked to vehicle technology; the more recent is the technology the more likely that the vehicle is more fuel-efficient and less polluting (Anable *et al.*, cited in Stead, 1999).

- (iii) Age is linked to the likelihood that the engine is operating under a specific state. Kazopoulo *et al.* (2005) tested a sample of the Lebanese vehicle fleet, which is mainly including either German or Japanese vehicles. These researches demonstrated, using I/M data of 100 vehicles in the model year range between 1972 and 2002, that a large percentage of the old vehicles (≤ 1986) operate under fuel-rich operations, a large proportion of the vehicles between 1987 and 1993 operate under fuel-lean operations, and a large proportion of the new vehicles (≥ 1994) operate under stoichiometric combustion.

Also, vehicle emissions are increased with the accumulation of vehicle kilometres travelled. Vehicle kilometres travelled are strongly correlated with vehicle age. Nonetheless, Washburn *et al.* (2001) considered the intensive use of a vehicle is more critical than age for the determination of the levels of emissions. For, the usage of the vehicle is normally intensified into a short period instead of being distributed over time.

3.3.4.4 Maintenance-status

Maintenance practices that do not meet manufactures' original specifications elevate vehicle emissions. In contrast, good maintenance practices that meet original specifications reduce vehicle emissions substantially. Both EPA and Ross *et al.* (cited in Pickrell, 1999) estimated that the maintenance of malfunctioning

vehicles that are identified by on-board diagnostics (OBD) devices would reduce HC by 32 percent, CO by 17 percent, and NO_x by 25 percent.

Inspection and maintenance (I/M) programmes enhance the reduction of emissions. Walsh (cited in Hickman, 1994) estimated that I/M programmes would reduce both HC and CO by 25 percent and NO_x by 10 percent. Also, the US EPA estimated (Clock *et al.*, 1998) that inspection and maintenance (I/M) programmes would reduce CO between 15 percent and 20 percent. Due to the significance of inspection and maintenance (I/M) programmes in reducing emissions, they were adapted in many countries. In Sweden, for example, I/M programmes reduced CO by 20 percent and HC by 7 percent (Faiz *et al.*, 1998). In Switzerland, also, I/M programmes reduced CO by 30 percent and HC by 20 percent (Faiz *et al.*, 1998).

Some inspection programmes, such as engine tuning-up, that are designed to reduce HC and CO will often increase NO_x (Hickman, 1994; Faiz *et al.*, 1998). Servicing vehicles may also decrease both CO and HC, and increase NO_x. A study by the French Institute National de Recherche sur les Transports et Leur Sécurité (INRETS) (cited in Faiz *et al.*, 1998) tested vehicles before and after being tuned to manufactures' specifications and found after vehicles were tuned that both CO and HC decreased significantly, and NO_x increased. Another study by Potter and Savage (cited in Hickman, 1994) showed that after vehicles were serviced both CO and HC decreased, and NO_x increased.

Similar to I/M programmes, the enhanced inspection and maintenance programmes are effective in preventing the aggravation of emissions from in-use vehicles (Pickrell, 1999; Wiederkehr, 1995). These programmes are more cost-effective than other inspection programmes (Pickrell, 1999). In contrast, Harrington *et al.* (cited in Okmyung, 2003) found that the enhanced I/M programmes in Arizona were not cost effective programmes as was predicted by the US EPA. A much more cost-effective programmes than I/M are small-scale retirement programmes, especially in regions where reducing HC is likely to be the best strategy to control ozone (Deysher and Pickrell, 1997). Comprehensive vehicle retirement programmes in one year reduced HC by 5.3 percent and NO_x by 2.3 percent (Deysher and Pickrell, 1997).

3.3.5 Vehicle Driving-Profile

Emission models have primarily been trip-based (Ito *et al.*, 2000). Emissions are measured on a test drive-cycle that represents a trip from an origin to a destination, and then are recorded for the average speed over a trip (Ito *et al.*, 2000). Travel demand models are mainly link-based, and data are aggregated for each link (Ito *et al.*, 2000).

Emissions measured by laboratory-based testing are aggregated over a test drive-cycle. A test drive-cycle represents modal operations of the traffic for an average trip at an average speed (Sierra Research Inc., cited in Ito *et al.*, 2000). A Special test drive-cycle were used for measuring emissions in the earlier studies, whereas standardised drive-cycles, such as FTP-75 and NEDC – the standardised test drive-cycle in the US and in the European Union respectively –, were used in later studies (Sturm, 1998).

Federal Test Procedure (FTP) is commonly used in many countries, but was designed in the 1970s. FTP does not represent accurately real-world traffic conditions (Venigalla *et al.*, 1995). For, FTP test drive cycle does not represent high speeding vehicles under lean and steady-state driving operations (DOTARS, 2001). In 1993, the US EPA (cited in Marsden *et al.*, 2001) acknowledged that FTP test drive-cycle does not represent adequately enrichment events common for real-world traffic conditions, because the maximum acceleration under the FTP test drive-cycle is only 3.3 mph/s (91.48 m/s²).

Since then, several revision studies have been undertaken to review the FTP drive-cycle. The most significant one was the FTP revision project. The project has collected data from real-world driving conditions using instrumented vehicles driven in Los Angeles, Atlanta, Baltimore, and Spokane. Based on the collected data, the US EPA has established a Supplemental Federal Test Procedure (SFTP) for the 2000 vintages. SFTP includes two single bag test drive-cycles, namely a new start control cycle (SC03) after the new 60-min soak, and a new aggressive drive-cycle (US06) under hot-stabilised conditions known as Bag 4 (Barth *et al.*, 1997). In addition to FTP test drive-cycle, several other test drive-cycles are used

for testing emissions, such as Inspection Maintenance (IM240), Idle testing, and Acceleration Simulation Mode (ASM). These are described in more details in Section 5.3 of Chapter 5.

Test drive-cycles are complemented by real world driving conditions in areas of very high speeds, such as the German autobahn cycles that are complemented by two cycles namely, city main street (CMS) and city secondary street (CSS) (Sturm, 1998). Test drive-cycles are necessary to represent real-world on-road driving conditions better. Therefore, several studies devise representative test drive-cycles using real-world driving conditions, e.g., André *et al.*, 1994; Ergeneman, 1997; Ergeneman *et al.*, 1997.

Additionally, various regions devise different standardised test drive-cycles to represent real-world driving conditions better. Lin and Niemeier (2003) found that the differences of driving in various regions are large enough to create important differences in test drive-cycles. Milkins and Watson (1983) demonstrated that test drive-cycles used in the US, Europe, and Japan, do not represent adequately urban driving conditions in Australian cities. Thereafter, Watson at the University of Melbourne in Australia devised Australian Urban Cycle (AUC) based on Melbourne real world driving conditions (DOTARS, 2001). AUC test drive-cycle is harsher with higher average speeds, and more frequent accelerations with wide-open throttle conditions, than both FTP and Euro tests (DOTARS, 2001). Recently, the Transport Systems Centre at the University of South Australia designed a new Australian drive cycle called Australian Composite Urban Emissions Drive Cycle (CUEDC) (Zito and Primerano, 2005). The drive cycle CUEDC is designed for the NISE2 study, and for assessing the performance of emissions for the vehicles on actual Australian on-road conditions and driving patterns (Zito and Primerano, 2005).

3.4 Summary of the Interfaces between Transport and Vehicle Emissions

Based on the comprehensive approach that we undertake in reviewing the interfaces between transport and vehicle emissions, we conclude herein the most important influences for the empirical treatments of this thesis, as follows:

- The design variables of vehicles are inter-related. Examining the results of various studies indicates that various emissions were affected by various traffic schemes to varying extents.
- We recognise four groups of the urban transport system that best define the relations between the transport system and emissions. These groups are traffic flow conditions, vehicle operational variables, driving behaviour, and vehicle technology (Figure 3-1). The groups include large numbers of variables that have potentially direct or indirect influences on vehicle emissions. Also, the groups represents the interactions between various components and vehicle emissions, as follows:
 - The driving behaviour group, such as accelerating and braking, and shifting-gears, represents the interactions between the driver, the vehicle, and emissions.
 - The traffic flow conditions group, such as driving modes and infrastructure designs, represents the interactions between the vehicle, infrastructure, and emissions.
 - The vehicle operational variables group, such as speeds and accelerations, represents the interactions between the vehicle, traffic, and emissions.
 - The vehicle technology group, such as engine design and engine capacity, represents the interactions between the engine, the vehicle, and emissions.

- Vehicle emissions are measured by several standardised test drive-cycles, such as FTP, IM240, and SS60 (Chapter 5). A standardised test drive-cycle represents traffic modal operations for an average trip at an average speed.
- Test drive-cycles do not represent well real world driving conditions.
- Servicing vehicles decrease both CO and HC, but increase NO_x.

Chapter Four

The Theoretical Context

4.1 Introduction

The review of the literature in Chapter 2 establishes that HC, CO, and NO_x emissions are three main emissions of conventional gasoline-fuelled vehicles that are crucial to control. These emissions are simultaneously influenced by three main groups of engine characteristics (Appendix III): (1) *Engine Design variables*, such as the combustion chamber, spark plugs, fuel injection system, and engine displacement. (2) *Operating parameters*, such as the engine speed and engine management system. (3) *Exhaust gas after treatment systems*, such as the catalytic converter and additional air injection. Chapter 2 also reveals that almost all existing models treat vehicle emissions in isolation from each other and relate each of the three main emissions to vehicle variables only.

Chapter 4 takes on a theoretical approach, and seeks to determine whether it is theoretically justified to estimate vehicle emissions independently from each other similar to the approach used in existing models, or to estimate vehicle emissions as jointly dependent variables similar to what we propose in this thesis. The Chapter also presents the principles of the process of combustion in conventional gasoline-fuelled vehicles, and focuses on the complexity of the process. It looks closely at major thermodynamic and chemical phenomena that govern the production of HC, CO, and NO_x emissions. Moreover, the chapter investigates the interdependency of chemical reactions of the combustion process. The investigations seek to determine whether it is theoretically justified to estimate HC, CO, and NO_x emissions simultaneously. Moreover, the chapter presents the thesis hypothesis that HC, CO, and NO_x emissions are jointly dependent such that when estimating one emission the other two emissions must be included as independent variables in the model.

4.2 Emissions of Complete and Incomplete Combustion

The combustion process in conventional gasoline-fuelled engines produces power, heat, and emissions (Houghton, 1995). The exhaust includes emissions of complete combustion, and incomplete oxidation of the fuel and other products of incomplete combustion, as shown in Figure 4-1.

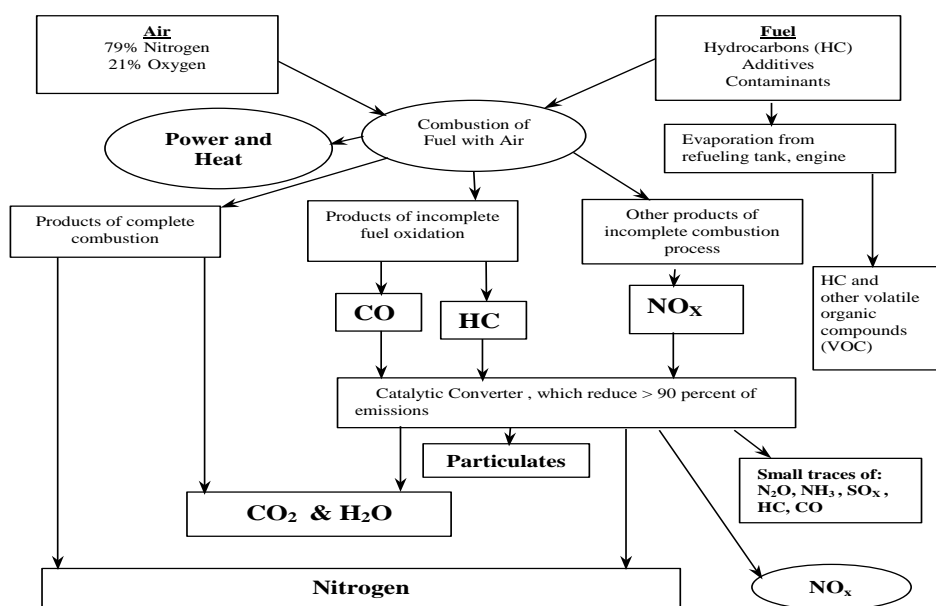


Figure 4-1 Emissions from Gasoline-Fueled Automobiles

Source: Houghton (1995)

HC, CO, and NO_x are three main products of the incomplete combustion process in the engine. The main compounds present in the exhaust are carbon dioxides (CO₂), water (H₂O), nitrogen (N₂), unburned or partially burned fuel (i.e., hydrocarbons (HC)), carbon monoxide (CO), nitrogen oxides (NO_x), and other traces, such as phosphorus (P), aldehydes (H-C-O), lead (Pb) for leaded fuels, and sulphur dioxides (SO₂) for fuels that contain sulphur (Schäfer and Basshuysen, 1995; Pulkrabek, 1997).

4.3 The Operating Cycle in Internal Combustion Engines

The operating cycle in internal combustion engines is not a perfect thermodynamic cycle. It is a mechanical cycle that includes chemical thermodynamics processes. The cycle converts the chemical energy in the fuel into mechanical power output. First, the chemical energy stored in the fuel is released as a thermal energy. Then, the thermal energy of the gases in the burnt air-fuel mixture is converted to a rotating mechanical energy via the gases expanding against the piston. Finally, the power output is transmitted by a connecting rod and a crank mechanism to the driving shaft.

4.3.1 The Four-Stroke Cycle

Most conventional gasoline-fuelled engines operate in a four-stroke cycle. The cycle is four strokes from its position, and each cylinder rotates two revolutions of the crankshaft to complete a cycle. The rotation of the cylinder causes the piston to travel in cyclical movements, and it comes to rest at two crank positions: top centre (TC) and bottom centre (BC) (Figure 4-2).

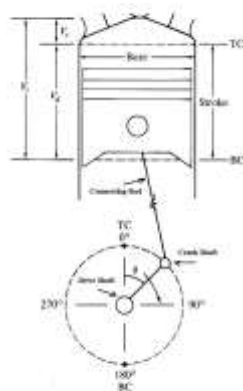


Figure 4-2 Dimensions of a Typical Cylinder in Spark-Ignition Engines

Source: (Heywood, 1988): V_t = total volume of the cylinder, V_c = clearance volume – minimum volume of the cylinder –, V_d = displaced volume = $V_t - V_c$, θ = crank angle

We describe overall the mechanism of the operating engine cycle (Figure 4-3), which is the basic operating cycle for all conventional petrol-fuelled vehicles including vehicles with electronic fuel injection and advanced engine management

systems (Pulkrabek,1997). We focus on the interdependent nature of the chemical thermodynamics processes of the engine cycle in Sections 4.4 and 4.7.

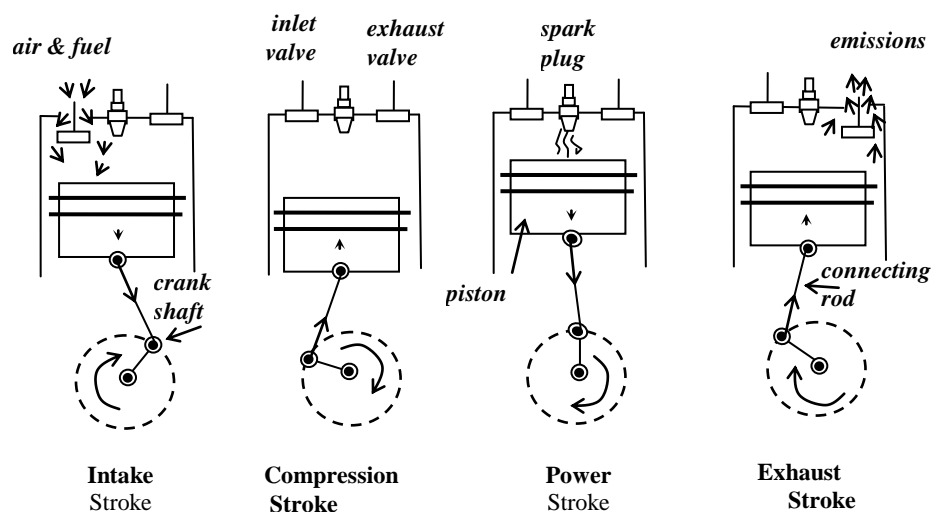


Figure 4-3 The Four-Stroke Cycle in Internal Combustion Engines

Source: Stone (1999)

The four-stroke cycle in internal combustion engines is, as follows (Stone, 1999):

1. **First Stroke: Intake Stroke --Induction--:** the intake valve opens and the piston starts moving downward, which in turn creates a vacuum. As a result, a pre-mixed air-fuel mixture is drawn into the cylinder and mixes with any residual gases from a previous cycle in the cylinder.
2. **Second Stroke: Compression Stroke:** at the end of the intake stroke, the intake valve closes, and the piston starts to move upward. This compresses the mixture raising both the pressure and the temperature in the cylinder. As the piston approaches the TC position, a spark plug gives a spark, and initiates combustion.
3. **Third Stroke: Power Stroke --Expansion--:** the spark ignites the compressed mixture, and combustion occurs. A turbulent flame propagates in the mixture – air, fuel, and any residual gases – across the cylinder. The flame raises the temperature in the cylinder and causes the burnt gases in the mixture to expand. The resulting pressure pushes the piston downwards.

4. **Fourth Stroke: Exhaust Stroke:** at the end of the power stroke, the exhaust valve opens and the piston starts moving upward. Then, the products of combustion exit through the exhaust valve.

4.3.2 Combustion

We describe, on the whole, the development of combustion in the sequence of events of the four-stroke cycle (Figure 4-4), and elaborate on the description of the combustion process in Section 4.4.

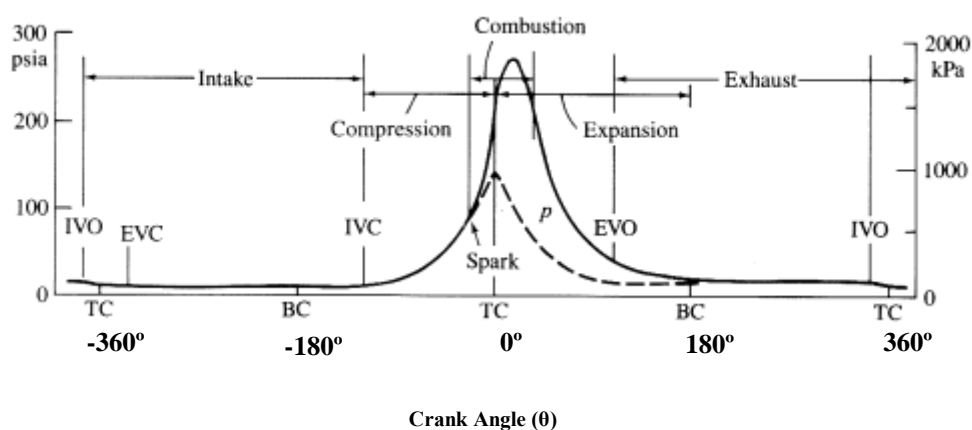


Figure 4-4 Sequence of the Events in the Engine Operating Cycle

Source: (Heywood, 1988)

- the cylinder pressure for a motored cycle (with no residual from previous cycle)
- the cylinder pressure for a firing cycle (with residual from a previous cycle)
- IVO, IVC: inlet valve opening and inlet valve closing, respectively
- EVO, EVC: exhaust valve opening and exhaust valve closing, respectively

The process of combustion occurs during a finite time of the very short engine cycle (Pulkrabek, 1997). The duration of burning in each cycle varies with engine design and operational variables. It is typically between 40° and 60° crank angle (Heywood, 1988). The process of combustion starts at the end of the second stroke (compression) and lasts into the third stroke (expansion). At the end of the compression stroke, an electrical discharge across the spark plug initiates combustion just before the piston will reach the TC position, i.e., between 10 and 40 degrees crank angle before TC. Combustion is half complete about 10° after TC, and is totally complete between 30° and 40° after TC. The peak pressure occurs at about 15° after TC.

The operating cycle of conventional gasoline-fuelled engines is approximated by the ideal air standard cycle – Otto cycle – (Stone, 1992). The ideal air standard cycle consists of four non-flow processes, of which compression and expansion are isentropic, i.e., adiabatic (no heat transfer across the boundary of the system) and reversible (frictionless). The main implications of using this approximate cycle for modelling the engine cycle, and the impacts on understanding the processes that occur in the cylinder including combustion are presented in Section 4.6.

4.4 The Process of Combustion

Combustion in general, is a rapid chemical reaction that releases heat and radiation, and more specifically is rapid oxidation reactions (Chomiak, 1990). In such reactions, chemical transformations (Sections 4.7 through to 4.10) occur as the gaseous molecules of both compounds of fuel and oxidiser collide with each other. In spark-ignition engines, the compounds are gasoline and the ambient air, the latter of which supplies the oxygen necessary for oxidation of the fuel (Section 4.10). The ambient air flows into the engine via the intake system, and fuel is added to the inflow air by fuel injectors or a carburettor (Figure 4-5).

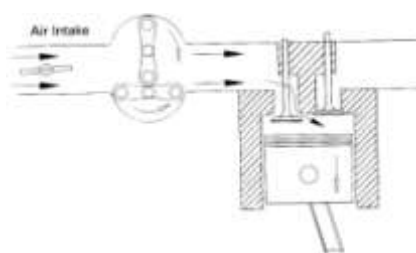


Figure 4-5 The Intake System

Source: (Pulkrabek, 1997)

The fuel enters the air stream as a liquid jet, and then atomises into droplets that vaporise and mix with the air. Then, during the first stroke the pre-mixed air-fuel mixture is drawn into the cylinder (Schäfer and Basshuysen, 1995; Heywood, 1988).

4.4.1 Development of the Flame

The flame resulting from combustion involves aspects of chemistry, fluid mechanics, and molecular physics. The laws for energy conservation, mass conservation, chemical reaction kinetics, thermal conduction, and molecular diffusion govern the development of the flame (Fristrom, 1995). The flame is created by either normal or abnormal combustion. Normal combustion is the ignition of the air-fuel mixture by a spark, while abnormal combustion is either pre-ignition or self-ignition (Stone, 1992). The flame created by normal combustion proceeds in three main stages, as follows (Pulkraberk, 1997):

1. **flame ignition:** the spark plug ignites the air-fuel mixture in the combustion chamber, and initiates a flame. Flames of combustion are exothermic chain reactions that propagate through space (Fristrom, 1995). It is the characteristic of spatial propagation that distinguishes the flame reactions from other combustion reactions in the cylinder.
2. **flame propagation:** the flame propagates after burning between 5 percent and 10 percent of the air-fuel mixture. The propagation of the flame results from the strong coupling of all chemical reactions with other processes of combustion, such as molecular diffusion, heat conduction, and fluid flow (Fristrom, 1995). The flame front – both pre-heat and reaction zones – propagates steadily throughout the mixture. The propagation of the flame elevates the temperature in the cylinder, and induces gradients of substance concentrations and temperatures (Heywood, 1988; Fristrom, 1995). The flame is initially at the ambient temperature and proceeds to reach the flame temperature (Glassman, 1995). The resulting gradients enhance fluxes of heat and reactive substances into the unburned mixture, and therefore accelerate the rates of the reactions. The faster the reaction, the steeper the resulting heat and concentrations gradients and the steeper the gradients the higher are the fluxes. The loop — fluxes, rate of the reaction, and gradients of heat and concentrations — is opposed by the flame propagation (Fristrom, 1995). The flame front is a source for CO and NO_x emissions, and quenching the flame produces HC and CO (Figure 4-6).

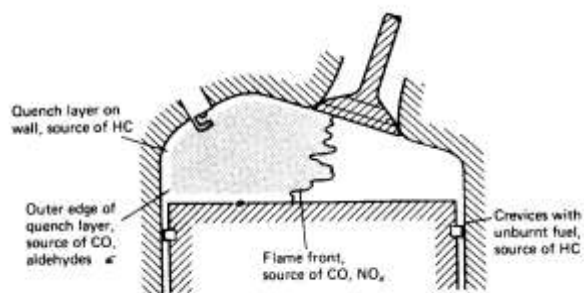


Figure 4-6 Propagation of the Flame

Source: (Mattavi and Amann, cited by Stone, 1992)

3. *flame termination*: the flame terminates after between 90 percent and 95 percent of the air-fuel mixture is burnt. The flame terminates due to the processes of heat conduction and viscous drag with the walls at the extreme edges of the chamber (Figure 4-7).

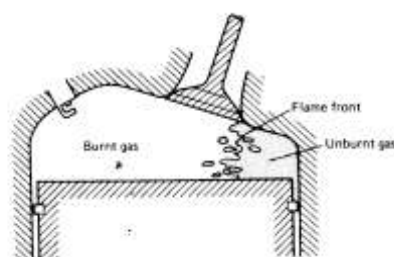


Figure 4-7 Termination of the Flame

Source: Stone (1992)

4.4.2 Variations in the Combustion Process

The rate of burning is not constant. It varies throughout the process of combustion in each cycle, and also it varies within different cylinders. Observations of the cylinder pressure for successive cycles (Figure 4-8) show that there are substantial variations throughout the combustion process in each cycle.

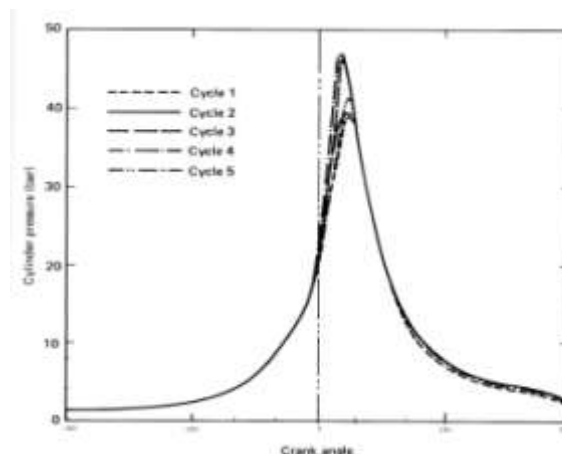


Figure 4-8 Pressure-Time Diagram for 5 Successive Cycles

Source: (Stone and Green-Armytage, cited by Stone, 1992)
 (Ricardo E6 engine, with compression ratio 8:1, stoichiometric air/iso-octane mixture, 1000 rpm, and 8.56 bar bmep)

Several factors are responsible for the variations throughout the combustion process in each cycle and within all cylinders (Heywood, 1988):

1. **Flow-patterns of the mixture:** characteristics of the flow of the medium, such as turbulence, swirl, squish, and tumble, contribute to variations in combustion. Turbulence is local fluctuations in the field flow due to high velocities (Heywood, 1988; Pulkrabek, 1997). Swirl is the rotational motion of the flow about the cylinder axis (Heywood, 1988). Squish and tumble is the radial inward motion of the gas mixture and the transverse gas motion that occurs toward the end of the compression stroke (Heywood, 1988; Pulkrabek, 1997).
2. **Quantities of fuel, air, and the recycled exhaust gas (EGR):** the quantity of inflow into a cylinder of fuel, air, and thus air/fuel ratio (Figure 4-9), in addition to the recycled exhaust gas for each cycle is not identical. As a result, mixing the fresh quantities with the residual gases from previous cycles is not homogenous, and creates variations in the rate of burning in local areas next to the spark gap.

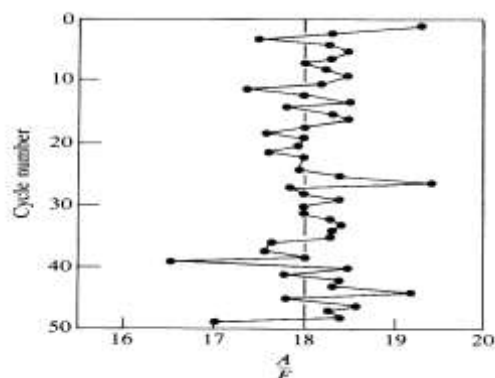


Figure 4-9 Air/Fuel Ratios in 50 Successive Cycles

Source: (Heywood, 1988)

Engine operated at 1400 rev/min, MBT timing, imep = 314 kPa.

Measurements are in the vicinity of the spark plug.

- 3. Composition of the mixture:** the composition of the mixture varies between cycles and within cylinders. The variations in the composition of the mixture induce variations in mixing the fresh mixture with the residual gases, especially in the vicinity to the spark plug.

4.4.3 Incomplete Combustion

The fuel that flows into conventional engines is not totally burned. Efficiency of combustion is typically between 95 and 98 percent (Pulkrabek, 1997). The combustion efficiency for stable combustion does not significantly vary with the engine operating and design variables. It varies only with the equivalence ratio of the mixture. The combustion efficiency decreases as the mixture becomes richer (Heywood, 1988). Incomplete combustion produces either partially burned or unburned fuel (HC), in addition to CO and NO_x. Several factors contribute to incomplete combustion, as follows (Heywood, 1988; Pulkrabek, 1997):

- 1. Quench effect:** the flame quenches at the walls of the combustion chamber. The flame quenches because of high residues under low engine loads and idling conditions, or because of a weak mistimed spark (Schäfer and Basshuysen, 1995). The quenching of the flame leaves a thin layer of unburned fuel on the walls. This layer burns up rapidly when on smooth walls with least surface-irregularities. Porous deposits build up on the walls, especially in old engines, inhibit burning the layer and, therefore, increase HC and CO emissions, but decrease NO_x emissions. Some

amounts of build up (unspecified in the source) produces 44 percent more HC emissions, 266 percent more CO, and 28 percent less NO_x (Figure 4-10).

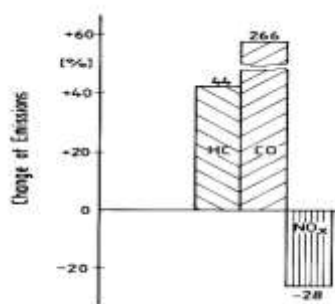


Figure 4-10 Effects of the Build up of Deposits on Emissions

Source: (Schafer and Basshysen, 1995)

2. **Quality of combustion:** bulk quenching of the flame under transient operations (Section 3.2 in Chapter 3) worsens the quality of combustion, and slows down the process of combustion.

3. **The crevices in the engine:** during compression and combustion, pressure in the cylinder increases, and forces the gases of the mixture into the crevices. Eighty percent of the total crevices are the narrow clearance connected to the combustion chamber between the piston and cylinder walls, five percent are imperfect fit in the threads of the spark plug or fuel injector, and between 10 and 15 percent are gaps in the gasket between head and block (Pulkrabek, 1997). Some of the trapped gases in the crevices will not burn, because the flame cannot reach into the crevices. However, during expansion and exhaust strokes, pressure in the cylinder decreases and, therefore, forces the trapped gases, burned and unburned, to return back into the cylinder. Also, there is a small flow from the unrounded corners at the edge of the combustion chamber and around the edges of valve faces (Pulkrabek, 1997).

4. **The oil film:** the thin film of the lubricating oil on the walls of the cylinder, the piston, and head, absorbs some fuel vapours before the start of combustion and during intake and compression strokes. Then, after

combustion, and during expansion and exhaust strokes, the oil film discharges hydrocarbons back into the cylinder and, therefore, some fuel remain unburned.

4.5 Air/ Fuel Mixtures

Air-fuel mixtures are mainly described by two parameters: air/fuel and fuel/air ratios, as follows (Stone, 1992):

$$\begin{aligned}\text{Air / Fuel ratio} &= \frac{m_a}{m_f} \\ \text{Fuel / Air ratio} &= \frac{m_f}{m_a} \quad (4-1)\end{aligned}$$

where: m_a = air mass (kg) m_b = fuel mass (kg)

Air-fuel mixtures are stoichiometric, i.e., theoretically chemically correct (Appendix III), when the air mass to the fuel mass equals 14.6 kg of air to 1.0 kg of fuel, for both gasoline-fuelled and diesel-fuelled engines (Schäfer and Basshuysen, 1995). Ideal combustion occurs when the air/fuel ratio equals 14.6. However, combustion is possible for air/fuel ratios between 6 and 19. When the air/fuel ratio is less than 6 the mixture is too rich to sustain combustion and when it is greater than 19 the mixture is too lean and there is insufficient fuel to cause combustion (Pulkrabek, 1997).

The strength of the air-fuel mixture is described by the fuel equivalence ratio (Φ) and the relative air/fuel ratio (λ). For example, for a mixture with 25 percent excess air the fuel equivalence ratio (Φ) and relative air/fuel ratio (λ) are, as follows (Stone, 1992; Heywood, 1988):

$$\Phi = \frac{\text{Actual(Fuel/ Air)}}{\text{Stoichiometric(Fuel/ Air)}} = \frac{\text{Stoichiometric(Air/ Fuel)}}{\text{Actual(Air/ Fuel)}} = \frac{1}{1.25} = 0.8$$

$$\lambda = \Phi^{-1} = \frac{\text{Actual(Air / Fuel)}}{\text{Stoichiometric(Air / Fuel)}} = 1.25 \quad (4-2)$$

Air-fuel mixtures vary with levels of power, engine-operating conditions, engine speeds, and engine loads (Heywood, 1988). Air-fuel mixtures must always be chemically correct, for complete combustion and reliable ignition (Stone, 1992). Theoretically, the optimum air-fuel mixture is the mixture that produces the smoothest operations, but emission control systems require a different air-fuel mixture, and also require re-circulating a fraction of the exhaust gases (EGR) into the intake system (Heywood, 1988), which therefore upsets the optimum air-fuel mixture.

The induction of correct and consistent air and fuel into the engine is difficult to achieve and, therefore, the supply of air-fuel mixtures varies between cycles and cylinders (Section 4.4.2). Additionally, the supply of fuel depends on the quality of the fuel injectors, and engine-operating conditions are limited by statistical averages (Pulkrabek, 1997). Gasoline-fuelled engines operate with Φ between 1.18 and 0.84, or with λ between 0.85 and 1.2 (Schafer and Basshuysen, 1995). When $\Phi = 1$ ($\lambda = 1$), the mixture is stoichiometric and maximum energy is released. For $\Phi > 1$ ($\lambda < 1$), the engine runs rich, and increases CO and HC. For $\Phi < 1$ ($\lambda > 1$), the engine runs lean and produces oxygen (O_2). A fuel-lean mixture burns slowly, and has lower temperatures and pressures.

Various air-fuel mixtures produce variable amounts of HC, CO, and NO_x , as shown in Figure 4-11. The figure illustrates the complexity of the formation of vehicle emissions. The process of combustion creates, in the combustion chamber, an environment of temperature, pressure, and substance concentrations (Section 4.8). The created environment determines the reactions and products of combustion, and it varies constantly within each cycle and between cylinders (4.4.2).

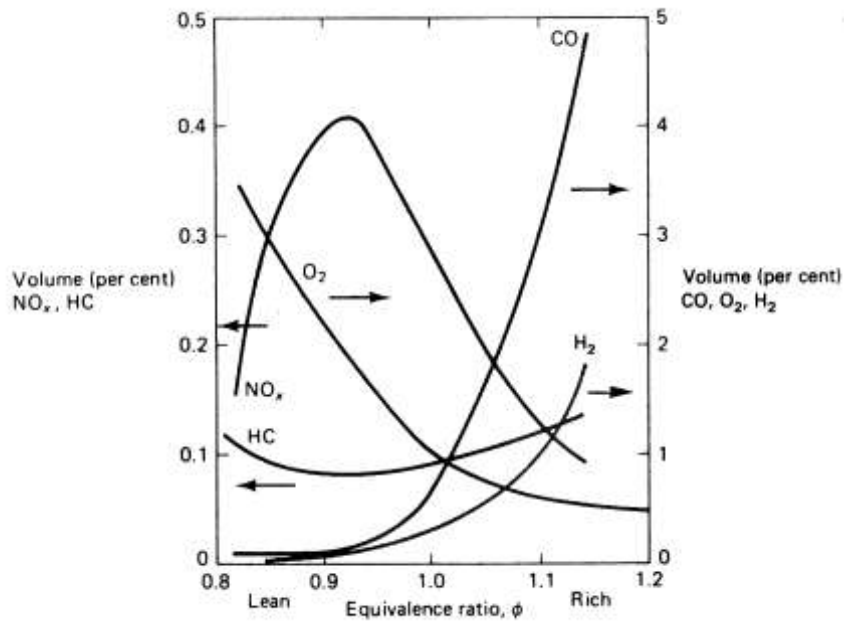


Figure 4-11 HC, CO, and NO_x in various Air-Fuel Mixtures

Source: (Matthey, cited in Stone, 1992)

4.6 A Complex System of Combustion

The combustion process is an open thermodynamic system that exchanges heat and work with the atmosphere (Heywood, 1988). The process consists of flows into the system and flows out of the system (Figure 4-12), in addition to chemical kinetics (Section 4.8).

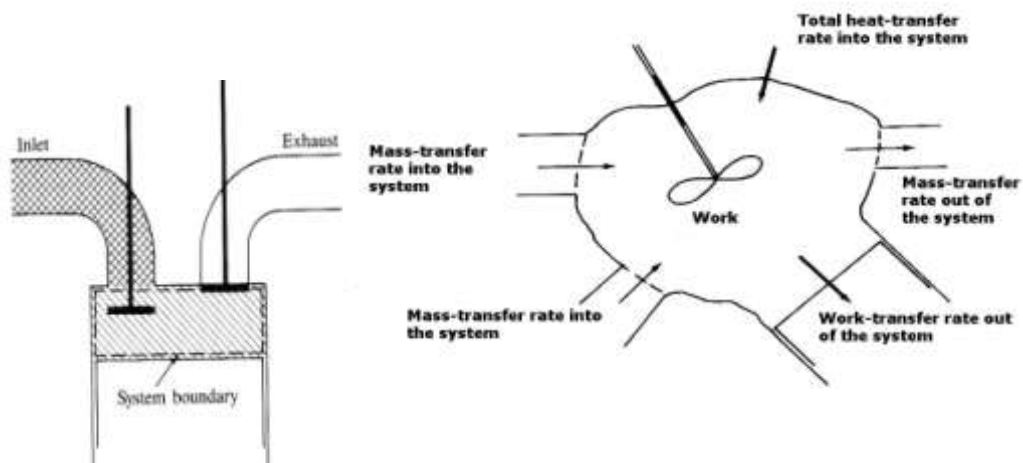


Figure 4-12 The System of Combustion

Source: (Heywood, 1988)

The combustion system is a complex system that involves interdisciplinary processes, i.e., processes of different areas of knowledge. The processes include fluid dynamics and turbulent flows, heat and mass transfers both across the boundary of the system (Figure 4-12) and at the molecular level (Section 4.8), chain reactions and phase (state) changes of the compounds, and flame diffusion and radiation.

Modelling the combustion process in the engine poses real challenges to researchers. There are aspects in modelling combustion that are not fully understood, such as the flows into the system and the reaction kinetics within the system. Also, modelling deviates from real-world conditions, because researchers use approximate cycle that represents approximate boundary conditions, such as isentropic compression and expansion, equilibrium chemical reactions, and heat-sealed walls (Schäfer and Basshuysen, 1995).

Based on Sections 4.2 through to 4.5, we conclude that the process of combustion is a complex system that includes interdisciplinary processes. We present the major points concluded on the macroscopic level – Section 4.11 discusses on the molecular level –, as follows:

1. The actual boundary conditions of the combustion system deviate from the assumed simplified conditions, as follows (Heywood, 1988; Stone, 1992; Pulkrabek, 1997):
 - Compression and expansion processes are non adiabatic. They occur with heat transfer, and thus are not isentropic.
 - The combustion cycle is irreversible; there is friction between the piston and cylinder walls, and within the cylinder because of the turbulent flow.
 - The mixture in the cylinder is not an ideal gas. It is not homogenous— not uniform in composition – and, therefore, reaction kinetics and the equation of state for ideal gases do not accurately describe the mixture.
 - The combustion cycle is an open system. There is heat transfer, work transfer, and mass flow across the boundary of the system.

- The system of combustion is not constant in volume. There are air leakages during induction and exhaust processes (Pulkrabek, 1997). Also, the quantity of fuel, air, and recycled exhaust gas inflow is not identical into all cylinders and, therefore, the composition of the mixture varies with each cycle.
2. The speed of flames and thus the process of combustion vary in each cycle. Among the factors that affect the speed of flames are the following (Chomiak, 1992):
- Changes in the state of the process, such as phase changes of the compounds, thermal conduction, and diffusion and radiation of the flame.
 - Dynamics of the continuous mixture, such as patterns of fluid flow.
 - Appearance of new compounds, such as the chemical transformations of the mixture into new compounds.
3. The process of combustion includes several interdisciplinary processes, i.e., processes of different areas of knowledge, (Chomiak, 1990):
- *Heat and mass transfer*: combustion involves heat and mass transfer both on a macroscopic level, i.e., across the boundary of the system, and on a molecular level (Sections 4.8 and 4.11). The transfers are constrained by laws of energy and mass conservation.
 - *Dynamic changes in the flow patterns*: combustion affects the pattern of the flow of the gas mixture in the cylinder, such as air, fuel vapour, the recycled exhaust, and the residual gases. The flow of the gas mixture in general is turbulent flow and in many patterns, such as swirl and squish (see Section 4.4.2).
 - *Radical chemical transformations*: combustion includes changes in multiple compounds, and the combustion reactions consist of several chain reactions (Sections 4.7 and 4.9). The chemical changes that take place during combustion are complex, and are so rapid that they adapt themselves to all the other processes in the cylinder (Chomiak, 1990).

4. The system of combustion is constrained by laws of conservation of energy and mass for every component in the system. Also, it is constrained by molecular transfer, and chemical kinetics including differential equations of the chemical reactions (Sections 4.8).
5. Combustion occurs almost instantaneously within a cycle, but emissions are measured either in grams per test or grams per unit distance (Figure 4-13). The flow of emissions is continuously sampled by CVS (constant volume sampling), and the mean volumetric concentrations of emissions, such as CO, HC, and NO_x, are continuously measured (Schäfer and Basshuysen, 1995).

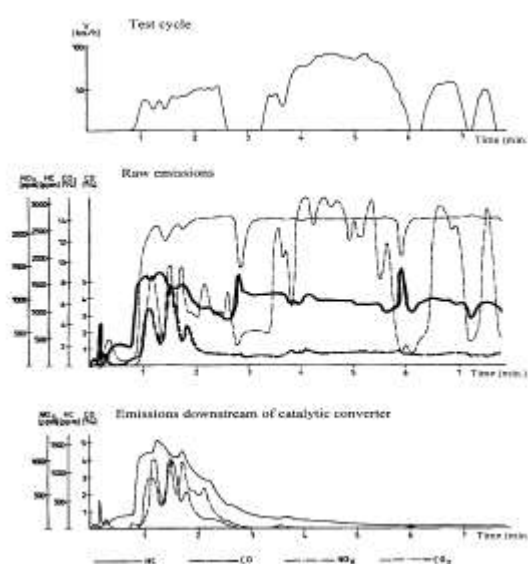


Figure 4-13 The Flow of Emissions in CVS for FTP-75

Source: (Schafer and Basshuysen, 1995)

6. Combustion occurs almost instantaneously within a cycle, and there is insufficient time for the reactions to reach equilibrium (Mattavi and Amann, cited by Stone, 1992). More details with regards to the reactions are discussed in Section 4.11.

4.7 Nature of the Combustion Reactions

So far, we have established the overall mechanism of the process of combustion, in terms of flame development and general characteristics of the combustion process. Also, we have presented the major points that exhibit the complexity of the system on the macroscopic level mainly. This section presents, in general, a brief description of the nature of the combustion reactions. Sections 4.8 through to 4.10 treat the reactions of combustion in more details.

Combustion reactions are not simple reactions that occur in one step. They are complex reactions that occur in a chain of unimolecular and bimolecular reactions, i.e., first and second order reactions. Furthermore, the order of the combustion reactions is not constant, and it changes with higher concentrations of intermediate products. The chemical mechanism of combustion reactions consists of a large number of simultaneous interdependent reactions. The reactions undergo a long sequence of changes, and consist of many intermediate compounds and reactions. The chain of combustion reactions consists largely of several groups of reactions, such as initiating, propagating, chain-branching, and terminating reactions. The initiating reactions produce highly reactive intermediate radicals from stable molecules, such as fuel and oxygen. Then, the reactions propagate and the radicals react with other reactant molecules in the propagating reactions. These give other intermediate products and more radicals, and the chain goes on. The propagating reactions are chain-branching that increase the number of radicals by producing two reactive radical molecules for each radical consumed. Finally, the chain terminates once the radicals are consumed by the terminating reactions.

4.8 Chemical Kinetics of the Combustion Reactions

The stability of chemical reactions is not absolute, and is determined by the activation energy (4.8.1). Chemical reactions are associated by either absorption or release of energy in the form of heat. Reactions that absorb heat are endothermic reactions, whereas reactions that release heat are exothermic reactions (4.8.1). Also, chemical reactions are either decomposition or recombination reactions (4.8.3).

Various disciplines employ several analytical models to investigate the combustion process and to predict the formation of emissions in the engine. Specifically, they attempt to focus on modelling the complex formation of nitrogen oxides (NO_x) in the combustion process (4.10.4). We review the work of Fristrom (1995), Chomiak (1992), and Glassman (1996; 1977), and present insights into some theoretical aspects of the chemical kinetics of the combustion reactions in conventional gasoline-fuelled engines, as follows:

4.8.1 Activation Energy

The activation energy is the energy barrier of the repulsion forces between the molecules. For a reaction to occur, the activation energy must exceed the average energy resulting from the thermal motion of the reactant molecules. The activation energy is required to alter the molecular structure of the reactants.

In other words, for a reaction to occur, the kinetic energy of the relative motion of the molecules must be greater than or equal to the activation energy (E). The probability that the energy of collision of the reactants is greater than or equal to the activation energy, is calculated using $\text{Exp}\left(\frac{-E}{RT}\right)$, (see Equation 4-7).

We elaborate on the energy of a reaction by illustrating the potential energy curve for an arbitrary bimolecular reaction, e.g., $AB + C \longrightarrow AC + B$, as shown in Figure 4-14.

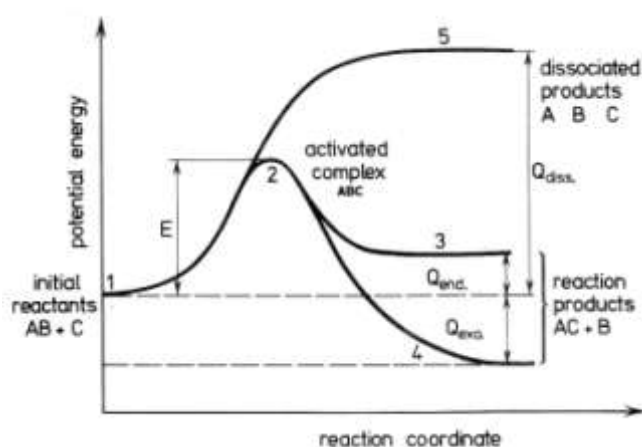


Figure 4-14 The Potential Energy of a Reaction

Source (Chomiak, 1992)

As the reactants AB and C approach each other, their potential energy increases due to the forces of repulsion between them. An activated complex (ABC) is formed with maximum potential energy. However, ABC is not a stable molecule. It is in a state of unstable equilibrium. The three atoms are bound with three equal forces.

As soon as the C molecule has a kinetic energy higher than E, it will overcome the repulsion forces. This leads to a complete decomposition of the ABC compounds, and three independent atoms, i.e., A, B, and C (curve 1-5), are formed. The difference between the potential energies before and after collision is the energy of dissociation (Q_{diss}).

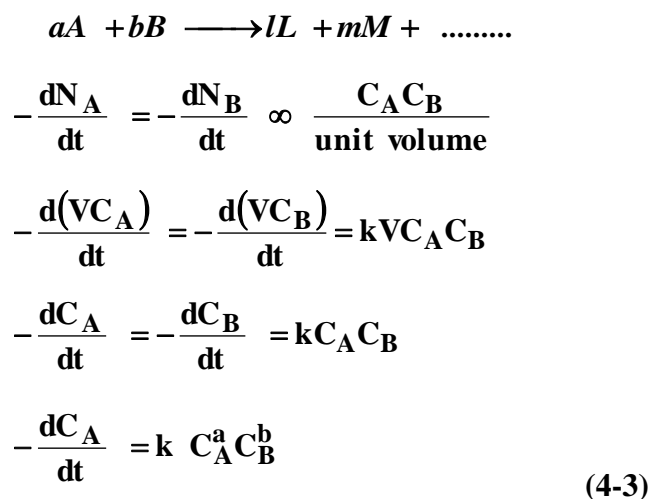
When the attraction forces between A and C are greater than the attraction forces between A and B, a stable AC molecule is formed. The reaction (AC +B) is either endothermic (Q_{end}) that absorbs heat (curve 1-3) or exothermic (Q_{exo}) that releases heat (curve 1-4).

4.8.2 The Rate of Reaction

The rate of a reaction is the rate of change of the number of molecules or moles in the system. Combustion reactions, according to the principle of le Châtelier, attempt to reach equilibrium and eliminate any external changes imposed on the system of reactions. The rate of a reaction depends on three main factors (Stone, 1992). We describe overall the main factors (Chomiak, 1992):

- (1) **Molar concentrations – the number of moles per a unit of volume** –: A change in the concentration of a constituent would shift the reactions in a direction to lower the concentration of the constituent.

We write the rate of a reaction in terms of molar concentrations for a bimolecular reaction, which is typical of combustion reactions in a system of constant volume and mass, as follows:



where:

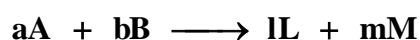
N_A, N_B : number of moles of A and B compounds respectively.
 $dN_A/dt, dN_B/dt$: rate of change of N_A, N_B respectively
 V : volume
 k : reaction rate constant; it varies with temperature and heat of the reaction
 C_A, C_B : molar concentrations of A and B compounds respectively.

- (2) **Pressure:** An increase in the pressure of the system shifts the reactions towards reducing the total number of moles, and thus reducing the pressure.

We express the rate of the reaction in terms of pressure, for a system of constant volume and mass. We express initially the rate of an arbitrary n order reaction (Equations 4-4). Then, for a second order reaction, we express it in more details using the equation of state for ideal gases (Equations 4-5).

$$\begin{aligned}
 -\frac{dC_A}{dt} &\propto p^n \\
 -\frac{dC_A}{dt} &= k_A p^n X_A^{n1} X_B^{n2} X_C^{n3} \dots\dots
 \end{aligned} \tag{4-4}$$

$$n = n1 + n2 + n3$$



$$pV = nRT$$

$$p = \frac{n}{V} RT$$

$$p = zRT$$

$$p_A = C_A RT \quad , \quad p_B = C_B RT$$

$$p_A = \frac{C_A}{z} p \quad , \quad p_B = \frac{C_B}{z} p$$

$$C_A = \frac{pX_A}{RT} \quad , \quad C_B = \frac{pX_B}{RT} \quad (4-5)$$

$$-\frac{dC_A}{dt} = k_A X_A^a X_B^b \frac{P^2}{(RT)^2}$$

where:

p: total pressure

V: volume

n: the total number of moles: the overall reaction order

n₁, n₂, n₃: the number of moles of A, B, and C respectively

R: universal gas constant

T: absolute temperature

z: number of moles per unit of volume

p_A and p_B: partial pressure of A and B respectively

C_A, C_B molar concentration of A and B respectively

C_A/z, C_B/z :molar fraction of A and B respectively

X_A, X_B: volume fraction of A and B respectively

k_A reaction rate constant

- (3) **Temperature:** A raise in the temperature of the system shifts the reactions towards absorbing the heat. A chemical reaction depends on the probability of collisions between molecules per unit time. The number of collisions increases proportionally with the square root of temperature, as follows:

$$\text{number of collisions} \propto T^{0.50} \quad (4-6)$$

Therefore, a rise in temperature increases the rate of a reaction. Nonetheless, experiments show that the rate of a reaction increases even faster with increasing the temperature. Thus, it is difficult to predict accurately the rate of a reaction.

The reaction rate constant is theoretically calculated by Arrhenius formula (Chiomak, 1992; Schäfer and Basshuysen), as follows:

$$K = BT^\alpha \text{Exp}\left(-\frac{E}{RT}\right) \quad (4-7)$$

Where:

$BT^\alpha = c$: frequency factor (pre-exponential) and is empirically calculated by experimental data

B is a coefficient, and is determined by the theory of probability for the collisions of gases

α is an empirical temperature factor and, in general, $-1 < \alpha < 2$.

E is the activation energy

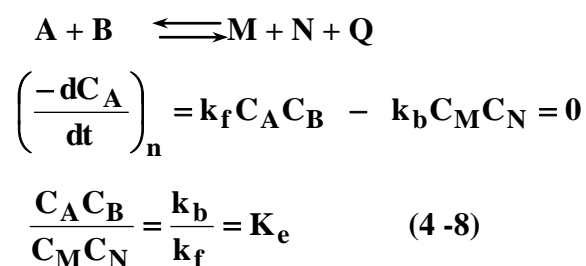
R universal gas constant

T absolute temperature

4.8.3 Equilibrium Reactions

Equilibrium constant (K_e) determines the direction towards which the reaction will be shifted, i.e., a recombination reaction or a decomposition reaction; the larger is K_e the more towards the right is the reaction.

We express the equilibrium constant (K_e), for a bimolecular reaction, as follows:



Where:

K_e = equilibrium constant and is a function of temperature and the heat of a reaction

k_b = rate of the backward reaction

k_f = rate of the forward reaction

Q = the heat transfer in the reaction

C_A, C_B = molar concentration of A and B respectively

C_M, C_N = molar concentration of M and N respectively

K_e varies with the temperature and the heat of a reaction, and is determined by Van't Hoff formula, as follows:

$$\frac{d \ln K_e}{dT} = -\frac{Q}{RT^2} \quad (4-9)$$

The difference between the activation energies of the forward and backward reactions is equal to the overall thermal effect of the reaction ($E_b - E_f = Q$).

4.9 Chain of the Combustion Reactions

The mechanism of combustion reactions is determined by experimental estimates of the kinetic data of the reactions. The mechanism of combustion reactions is complex, and not all details are known. After 50 years of extensive studies, the overall kinetics of the oxidation of hydrocarbons has started to emerge (Glassman, 1977). For example, we present a summary of the main reactions involved in the oxidation of methane (CH_4) (Figure 4-15).

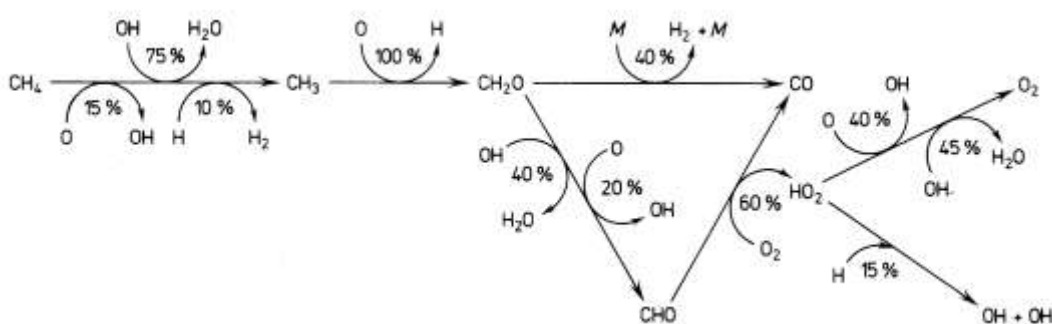


Figure 4-15 The Chain Scheme of the Oxidation of Methane

Source: (Chomiak, 1990)

A mechanism of the combustion reactions consists of an infinite number of routes and, therefore, one scheme is not necessarily an accurate representative of all possible routes. We present the scheme for the combustion of methanol with air, and also present the associated kinetic data (Section 4.8), as shown in Table 4-1:

Table 4-1 Chain Reactions for the Combustion of Methanol with Air

No.	Reactants	Products	B ($m^{3k}/kmol^k.s$)	E/R	α
1	CH ₃ OH + M	CH ₃ + OH + M	1.0*10 ¹⁵	34200	0
2	CH ₃ OH + CH ₃	CH ₂ + CH ₄	1.8*10 ⁸	4940	0
3	CH ₃ OH + O	CH ₂ OH + OH	1.7*10 ⁹	1150	0
4	CH ₃ OH + H	CH ₃ + H ₂ O	1.3*10 ¹⁰	2670	0
5	CH ₃ OH + OH	CH ₂ OH + H ₂ O	3.0*10 ¹¹	3000	0
6	CH ₂ OH + O ₂	CH ₂ O + HO ₂	5.0*10 ⁷	0	0
7	CH ₂ OH + M	CH ₂ O + H + M	2.5*10 ¹¹	14600	0
8	CH ₄ + O ₂	CH ₃ + HO ₂	8.0*10 ¹¹	28300	
9	CH ₃ + O ₂	OH + CH ₂ O	2.0*10 ⁷		0
10	CH ₄ + OH	CH ₃ + H ₂ O	6.0*10 ¹¹	6290	0
11	HCO + O ₂	CO + HO ₂	1.0*10 ¹¹	3434	
12	CH ₄ + HO ₂	CH ₃ + H ₂ O ₂	2.0*10 ¹⁰	9091	
13	CH ₄ + H	CH ₃ + H ₂	2.2*10 ¹	4400	3
14	CH ₄ + O	CH ₃ + OH	2.1*10 ¹⁰	4560	0
15	CO + HO ₂	CO ₂ + OH	1.0*10 ¹⁴	11616	0
16	CH ₂ O + O ₂	HCO + HO ₂	1.0*10 ¹¹	16162	
17	HCO + M	CO + H + M	5.0*10 ¹¹	9570	
18	CO + OH	CO ₂ + H	4.0*10 ⁹	4030	
19	CH ₂ O + OH	H ₂ O + HCO	5.4*10 ¹¹	3170	0
20	CH ₃ + O	CH ₂ O + H	1.0*10 ¹¹		
21	CH ₂ O + H	HCO + H ₂	1.35*10 ¹⁰	1890	
22	CH ₂ O + O	HCO + OH	5.0*10 ¹⁰	2300	
23	HCO + OH	CO + H ₂ O	1.0*10 ¹¹	0	0
24	CH ₃ + O ₂	H ₂ + CO + OH	4.0*10 ⁹	9091	0
25	CO + O + M	CO ₂ + M	6.0*10 ⁷	0	0
26	CH ₂ O + M	CHO + H + M	1.0*10 ¹¹	18500	
27	CHO + H	CO + H ₂	2.0*10 ¹¹	0	0
28	CHO + O	CO + OH	1.0*10 ¹¹	0	0
29	H + H + M	H ₂ + M	1.0*10 ¹²	0	-1
30	O + O + M	O ₂ + M	1.0*10 ⁸	0	0
31	O + H + M	OH + M	3.0*10 ⁸	0	0
32	H + O ₂	OH + O	2.2*10 ¹¹	8462	0
33	O + H ₂	OH + H	1.8*10 ⁷	4482	1
34	OH + H ₂	H ₂ O + H	2.2*10 ⁸	2593	0
35	H + OH + M	H ₂ O + M	1.5*10 ¹¹	0	-0.5
36	2OH	H ₂ O + O	6.3*10 ⁹	553	0
37	H ₂ + O ₂	2OH	1.36*10 ¹⁰	24318	0

38	H + HO ₂	2OH	7.3*10 ¹¹	0	0
39	N ₂ + M	2N + M	2.0*10 ¹⁸	113316	-1.5
40	NO + M	N + O + M	5.5*10 ¹⁷	75544	-1.5
41	NO + O	N + O ₂	1.55*10 ⁶	19439	1
42	O + N ₂	NO + N	1.36*10 ¹¹	37974	0
43	N ₂ O + M	N ₂ + O + M	1.0*10 ¹²	30722	0
44	2NO	N ₂ O + O	2.6*10 ⁹	32130	0
45	NO + O ₂	NO ₂ + O	7.8*10 ⁸	22930	0
46	N ₂ + O ₂	NO + NO	9.1*10 ²⁰	64970	-2.5
47	NO ₂ + M	O + NO + M	6.0*10 ¹⁸	36060	-1.5
48	NO + O ₃	NO ₂ + O ₂	8.9*10 ⁸	1330	0
49	HNO + H	NO + O ₂	4.5*10 ⁹	0	0
50	N ₂ O + H	N ₂ + OH	3.0*10 ¹¹	8080	0
51	HNO + OH	NO + H ₂ O	3.0*10 ⁹	1200	0.5
52	H + NO + M	HNO + M	5.4*10 ⁹	-300	0
53	HNO + NO	N ₂ O + OH	6.14*10 ⁹	17222	0
54	NH ₃ + NO	NH ₂ + HNO	1.0*10 ⁷	0	0
55	NH ₂ + H + M	NH ₃ + M	4.8*10 ⁸	-8300	0
56	NH ₃ + H	NH ₂ + H ₂	5.0*10 ⁸	1000	0.5
57	N + OH	H + NO	1.2*10 ¹⁰	0	0
58	NH ₃ + N	NH ₂ + NH	5.0*10 ⁸	1010	0.5
59	NH ₃ + OH	NH ₂ + H ₂ O	5.4*10 ¹²		0
60	NH ₃ + O	NH ₂ + OH	1.0*10 ⁸	2475	0
61	NH + HNO	NH ₂ + NO	2.0*10 ⁸	1010	0.5
62	HNO ₃ + M	OH + NO ₂ + M	1.6*10 ¹²	15450	0
63	NH ₂ + OH	NH + H ₂ O	3.0*10 ⁷	656	0.679
64	NH ₂ + NO	N ₂ + H ₂ O	1.0*10 ¹⁰	0	0

Source: (Schäfer and Basshuysen, 1995).

M represents transfer of thermal energy – heat transfer –

k = 1 and 2 for bimolecular and tri-molecular reactions respectively

4.10 The Combustion Reactions

We express the chain reactions of the combustion process by high order reactions in a system of constant mass and volume (4.10.2, 4.10.3, and 4.10.4). However, such reactions do not represent accurately the combustion reactions, because:

- The process of combustion does not occur at a constant volume and mass.
- High order reactions do not describe accurately the composition of the mixture. The composition of the mixture is not necessarily homogenous, and varies between cylinders (4.4.2).
- The combustion reactions are either combination or decomposition reactions (4.8.3).

- The reactions of combustion consist of a number of intermediate reactions and intermediate products (Sections 4.7 and 4.9).
- The reactions state changes over time; various compounds have various lifetimes (Schäfer and Basshuysen, 1995).
- The combustion reactions are interdependent. The reactions are constrained by laws of mass conservation and energy conservation on the molecular level (Section 4.8).

The main two compounds in the combustion process are fuel and the ambient air. These supply the main elements of the combustion reactions. The ambient air supplies oxygen (O_2) and nitrogen (N_2), and the fuel supplies carbon (C) and hydrogen (H_2). Nitrogen is not an active element; however, heat released by other combustion reactions enhances the splitting of nitrogen (N_2) into two reactive molecules ($2N$) that initiates a chain of reactions with oxygen (O_2).

4.10.1 Hydrocarbon Fuels

Fuels, such as gasoline and diesel, are mixtures of hydrocarbons with bonds between hydrogen (H_2) and carbon (C) atoms (Stone, 1992). Some hydrocarbons contain oxygen in the form of OH groups, e.g. methanol (CH_3OH) (Schäfer and Basshuysen, 1995). Gasoline, the main fuel for spark-ignition engines, is manufactured from crude petroleum, and comprises a mixture of several hydrocarbons that varies with regions (Pulkrabek, 1997). Crude petroleum consists by weight of 87 percent carbon (C), between 11 and 14 percent hydrogen (H_2), and other traces (Pulkrabek, 1997).

Hydrocarbons consist of one atom of carbon that has 4 bonds in a molecular structure, and an atom of hydrogen that has one bond in a molecular structure. The hydrocarbon molecules can be saturated with a single bond between two carbon atoms, or unsaturated with double or triple bonds between two carbon atoms. Hydrocarbon molecules are formed in several families (Pulkrabek, 1997):

Paraffins (C_nH_{2n+2}): examples are methane (CH_4), butane (C_4H_{10}), and isooctane (C_8H_{18}) (Figure 4-12). **Olefins** (C_nH_{2n}): are chain molecules that contain

one double carbon-carbon bond, e.g., ethane (C_2H_4) and butene-1 (C_4H_8) (Figure 4-12).

Diolefins (C_nH_{2n-2}): similar to olefins are chain molecules that have two double carbon-carbon bonds, e.g., 2-heptadiene (C_7H_{12}) (Figure 4-12).

Acetylene (C_nH_{2n-2}): unlike diolefins, are chain molecules that have a triple carbon-carbon bond, e.g., acetylene (C_2H_2) (Figure 4-12).

Cycloparaffins (C_nH_{2n}): unlike olefins, are unsaturated ring structures with a single bond, e.g., cyclobutane (C_4H_8) (Figure 4-12).

Aromatics (C_nH_{2n-6}): are unsaturated ring structures with double carbon-carbon bonds, e.g., the benzene ring (C_6H_6) (Figure 4-12).

Alcohol is similar to paraffins with one of the hydrogen atoms replaced with hydroxyl (OH), e.g., methyl alcohol or methanol (CH_3OH) (Figure 4-12).

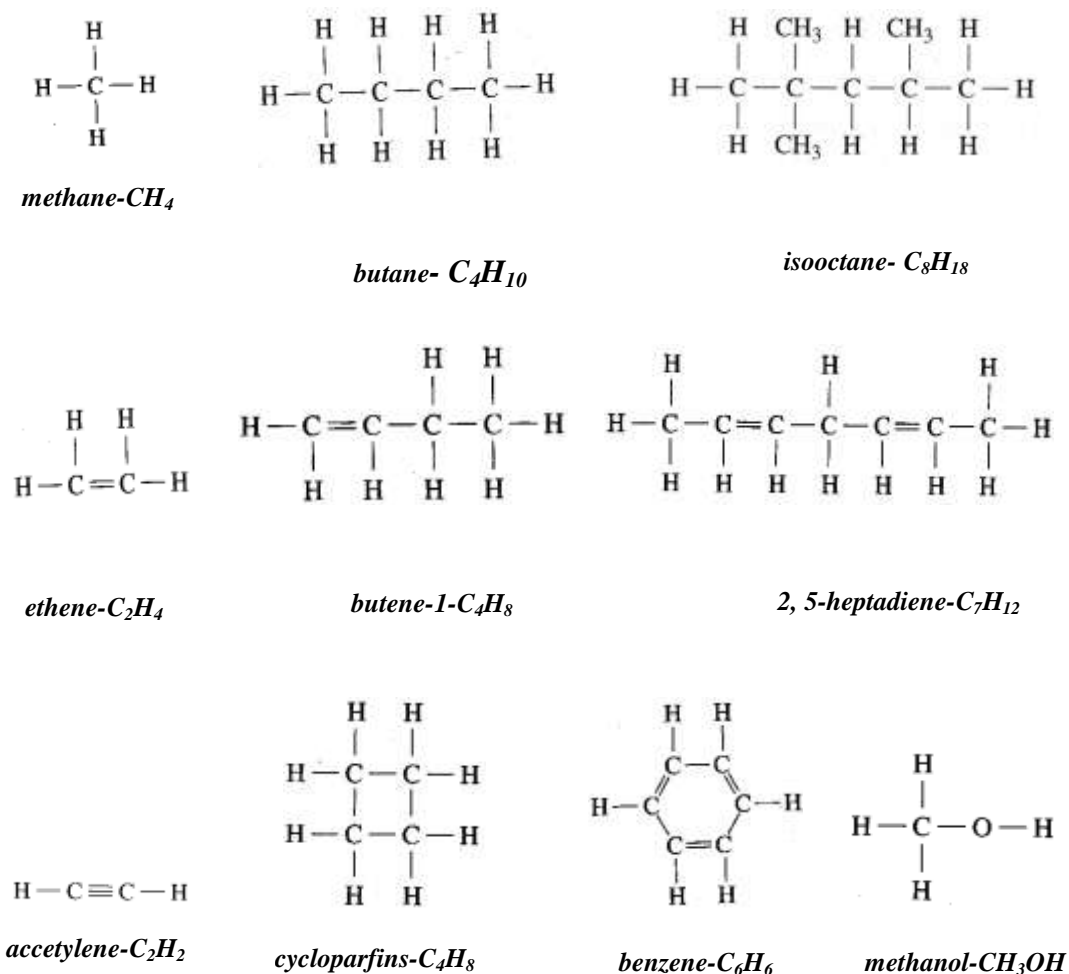


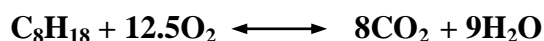
Figure 4-16 Molecular Structures of Various Hydrocarbons Families

Source: (Pulkrabek, 1997)

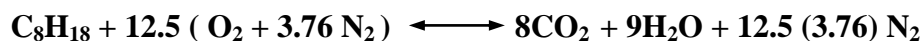
We assume that the combustion system has constant volume, and the mixture in the chamber is homogenous, i.e., uniform in composition. We then write high order reactions to describe overall the combustion reactions in stoichiometric air and oxygen, and in non-stoichiometric air, in addition to Zeldovich's chain of reactions that produce NO_x .

4.10.2 Stoichiometric Combustion Reactions

A complete combustion of the fuel in stoichiometric oxygen releases carbon dioxide (CO_2) and water (H_2O) (Schäfer and Basshuysen, 1995). The stoichiometric oxygen is the oxygen necessary to convert all carbon in the fuel to CO_2 and all hydrogen to H_2O , and no oxygen remains. For example, the overall reaction of a complete oxidation of isooctane (C_8H_{18}) is as follows (Schäfer and Basshuysen, 1995):



However, the ambient air supplies the oxygen (O_2) needed for the reaction. The ambient air consists, in molar terms, of 21 percent oxygen (O_2) and 79 percent atmospheric nitrogen (N_2^*), of which 78 percent is nitrogen (N_2), and 1 percent is argon and other traces (Stone, 1992). Nitrogen (N_2) is a stable element, but dissociates into 2N with high combustion temperatures. Nitrogen and argon in the ambient air affect the temperature and pressure in the combustion chamber (Schäfer and Basshuysen, 1995). The combustion of isooctane with stoichiometric air is, assuming 79 percent N_2 and 21 percent oxygen, as follows (Pulkrabek, 1997):

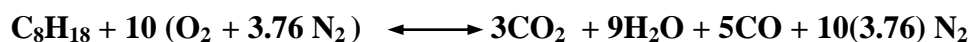


4.10.3 Non-Stoichiometric Combustion Reactions

Combustion occurs with stoichiometric oxygen, and also occurs with more than stoichiometric oxygen or with less than stoichiometric oxygen. For example, burning isooctane with 150 percent of the stoichiometric air, i.e., more than stoichiometric oxygen, produces oxygen in the products, as follows:

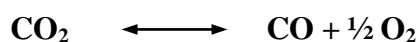


On the other hand, burning isooctane in 80 percent of the stoichiometric air, i.e., less than stoichiometric air does not produce enough oxygen to convert all carbon atoms into CO₂ and, therefore, carbon monoxide (CO) ends up in the products, as follows:

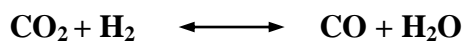


CO increases with fuel-rich mixtures, because there is not enough oxygen in the air-fuel mixture to transform all carbon (C) atoms into CO₂ (Schäfer and Basshuysen, 1995). CO is not only an emission, but also absorbs some of the thermal energy released into the system (Pulkrabek, 1997), and thus decrease NO_x.

In contrast, the production of CO in mixtures with more than stoichiometric O₂ is, as follows (Schäfer and Basshuysen, 1995):

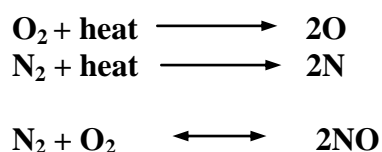


While the production of CO in mixtures with less than stoichiometric O₂ is better described with the water gas gross reaction (Schäfer and Basshuysen, 1995):

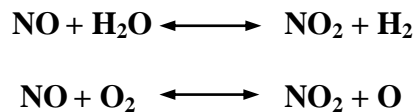


4.10.4 Formation of NO_x (NO and NO₂)

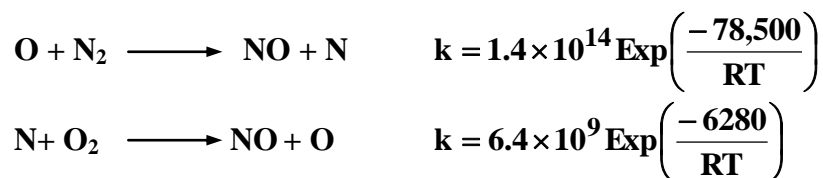
Several mechanisms for the formation of NO_x have been suggested in the literature, such as Zeldovich and Fenimore. Normally stable compounds and elements, such as N₂, dissociates at high temperatures. N₂ dissociates into 2N, and reacts with O to form NO at very high temperatures, in a chain of complex reactions, such as Zeldovich's mechanism (Stone, 1992):



NO reacts further to produce NO₂, as follows (Pulkrabek, 1997):

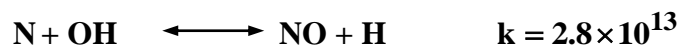


Zeldovich's mechanism is initiated by O atoms. The O atoms are formed by the dissociation of O₂ or by collisions between an H atom and O₂. The collisions between the O atoms and nitrogen molecules (N₂) start the kinetic route for NO in Zeldovich's mechanism, as follows (Glassman, 1995):



Zeldovich's mechanism is the main source for the thermal NO. However, Fenimore's mechanism suggests that other reactions than Zeldovich's reactions are important, and these produce small percentages of NO in the flame region, "prompt NO" (Glassman, 1977).

For very fuel-rich mixtures with equivalence ratio (Φ) > 1.2 (Section 4.5), the formation of NO is better described by (Schäfer and Basshuysen, 1995; Glassman, 1995):



The oxidation reactions of the fuel and the formation of NO in the combustion process are intimately linked (Heywood, 1988). We elaborate and state that the combustion reactions, including the formation of NO, are interdependent. There is heat and mass transfer at the molecular level in the combustion reactions (Section 4.8 and Section 4.11). Specifically, the chain of reactions that is responsible for the formation of NO_x is initiated by the release of the thermal energy from other combustion reactions. Also, oxygen atoms (O) that initiate Zeldovich's chain of

reactions are made available by other reactions in the chain of combustion reactions (Section 4.9). The concentration of NO reaches a maximum, as the heat transfer reaches the maximum in the system (Figure 4-17).

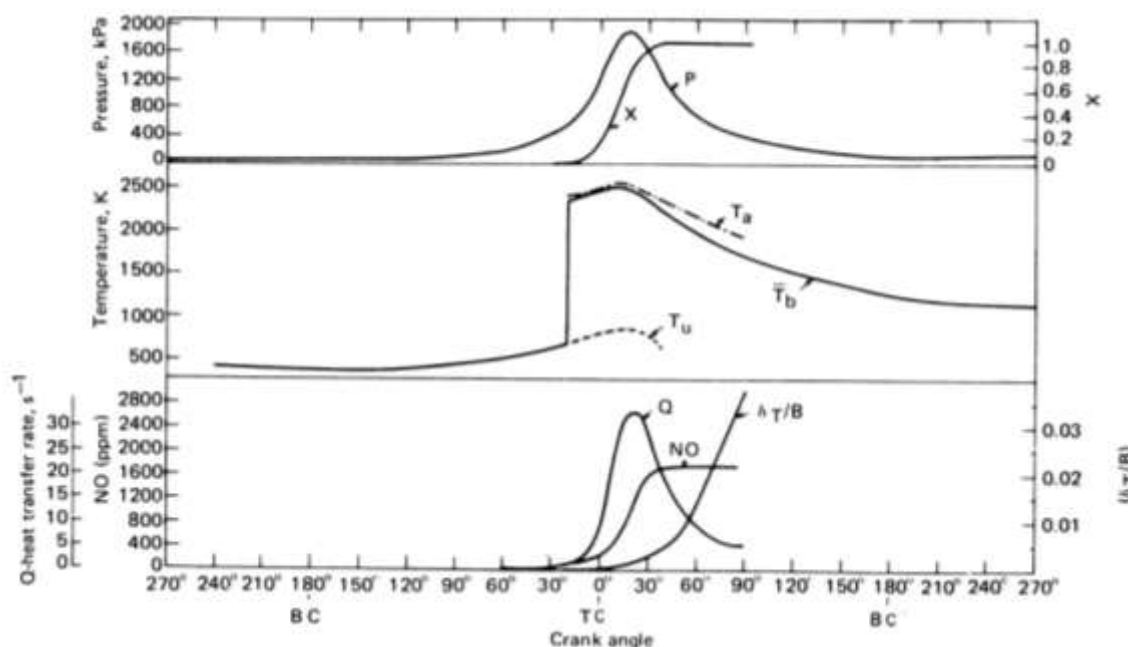


Figure 4-17 NO in relation with Heat Transfer

Source: (Heywood et al., cited in Stone, 1992)

Where:

- X : mass fraction burnt
- T_u : temperature of unburnt mixture
- \bar{T}_b : mean temperature of burnt gas
- P : cylinder pressure
- T_a : temperature of burnt gas adiabatic core
- Q: instantaneous heat transfer rate
- NO: nitric oxide concentration
- δ_T : thickness of thermal boundary layer
- B: the cylinder bore

4.11 Interdependencies of the Combustion Reactions

We have so far established the chemical thermodynamic nature of the process of combustion in the engine. Based on the thermodynamic characteristics of the combustion process and on Sections 4.7 through to 4.10, we conclude that

combustion reactions are interdependent. We present the major characteristics of the combustion reactions concluded, as follows:

1. The process of combustion is a dynamic process that creates in the combustion chamber an environment of temperature, pressure, and substance concentrations. The created environment determines the reactions and products of combustion -- see the second in this list --. The created environment is dynamic, and varies constantly within each cycle and between cylinders (Section 4.4.2). Figure 4-18 shows variations of the products of equilibrium combustion reactions with changes in the created environment, and at three different temperatures and a constant pressure.

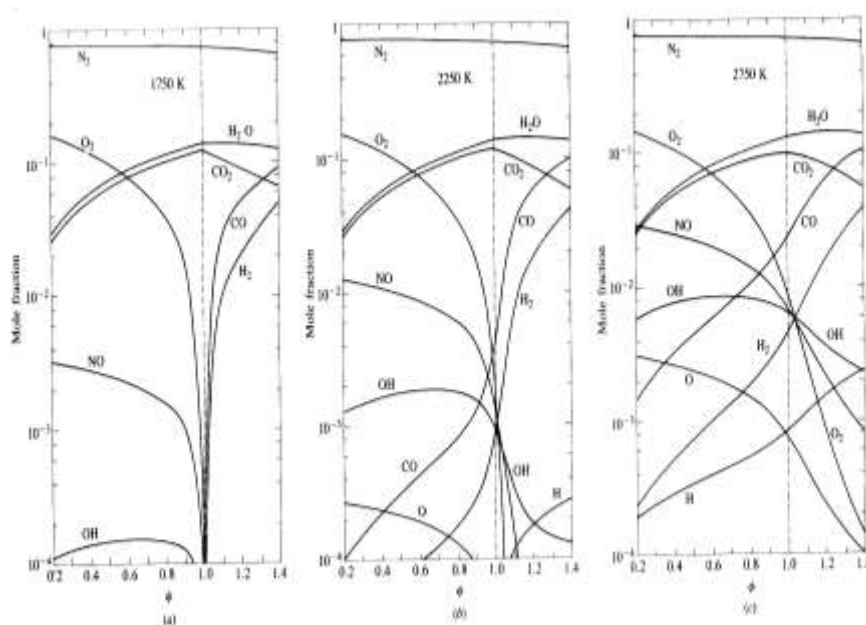


Figure 4-18 Mole Fraction of Equilibrium Combustion Products versus Fuel Equivalence Ratio at 3 Different Temperatures and 30 Atmospheres Pressure

Source: (Heywood, 1988)

2. The combustion reactions are dynamic and interdependent. The propagation of the flame elevates the temperature in the cylinder, and induces gradients of temperatures and substance concentrations (Heywood, 1988; Fristrom, 1995). The resulting gradients enhance fluxes of heat and reactive substances into the unburned mixture, and therefore accelerate the rates of the reaction. The faster the reaction, the steeper the resulting

gradients of heat and concentration, and the steeper the gradients the higher are the fluxes. The loop — gradients of thermal energy and concentration and then the fluxes, and the rate of the reaction — is opposed by the flame propagation (Firstrom, 1995).

3. Combustion reactions are not simple reactions that occur in one step. They are complex reactions that occur in a chain of reactions. The reactions undergo a long sequence of changes, and consist of many intermediate compounds and reactions (Section 4.9).
4. The chemical mechanism of combustion reactions consists of a large number of simultaneous interdependent reactions (Figure 4-15). The chemical reactions involve heat and mass transfer (Section 4.8) that are constrained by laws of energy and mass conversations.
5. The chemical reactions are complex, and require several non-instantaneous chemical reactions with complex kinetics (Mattavi and Amann, cited by Stone, 1992):
 - Research is being undertaken to predict accurately CO and NO_x emissions.
 - There is insufficient time for the reactions to reach equilibrium.
 - The concentrations of CO and NO_x are higher than predicted by thermodynamics. The rate of forward reaction is different from the rate of backward reaction.

4.12 Controlling CO, HC, and NO_x Emissions

It is not possible to minimise all emissions simultaneously. For example, General Motors used an internal combustion engine simulation program for modelling the combustion process and the exhaust system during an engine cycle. They found that the concentrations of CO and NO are negatively related in the combustion process for several fuel equivalence ratios (Figure 4-19).

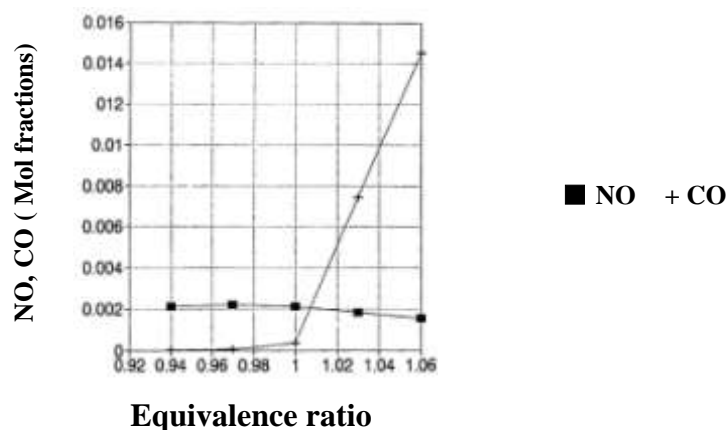


Figure 4-19 Emissions of CO and NO versus Fuel Equivalence ratio

Source: (Pulkrabek, 1997)

CO emissions can be reduced with fuel-lean operations; however lean operations have negative effects on the power of the engine. HC, similar to CO, is reduced with fuel-lean operations until there is a reduction in the flammability of the mixture, thereafter lean operations increase HC emissions. Also, HC can be reduced if a second spark plug is added to the chamber; starting the flame at two points will reduce both the path for the flame to proceed and the time needed for the reaction, and thereby will reduce flame quenching (Pulkrabek, 1997).

NO_x can be reduced in more ways than HC and CO. NO_x is reduced by reducing either the duration or the temperature of combustion. Also, NO_x is reduced by retarding ignition, because it reduces the peak temperature and pressure of combustion. However, retarding ignition has negative effects on both the power and the fuel economy. Additionally, re-circulating a fraction of the exhaust gas reduces NO_x . Exhaust gas recirculation (EGR) increases residual gases in the cylinder; EGR reduces both the temperature of combustion and the flame speed and, thereby, reduces NO_x . An EGR between 5 percent and 10 percent is likely to halve NO_x (Stone, 1992), but also is likely to lower the overall engine efficiency by reducing its limits to lean operation. To control nitrogen oxides, the combustion temperature in the engine is lowered. However, lowering the temperatures of combustion also reduces the thermal efficiency of the engine and, hence, increases CO.

4.13 Conclusions

First, we present a summary of the theory of combustion in gasoline-fuelled engines. Then we explain why it is meaningful to confirm theoretical knowledge through empirical studies. Finally, we state in view of that the hypothesis of the thesis. Chapter 5 presents the empirical framework for investigating the hypothesis of the thesis.

4.13.1 Summary of the Theory of Combustion in Gasoline-Fuelled Engines

The combustion process is a very rapid process that occurs almost instantaneously in a finite time of the short engine cycle and, thereby, emissions are simultaneously produced. A mixture of air-fuel flows in the engine in the first stroke. Then, the process of combustion starts at the end of the second stroke. The presence of O₂, N₂, and HC in the cylinder with a spark from the spark plug initiates several reactions during a finite but very short time of combustion, i.e., between 40° and 60° crank angle.

Additionally, the combustion process causes flames. The resultant flames by themselves are reactions. Fristrom (1995) defines flames as being chain and exothermic reactions that propagate through space. The flame propagation within the combustion chamber elevates the temperature in the cylinder, and causes gradients of thermal energy and reactive substance concentrations (Heywood, 1988; Fristrom, 1995). The development of the flame is governed by laws of energy conservation and mass conservation, Kinetics of chemical reactions, thermal conduction, and molecular diffusion (Fristrom, 1995).

Combustion reactions are interdependent. There is a cause-effects relationship between HC, CO, and NO_x emissions. The gradients of thermal energy and substance concentrations caused by the propagation of the flame enhance fluxes of heat and reactive substances into the unburned mixture. Thus, accelerate the rates of the combustion reactions. The faster are the reactions, the steeper are the resulting gradients of thermal energy and substance concentrations. Also, the steeper are the resulting gradients, the higher are the fluxes of heat and reactive substances into the unburned mixture. The loop of gradients, concentration, and

then fluxes and rate of the reaction is opposed by the propagation of the flame (Firstrom, 1995).

The combustion reactions, including the formation of NO, are interdependent. The oxidation of fuel and the formation of NO_x are closely related. The heat and mass transfer at the molecular level between the combustion reactions enhance the chain of the combustion reactions and cause the reactions to chain branching. The chain of reactions that is responsible for the formation of NO_x is initiated by the release of the thermal energy from other combustion reactions. Also, oxygen atoms (O) that initiate Zeldovich's chain of reactions are made available by other reactions in the chain of combustion reactions. The concentrations of NO reach a maximum as the heat transfer reaches the maximum in the system.

The theory of combustion in conventional gasoline-fuelled engines suggests a proportional relation between CO and HC. Both HC and CO are the products of incomplete oxidation of the fuel (Section 4.2 and 4.4.1 (2)). The theory also suggests an inverse relation between CO and NO_x (4.4.1(2)). The increases in the heat of the combustion process would enhance forming NO_x and would inhibit forming CO. The combustion reactions are opposed by the propagation of the flame.

While, Chapter 4 demonstrates complex nature of behaviours for HC, CO, and NO_x emissions, it is not very obvious what the nature of these behaviours is across vehicles population and driving patterns. Moreover, although the theory of combustion postulates a positive (proportional) relationship between HC and CO emissions and a negative (inverse) relationship between CO and NO_x, the theory is not very informative in terms of how much an emission goes up or down as a result of changes in the other two emissions. It does not provide numerical measures of the relationship between emissions. Empirical studies provide the numerical estimations of such relationships.

Additionally, although that the laboratory research that is based on the theory of combustion has broaden our knowledge about vehicle emissions, it is equally important to understand well the operational behaviour of vehicle emissions.

Theoretical studies are based on laboratory experiments, and performed usually under effective control (Phipps and Quine, 2001). Uncontrollable variations in vehicle emissions are inherent in the measurements, and therefore statistical analysis, which allow for the uncontrollable variations, is needed to enable analysis of the important factors. It is important to confirm the theoretical knowledge through empirical and quantitative technical studies. Moreover, rational comprehensive manner of studying vehicle emissions, has led to more emphases on the empirical statistical studies of vehicle emissions.

Research studies have not predicted accurately the combustion process, nor have determined the exact chemical reactions that attain equilibrium in the system. Combustion reactions are not in equilibrium. Reactions that produce CO and NO_x are complex and they do not reach equilibrium. Research is still underway to predict these reactions accurately.

4.13.2 The Hypotheses of the Thesis

Based on the theory of combustion in gasoline-fuelled engines, this section presents the hypotheses of the thesis. The thesis hypothesises that CO, HC, and NO_x emissions are statistically significantly interdependent. While the null hypothesis is that they are not statistically significantly interdependent.

We express the null hypothesis (H_0) and the alternative hypothesis, i.e., the thesis hypothesis (H_1), as follows:

H_0 : The null hypothesis is a joint hypothesis that CO, HC, and NO_x emissions are not statistically significantly interdependent.

H_1 : The alternative hypothesis, that CO, HC, and NO_x emissions are statistically significantly interdependent.

Chapter Five

Empirical Framework for Investigating Vehicle Emissions Interdependencies

5.1 Introduction

So far, the thesis has established that there is the potential for a large number of factors to have direct or indirect influence on vehicle emissions. The thesis has also established that vehicle design variables are inter-related and work in combination with other operational factors to influence the levels of emissions. It is difficult to isolate the effects of one single variable. A change that reduces one emission will often increase other emissions.

More importantly, Chapter 4 establishes that vehicle emissions are jointly dependent. It establishes that it is justified theoretically to estimate HC, CO, and NO_x emissions simultaneously. Chapter 4 also presents the hypothesis of the thesis (Section 4.13). However, sourcing a suitable database that consists of candidate variables for testing the hypothesis of the thesis is an empirical challenge for this thesis.

This chapter presents a framework to investigate empirically the hypothesis of the thesis. It proposes potential variables for testing interdependencies of vehicle emissions. It also proposes several statistical models, each of which includes three simultaneous-equations that are investigated under a specific test drive-cycle. The equations each relate one of three emissions to exogenous vehicle variables, and also to the other two emissions, as endogenous variables.

5.2 Dimensions for Investigating Emissions Interdependencies

Traffic activities produce HC, CO, and NO_x emissions. We hypothesise that these emissions are interdependent. This hypothesis is theoretically justified by the theory of combustion and the chemical thermodynamic principles of burning fuel with air in conventional internal combustion engines (Chapter 4). Nonetheless,

vehicle design variables and operational factors act together to determine the levels of emissions. Moreover, vehicle design variables are interrelated and affect collectively vehicle emissions. Therefore, the impacts of the urban transport system and the real-world road-driving environment on vehicle emissions are complex. The impacts are not explained only by vehicle variables or by the chemical thermodynamic principles.

We acknowledge that vehicle emissions are not only related to vehicle variables and the road-driving environment, but also are interdependent (Chapter 4). Thus, we recognise the necessity to estimate vehicle emissions not only as being related to the physical and operational variables of the vehicle, but also as being interdependent.

In the course of investigating vehicle emissions interdependencies, we relate one emission to explanatory vehicle variables and the other two emissions, as follows:

$$Y_i = E (X_i, Y_j, Y_k) \quad (5 -1)$$

where,

Y_i, Y_j, Y_k : are i, j , and k emissions respectively;

X_i : is a vector of vehicle variables that influence emission i under a specific test drive-cycle.

We limit our research to conventional gasoline-fuelled vehicles in urban driving conditions. We estimate the interdependencies of HC, CO, and NO_x emissions at the macro level, which represents average traffic activities over a trip. We investigate the effects of average traffic conditions and traffic operational variables under several test drive-cycles.

5.3 Empirical Framework for Modelling Emissions Interdependencies

Many variables in the road-driving environment have important influences on vehicle emissions (Chapter 3). Our empirical treatments have two main focuses.

First, is to find a measurable set of exogenous variables that represent traffic variables. Second, is to make sure that the endogenous relationships between emissions are testable.

We write initially the statistical models to investigate the hypothesis of the thesis that emissions are mutually or jointly dependent variables and are related to vehicle variables as shown in equations 5-2:

$$\begin{aligned}
 Y_i &= \alpha + \delta_i X_i + \lambda_{ij} Y_j + \lambda_{ik} Y_k + \varepsilon_i & \lambda_{ij} Y_j + \lambda_{ik} Y_k &\neq 0 \\
 Y_j &= \beta + \delta_j X_j + \lambda_{jk} Y_k + \lambda_{ji} Y_i + \varepsilon_j & \lambda_{jk} Y_k + \lambda_{ji} Y_i &\neq 0 \\
 Y_k &= \gamma + \delta_k X_k + \lambda_{ki} Y_i + \lambda_{kj} Y_j + \varepsilon_k & \lambda_{ki} Y_i + \lambda_{kj} Y_j &\neq 0
 \end{aligned}
 \tag{5-2}$$

Thus, we represent the hypothesis of the thesis, as follows:

$$\mathbf{H_0 : } \lambda_i = \lambda_j = \lambda_k = \mathbf{0}$$

H₀: The null hypothesis is a joint hypothesis that all λ 's slope coefficients are jointly or simultaneously equal to zero

$$\mathbf{H_1 : } \lambda_i \text{ and/or } \lambda_j \\ \text{and/or } \lambda_k \neq \mathbf{0}$$

H₁: The alternative hypothesis; not all λ 's slope coefficients are simultaneously zero

We consider several important issues to estimate parameters of proposed statistical models for inter-relationships among vehicle emissions:

- variables included in the models (Section 5.4);
- the models (Section 5.5): expressions of parameters, dependent variables, independent variables, and emissions; and probabilistic assumptions of the error terms in the model.
- testing the models (Section 5.6)

5.4 Variables in the Road Driving-Environment

One very important aim of the empirical treatment is to identify potential variables for estimating parameters of proposed models. Chapter 3 identifies four classes in the urban transport systems that contribute to vehicle emissions, namely traffic flow conditions, operational conditions, driving behaviour, and vehicle technology. These represent interactions between the urban transport system and vehicle emissions (Figure 3-1 in Chapter 3).

We suggest using these classes to identify variables for testing the hypothesis of the thesis. The variables could either be used directly in the statistical models or could be captured indirectly by contextual variables. We propose using vehicle variables for explanatory direct variables. Also, we consider driving modes, infrastructure designs, and vehicle operational variables for contextual indirect variables of the road-driving environment. We discuss direct variables and contextual variables, as follows:

5.4.1 Direct Variables

The review of the contributions of the urban transport system to vehicle emissions (Chapter 3 and Appendix III) suggests at least 15 variables could give reliable empirical evidences on vehicle technological variables. These represent the vehicle technology group (Figure 3-1 in Chapter 3), and are candidate data for investigations into the empirical treatments, as follows:

- **Vehicle make:** manufacturers use various technologies; vehicle emissions vary with vehicle makes
- **Body size:** various studies suggest that larger vehicles consume more fuel and produce higher levels of emissions.
- **Vehicle weight:** research indicates that the mass of a vehicle is very important in determining fuel consumption, and thereby emissions. Heavier vehicles consume more fuel and produce higher levels of emissions.

- **Engine capacity:** the engine cavity is a significant source for HC; the larger is the engine capacity, the higher the HC emissions.
- **Engine type:** engine configuration affects fuel consumption and vehicle emissions. Engines are configured inline or V-shape; V-shape engines consume more fuel and produce higher emissions.
- **Odometer-reading:** research indicates that the accumulation in vehicle kilometres travelled elevate emissions (Section 3.3.4.3 in Chapter 3).
- **Transmission system type and gears:** vehicles with automatic transmissions consume more fuel than vehicles with manual transmissions and have higher emissions (Wong, 2001). However, this is not necessarily always true, especially in case of vehicles with modern transmission system. Also, fuel consumption depends on several other factors such as, driver behaviour and driving conditions (Touw van der *et al.*, 1983), (Section 3.3.2 and Section 3.3.3 in Chapter 3). Transmissions are either manual or automatic, with manual transmissions have 3 to 5 gears.
- **Presence of an electronic engine management system:** electronic engine systems are capable of adjusting many variables of the engine, e.g., ignition timing, and affect both fuel consumption and emissions.
- **Fuel delivery type:** either a fuel injection system or a carburettor delivers the fuel required to form the air-fuel mixtures. Fuel injection controls the flow of fuel better than a carburettor and has lower emissions.
- **Exhaust gas recirculation (EGR):** EGR re-circulates the flow in the exhaust into the air inlet, which reduces NO_x.
- **Exhaust after-treatment system:** a three-way catalytic converter is the most common type of exhaust after treatment system for gasoline-fuelled vehicles; a catalyst reduces more than 90 percent of HC, CO and NO_x.

- **Oxygen sensor:** oxygen sensors adjust the strength of the air-fuel mixture to a chemically balanced mixture. Chemically correct mixtures are necessary to achieve higher conversion capacity of the three-way catalytic converter.
- **The maintenance status of the vehicle:** several studies have demonstrated that in-service vehicles emit higher emissions than new models. The conditions of several elements in the vehicle, such as level of oil in the engine, level of fluid, level of coolant in the radiator, level of water in the battery, fuel filter, air filter, and spark plugs, indicate the level of maintenance status for a vehicle.

This thesis investigates the potential interdependency among vehicle emissions, but it does not develop any predictive vehicle emissions models. We begin with an exploratory investigation to identify candidate variables for the confirmatory analysis (Chapter 9). The exploratory analysis investigates the power of the identified variables in explaining each of HC, CO and NO_x emissions in turn, in order to establish parsimony in the number of input variables into the models used to test the hypotheses of the thesis (Chapter 10). The thesis employs 3SLS regression to estimate the models (Section 5.5). We use maximum likelihood estimation to estimate all the coefficients in a simultaneous-equations (three equations model) system, each of which relate one emission to exogenous vehicle variables and also to the other two emissions, those which appear in the system as endogenous explanatory variables (see Equations 5-3).

5.4.2 Contextual Variables

It is not possible to represent every operational variable for a vehicle. Therefore, researchers employ test drive-cycles to represent real-world traffic conditions (Section 6.4 in Chapter 6). Candidate observations for HC, CO, and NO_x emissions could be obtained by measuring vehicle emissions under several test drive-cycles. Test drive-cycles represent modal operations at an average vehicle speed over a trip (Sierra Research Inc, cited in Ito *et al.* 2000), and a sub test drive-cycles represent one modal operation (Chapter 6).

Test drive-cycles represent four groups of variables: (i) traffic operational variables, such as speed and acceleration, (ii) infrastructure designs, such as types and designs, and (iii) driving modes, such as cold start or hot stabilised. Also, test drive-cycles represent implicitly driving behaviours.

Various test drive-cycles have different speeds, distances, and times (Chapter 6), and thereby have various degrees of effects on different emissions. Laurikko (1995) illustrated that the levels of emissions depend on test procedures and driving schedules employed. Also, Laurikko (1997) demonstrated that the time required for the catalyst to light off (Appendix III) is strongly related to the test drive-cycle employed. Moreover, Wenzel *et al.* (2000) found that intermittent malfunctions of the vehicle (Chapter 7) induce big variations from one test to another, even with all other things being equal. Consequently, it is unlikely that various test drive-cycles will give identical observations. Nevertheless, upper and lower limits may include all these observations. We suggest that the changes in the levels of emissions with respect to other emissions could be quantified within a band, and indicators could be derived for an emission response to changes with respect to the other emissions.

5.5 Three-Stage Least Squares (3SLS) Model

This section presents the formal model for testing emissions interdependencies. The model includes a system of three simultaneous-equations. In the system of these simultaneous-equations, the jointly dependent variables are HC, CO, and NO_x emissions. HC, CO, and NO_x emissions are endogenous dependent variables, and also are endogenous explanatory variables. They appear on the left hand side (lhs) and the right hand side (rhs) of the system, respectively. The three-stage least squares method uses the two-stage least squares estimated moment matrix of the structural disturbances to estimate all coefficients of the entire system simultaneously (Zellner and Theil, 1962). The system of simultaneous-equations regress endogenous variables, on all exogenous variables, and then uses these regression results to regress the overall equation system, and to estimate all coefficients of the entire equation system simultaneously (Washburn *et al.*, 2001; Zellner and Theil, 1962). As a consequence, the rhs endogenous explanatory

variables are stochastic and are correlated with the disturbance terms, for a detailed description of the 3SLS estimation, see Green (1997).

The simultaneous-equations system is formally defined in Equations (5-3):

$$\begin{aligned}
 HC_n &= \alpha + \delta_i X_{in} + \lambda_{ij} CO_n + \lambda_{ik} NO_{Xn} + \varepsilon_{in} \\
 CO_n &= \beta + \delta_j X_{jn} + \lambda_{ji} HC_n + \lambda_{jk} NO_{Xn} + \varepsilon_{jn} \\
 NO_{Xn} &= \gamma + \delta_k X_{kn} + \lambda_{ki} HC_n + \lambda_{kj} CO_n + \varepsilon_{kn}
 \end{aligned} \tag{5-3}$$

where:

HC_n = hydrocarbons emissions for the n^{th} observation
 CO_n = carbon monoxide emissions for the n^{th} observation
 NO_{Xn} = oxides of nitrogen for the n^{th} observation

$\delta_{in}, \delta_{jn}, \delta_{kn}$ = vectors of variables influencing HC, CO, and NO_X emissions, respectively, for the n^{th} observation

α, β, γ = constant terms for HC, CO, and NO_X equations, respectively, for the n^{th} observation

$\varepsilon_{in}, \varepsilon_{jn}, \varepsilon_{kn}$ = disturbance terms for HC, CO, and NO_X equations, respectively, for the n^{th} observation

$\lambda_{ij}, \lambda_{ik}$ = coefficients for CO and NO_X , respectively, in the HC equation

$\lambda_{ji}, \lambda_{jk}$ = coefficients for HC and NO_X , respectively, in the CO equation

$\lambda_{ki}, \lambda_{kj}$ = coefficients for HC and CO, respectively, in the NO_X equation

The impact of the changes in one of the endogenous variables on another endogenous variable is not the same as the coefficient in any one equation. The changes in the endogenous variables in any one equation will have effects on the endogenous dependant variable for that equation, which in turn will affect the other endogenous variables in the other equations, consequently will affect the whole system of equations. The impact of the changes in one endogenous variable on the other variables is determined through the final equilibrium of the system of equations, which converges to the maximum likelihood estimator.

Three-stage least squares (3SLS) regression is proposed to estimate the coefficients in the entire system of equations, because the right-hand side (rhs) endogenous variables are correlated with the disturbance terms. Ordinary least squares (OLS) regression, which is used in current models, is not appropriate for testing the hypothesis of the thesis for vehicle emissions interdependencies. OLS assumes that (Gujarati, 1995): (i) residuals are uncorrelated with the predicted left-hand side variable, and (ii) residuals are uncorrelated with explanatory variables.

Three stage least squares (3SLS) under the assumption that the error terms are normally distributed gives unbiased and efficient coefficient estimates, and accounts for simultaneous correlation of error terms when solving for the coefficients of the overwhole system (Zellner and Theil, 1962). Full information maximum likelihood (FIML) is equivalent to 3SLS in accounting for simultaneous correlation of error terms. However, the 3SLS method with no constraints imposed converges to the maximum likelihood estimator (Greene, 1998). In addition, the 3SLS method produces a unique set of estimates for the coefficients, and gives the smallest possible value for sums of the residual squares (Gujarati, 1995; Rao, 1971).

5.6 Testing Emissions Interdependencies Models

Model adequacy: the F-test determines the structural stability of the model. If the F-ratio exceeds the critical F-ratio at a level of significance of 0.05, [$F > F_{\alpha}(k-1, df)$], or when probability of the F-ratio is sufficiently low, we reject the joint null hypothesis that the regression coefficients are jointly or simultaneously equal to zero.

Coefficient estimates: the t-value of every explanatory variable determines whether a coefficient is not significantly different from zero and that the variable has no effect on the dependent variables. We retained only the statistically significant coefficients for a level of significance of $\alpha = 0.05$ and confidence interval $(1 - \alpha) = 0.95$. The level of significance, α , is the probability of the hypothesis under the t-distribution. We retain variables that have an absolute t-statistic greater than 1.96, that is equivalent to $(|t| > t_{\alpha/2, df} > t_{0.025, \infty} > 1.96)$.

Significance of emissions interdependencies: t-test determines whether there is enough evidence to suggest that emissions are significantly related. If we reject the null hypothesis, i.e., statistically insignificant regression coefficients, then there is insufficient evidence to reject that emissions are interdependent.

5.7 Concluding Remarks

We present an empirical framework to investigate the hypothesis of the thesis. We propose a regression method that relates an emission to exogenous variables of vehicle variables and endogenous variables of other emissions, to test the hypothesis of the thesis. Three stage least-squares (3SLS) regression is appropriate for testing emissions interdependencies, because: (i) it allows for the simultaneous effects among vehicle emissions since vehicle emissions are inter-related, (ii) it specifies a number of simultaneous equations to estimate the effects of vehicle variables and other emissions under various test drive-cycles, (iii) it converges to the maximum likelihood function, and (iv) it gives consistent estimators. We identify dimensions for potential data to test the hypothesis of the thesis for emissions interdependencies under several test drive-cycles. Contextual variables that capture several driving conditions permit investigations of the thesis hypothesis under several driving modes. In Chapter 6, we explore the actual data obtained and identify suitable sub sets in the data for testing the hypothesis of the thesis.

Chapter Six

The Raw Data

6.1 Introduction

Chapter 6 reports on exploring the veracity of the raw data. It introduces preliminary measures to examine and prepare the raw data for further applications, namely classification and regression trees (CART) and three stage least-squares (3SLS) regression. The chapter presents and appraises the quality of the raw data. It also serves as a scheme for screening the data and for assessing its suitability for testing the hypothesis of the thesis. The chapter describes sourcing the data. It also introduces the test drive-cycles employed for measuring emissions from our sample, and the procedures undertaken for tuning up the vehicles.

6.2 Data Sourcing

The raw data obtained are the outcomes of laboratory-based testing of vehicle emissions in the context of Australian National In-Service Emissions (NISE) study. NISE was undertaken to identify the emissions characteristics of passenger vehicles in Australia. It was managed by Federal Office for Road Safety (FORS) in Canberra between May 1994 and April 1996. We highlight the age of the data, in recognition that the technological characteristics of the vehicles available post 1991 differ from the sample of vehicles considered herein (see Section 6.6, for discussion). NISE includes a sequence of standardised test drive-cycles on a sample of 542 gasoline-fuelled passenger vehicles. Emissions were measured in three specialist laboratories run by New South Wales Environmental Protection Authority (NSW EPA), Environment Protection Authority of Victoria, and Ford Motor Company. We depict in a flow chart the sequence of the programme for measuring emissions of the sample of vehicles, as shown in Figure 6-1.

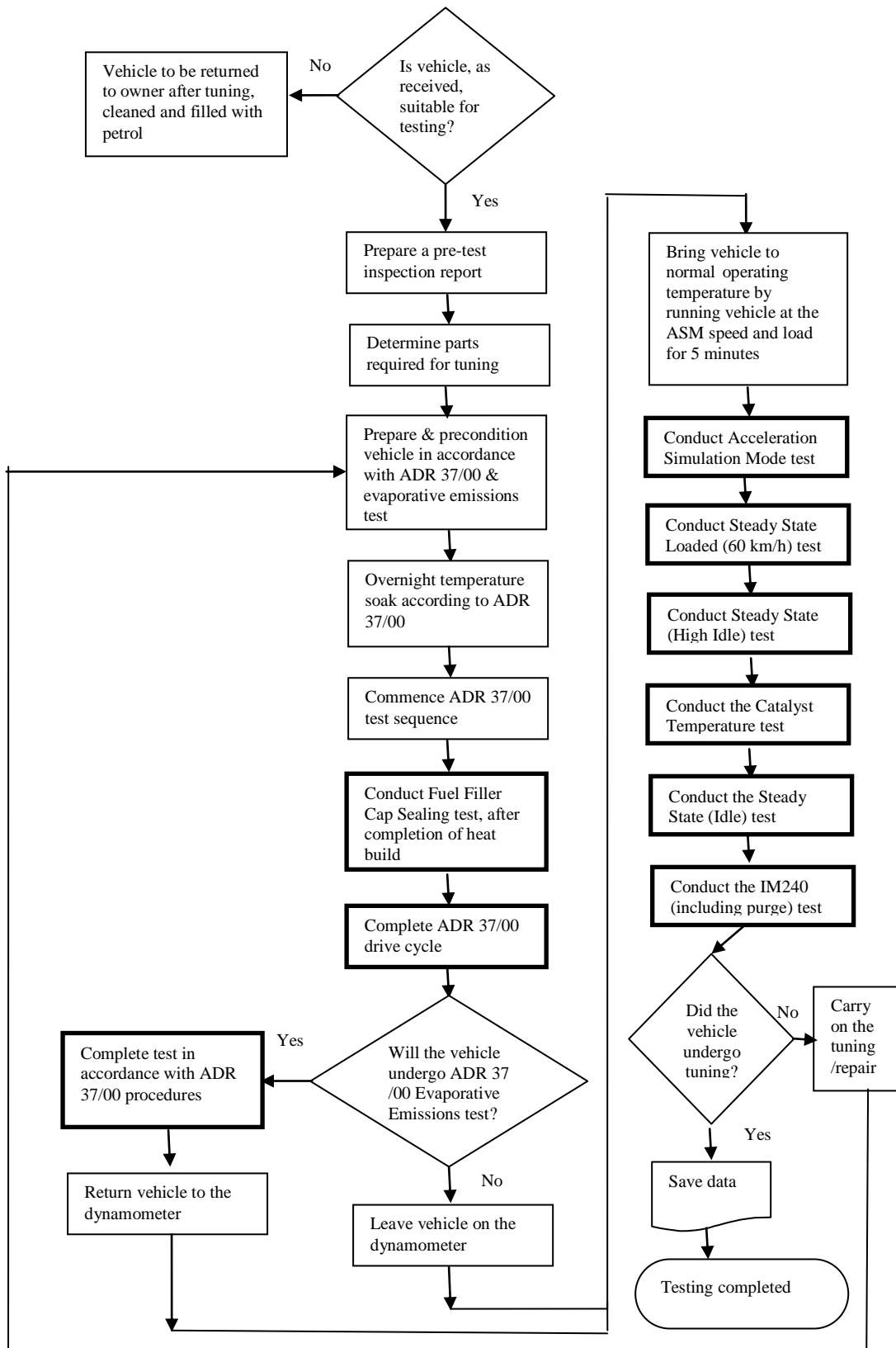


Figure 6-1 The Programme for testing the sample: A Sequence for measuring vehicle emissions

The programme identifies the steps taken before and during testing the sample of vehicles on a chassis dynamometer. One important step is preconditioning. It specifies the soak duration, temperature of the fuel, fuel type (indolene or tank fuel), quantity of the fuel (half or full tank), and Reid vapour pressure (RVP) of the fuel (Fomunung, 1999; FORS, 1996). The test fuel used in the sample has the following specifications (FORS, 1996): research octane number (RON) = 91.3, lead content = 0.002 g/l, sulphur content = 0.02 percent by mass, Reid vapour pressure (RVP) = 76.5 kPa, volatility index = 102.8, benzene content = 4.1 percent by volume, and density at 15 °C = 0.7343 g/ml.

Emissions of hydrocarbons (HC), carbon monoxide (CO), and nitrogen oxides (NO_x) were measured for 542 vehicles, for each of before and after they were tuned. For each of the 542 observations about 40 continuous and categorical variables were measured.

6.3 The Sample

Foreman (1993) designed the sample through a 1993 survey for 6,000 householders in Sydney and Melbourne metropolitan areas. Three thousand householders were surveyed in both Sydney and Melbourne metropolitan areas to obtain 300 vehicles from each city. Foreman (1993) considered two issues when drawing a sample from the population of vehicles in Australia. The two agree with existing literature, such as Wenzel *et al.*, 2000, as follows:

- **sample size:** Any sample size depends mainly on two factors (Wenzel *et al.*, 2000): (i) the shape of the distribution of the collected observations; and (ii) the hypothesis under studying.

Although the sample size of the NISE study needed to be large enough to represent well the population of vehicles in Australia, the sample size was limited to 542 observations. In this regard, two main factors were significant: (i) large costs incurred by laboratory-based testing; and (ii) the limited capacity of the facilities available for testing the sample.

- *selection / response bias*: the sample was randomly chosen from a survey of 6,000 householders. The householders that have more than one vehicle, the next vehicle due for registration was sourced. In order to avoid any sample bias caused by the owners offering the well-maintained one.

The sample consists of 542 gasoline-fuelled passenger vehicles, and each vehicle is required to meet three criteria: (i) vintages between 1980 and 1991, (ii) makes are Holden, Ford, Toyota, Nissan, and Mitsubishi, and (iii) in Sydney or Melbourne metropolitan areas. The makes selected were the most common in-service makes and models in Australia. The vintages between 1980 and 1991 were chosen, because they were numerous on the roads and intensively driven (FORS, 1996). Nonetheless, it was not easy to select a suitable sample from the vintages registered in New South Wales and Victoria between 1980 and 1991, because (Foreman, 1993):

- such sample will not differentiate between responsive and contactable owners in Sydney and Melbourne metropolitan areas that are willing to offer their vehicle for testing;
- it is difficult to locate the owners of the registered vehicles; and
- it is expensive and cumbersome to prepare tables by make and year of the current registered vehicles in New South Wales and Victoria. Also, it is cumbersome to link these to the partial census made, so that to obtain an efficient sample size.

Prior to sourcing the sample of vehicles, Foreman (1993) conducted a series of interviews over 20 months. He designed in advance quotas for every vintage and make in the sample (Tables 6-1 and 6-2). The first table shows quotas by make and vintage, and the latter table shows vehicles selected by make, model, size, and number of cylinders.

Table 6-1 The Sample Quota by Make and Vintage

Model year	Holden	Ford	Toyota	Mitsubishi & Nissan
1980 & 1981	19	19	20	9
1982 & 1983	16	20	12	18
1984 & 1985	14	21	11	21
1986	12	26	14	15
1987	13	23	15	15
1988	12	20	18	17
1989	12	21	18	16
1990	12	18	19	16
1991	13	18	21	15

Source: Foreman (1993)

Table 6-2 The Selected Vehicles by Make and Model

Vehicle make	Vehicle model	Vehicle size	No. of cylinders
Ford	Falcon / Fairmont / Fairlane	Large	
	Telstar	Small	
	Laser / Meteor	Small	
	Cortina	Small	
	Escort	Small	
Holden	Commodore / Berlina / Calais / Vacationer		
	Statesman	Large	4 / 6 / V8
	Camira	Large	V8
	Apollo	Small	4
	Astra	Small	4
	Nova	Small	4
	Torana / Sunbird	Small	4
Nissan	Pintara	Small	4
	Bluebird	Small	4
	Pulsar	Small	4
	Datsun 120Y	Small	4
	Datsun 200B	Small	4
Mitsubishi	Magna	Large	4
	Sigma	Small	4
	Colt	Small	4

Vehicle make	Vehicle model	Vehicle size	No. of cylinders
Toyota	Lexcen	Large	V6
	Camry	Large	4 / V6
	Corona	Small	4
	Corolla	Small	4

Source: Foreman (1993)

6.4 Laboratory-Based Testing

Laboratory-based testing measures vehicle emissions through a pre-defined test drive-cycle. A vehicle is mounted on a chassis dynamometer with the wheels in contact with the rollers, which are adjusted to simulate friction and aerodynamic resistances of the vehicle (Figure 6-2). The chassis dynamometer rotates according to pre-defined speeds and distances that simulate traffic conditions and engine loads in urban driving conditions (FORS, 1996). The control panel in front of the driver (Figure 6-2) stores the time-speed profiles of the test drive-cycle in use.

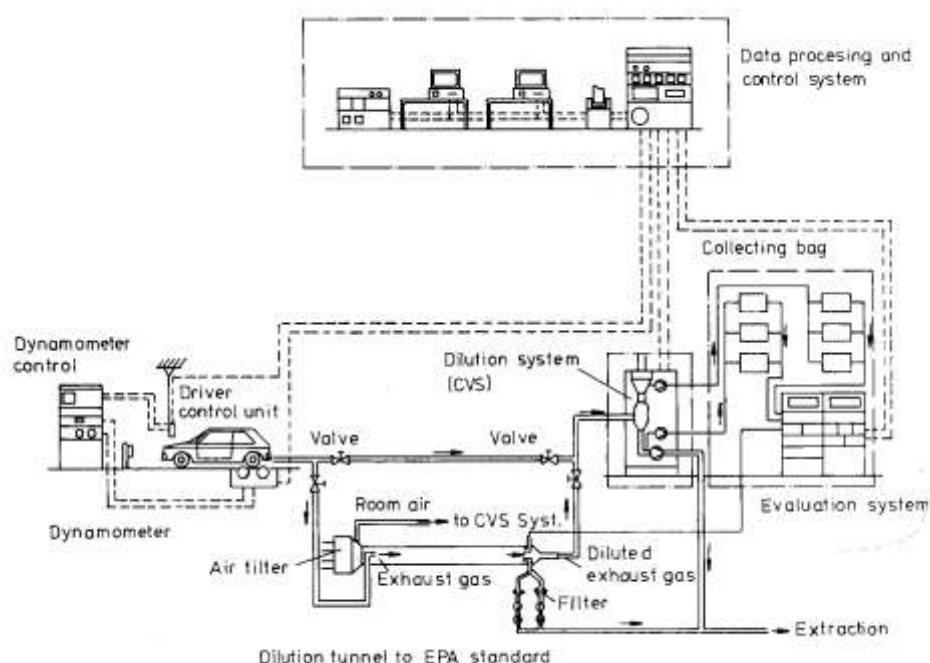


Figure 6-2 The Dynamometer and the System of Emissions Analysis

Source: (Schäfer and Basshuysen, 1995)

We present data obtained (Table 6-3). We also present the main test drive-cycles employed by the three available laboratories for testing the sample (Table 6-4 and Figure 6-3). We also show in the table and the figure other tests, such as catalyst temperature and integrity, fuel filler cap sealing, and chemical treatment process.

Data recorded by the three laboratories include information on several characteristics of the engine and vehicle, and also details of the employed test drive-cycles and the measured emissions (Tables 6-3, 6-4, 6-5). For each of the observations obtained, CO, HC, and NO_x emissions were measured, and over 40 variables were recorded for every observation. Appendix I includes a complete set of the raw data as received, and then tabulated under preliminary schemes. The raw data for each of the 542 observations includes but are not restricted to vehicle and engine characteristics, as follows:

- name of the laboratory
- vehicle make
- vehicle model
- body type
- compliance date
- emission standard
- vehicle mass
- odometer reading
- type of engine management system
- type of air injection system
- engine displacement
- number of cylinders
- gear type
- fuel system type
- choke
- catalyst
- air conditioning
- inertia
- exhaust
- engine oil
- transmission
- radiator coolant level
- battery water level
- fuel filter

Table 6-3 The Collected Data

Feature	Readings
Weight of vehicle (fuel tank full)	weight in kg
Catalyst temperature	in °C at inlet, outlet, and the difference
Flow meter test	total volume of flow (L), at specified points
Bag and raw analysis bench gas calibration	readings for each cylinder from each bench
RPM check	raw analysis bench rpm reading, and corresponding ONO-SOKKI reading
Infra-red temperature check (Raynger PM4 Detector)	comparison of temperature readings between laboratory device and reference device

Source: (FORS, 1996)

Table 6-4 Details of Testing of Vehicles Pre-Tuning and Post-Tuning

No.	Test Name	HC	CO	NO _x	Fuel consumption
ADR 37/00 (FTP)					
Exhaust emissions					
1	Cold Start 505	g	g	g	
2	Transient 867	g	g	g	
3	Hot 505	g	g	g	
4	Full Cycle	g/km	g/km	g/km	L/100 km
5	Steady State Loaded (60km / hr) [SS60]	g/min	g/min	g/min	
6	IM240 Exhaust Emissions	g/km	g/km	g/km	
7	ADR27 Exhaust emissions	g/km	g/km	g/km	L/100km
8	Acceleration Simulation Mode (ASM2525)	ppm	%vol	ppm	
9	Steady State (Idle)	ppm	%vol	---	
10	Steady State (High Idle 2500 rev / min)	ppm	%vol	---	
11	ADR 37/00 evaporative emissions	g/test			
12	ADR 27/00 evaporative emissions	g/test			
13	Catalyst Temperature	temperatures(C) at inlet and outlet of catalytic converter and the difference between two values			
14	Catalyst Integrity	Rattle / no rattle			
15	Fuel Filler Cap Sealing	HC concentration (ppm)			
16	IM240 Purge	Total Volume of Flow (L)			

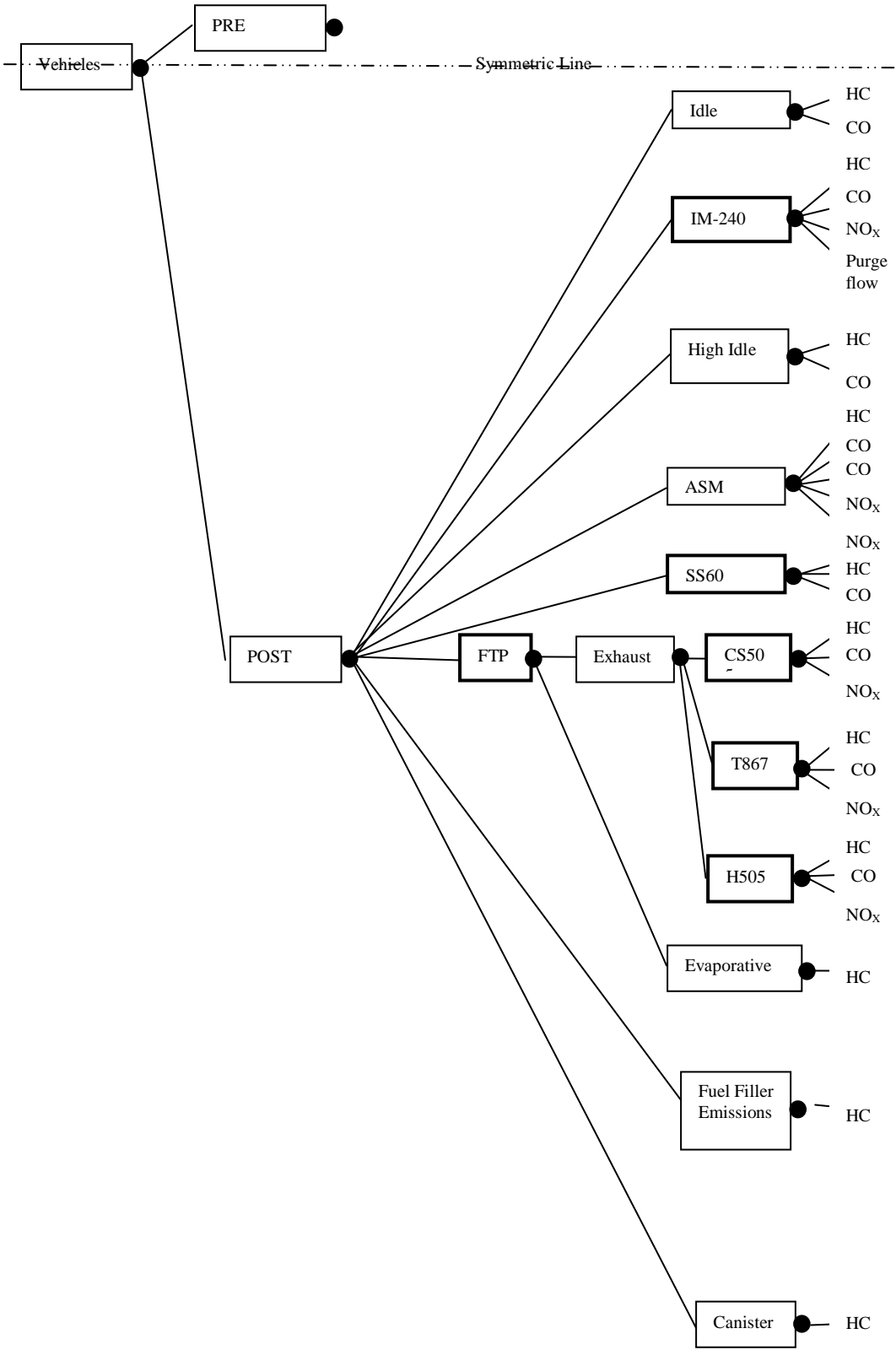


Figure 6-3 A Schematic Diagram of the Test Drive-Cycles Undertaken on the Sample

6.4.1 Test Drive-Cycles

We represent the tests selected for investigating the hypothesis of the thesis. These are the main test drive-cycles employed to measure the emissions of the sample, together with the FTP sub-cycles. FTP sub-cycles consists of three sub-cycles, namely a sub cycle to capture emissions from cold start, another sub cycle to capture emissions from hot stabilised operations, and a third sub cycle to measure transient emissions. We illustrate a complete list of the test drive-cycles employed to measure the emissions of the sample in the available facilities (Table 6-5). We, then, discuss these in the following list:

Table 6-5 The Test Drive-Cycles Employed by NISE Study

Test name	Emissions measured
ADR*37/00 exhaust emissions	CO, HC, NO _x
ADR*37/00 evaporative emissions	<i>HC</i>
IM 240	CO, HC, NO _x , Purge Flow
Acceleration Simulation Mode	CO, HC, NO _x
Steady State Loaded (60 km/h)	CO, HC, NO _x
Steady State (High Idle 2500 rev / min)	CO, HC
Steady State (Idle)	CO, HC

*ADRs require testing according to FTP drive-cycle.

Source: FORS (1996)

- (1) ***Federal Test Procedure (FTP)***: The US environmental protection agency (US EPA) devised FTP in the early seventies. FTP measures the running emissions throughout a pre-defined drive-cycle. The cycle runs for 12 km and up to 94 km/h (FORS, 1996). Also, FTP measures hot soak emissions produced after ceasing driving for a short period. Moreover, FTP measures diurnal emissions of the vehicle sitting inside an enclosed chamber. The exhaust is initially mixed with diluted air, and then three main emissions are collected in three large bags (Wenzel *et al.*, 2000): Bag 1 for cold start emissions, Bag 2 for

transient emissions, and Bag 3 for hot stabilised emissions, as shown in Figure 6-4.

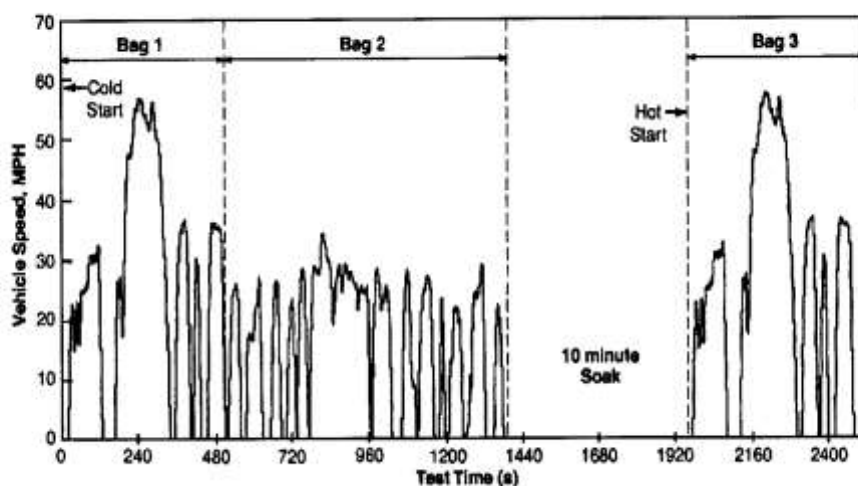


Figure 6-4 Test-Drive Cycle of the Federal Test Procedure (FTP)

Source: Teng *et al.* (2005)

The FTP takes 2467 seconds to complete. It consists of four driving profiles, as follows (FORS, 1996; Kelly and Groblicki, 1993): (i) the first 505 seconds are cold starts, (ii) then 867 seconds are transient operations, (iii) followed by 600 seconds soak period with the engine off, and (iv) the final 505 seconds are hot starts. The driving profile that represents hot stabilised operations is identical to the driving profile that represents cold starts (FORS, 1996).

- (2) ***Steady State Loaded 60 km/h (SS60)***: SS60 is a short test. It measures emissions from a vehicle that is driven on a chassis dynamometer at a constant speed of 60 km/h (FORS, 1996). FORS (1996) considered SS60 the most practical short test for measuring emissions, because its results correlate well with the results of FTP (Table 6-6).
- (3) ***Inspection Maintenance Test (IM240)***: IM240, similar to SS60 is another short test (FORS, 1996). The driving profile of IM240 is identical to the driving profile of the first 240 seconds of the FTP, i.e.,

the first 2 km (FORS, 1996). IM240 measures hot stabilised emissions under transient and loaded modes (Wenzel *et al.* 2000). Both Wenzel *et al.* (2000) and FORS (1996) suggested that the results of IM240 correlate well with the results of FTP test. Moreover, FORS (1996) demonstrated that the results of IM240 are highly correlated with the results of FTP test (see Table 6-6). Wenzel *et al.* (2000) considered IM240 is the most expensive and time-consuming standardised test for measuring vehicle emissions.

Table 6-6 The Correlation of both IM240 and SS60 with FTP

Test drive-cycle	ADR (37/00) according to FTP procedures		
	HC	CO	NO _x
IM240	0.94	0.90	0.90
SS60	0.80	0.84	0.72

Source: FORS (1996)

- (4) **Idle Testing or Steady State Idle:** Similar to both SS60 and IM240, idle testing is another short test. It measures emissions from a stationary vehicle under idle speeds while the accelerator is not pressed down (FORS, 1996). Unlike FTP, idle testing includes neither transient operations nor high loads operations. Thus, it is unsuitable for measuring NO_x emissions, because they are very low under idle testing (Wenzel *et al.*, 2000). The test measures HC and CO emissions under idle conditions, but not under high loads.
- (5) **Acceleration Simulation Mode (ASM2525):** the US state of California measures vehicle emissions under a 2525, i.e., 25 percent of maximum FTP load and at 25 miles per hour. ASM2525 measures HC, CO, and NO_x emissions as the vehicle is driven on a chassis dynamometer at 40 km/h (FORS, 1996). Wenzel *et al.* (2000) considered ASM2525 an improved test over the idle test, because it is capable of measuring emissions for a wide range of engine loads.

- (6) ***High Idle or Steady State High Idle Test***: is an improved test over steady state idle, and is suitable for measuring HC and CO under engine loads and speeds of 2500 revolutions per minute (rpm) (FORS, 1996; Wenzel *et al.*, 2000).

6.4.2 Vehicle Tuning Procedures

Initially, all vehicles in our sample were tested as delivered prior to any repairs made. Repairs do alter the emitting status of vehicles. Each vehicle was tested prior to tuning and before undertaking pre-conditionings. Then, it was tested after tuning and after repairing the fuel and ignition system according to manufacturers' specifications. Faulty components were replaced, provided that the total costs of their replacements are less than A\$150 per vehicle, i.e., less than the allocated budget. Faulty or malfunctioning catalytic converters were not replaced, but faulty oxygen sensors were replaced provided that the budget is available. Also, radiator, transmission, and battery fluids were topped up as necessary. The tuning procedures of vehicles were limited to the following items (FORS, 1996):

- replacing points and air filter;
- replacing fuel filter;
- using (SG20W-50 oil) and replacing oil filter;
- adjusting or replacing spark plugs and gaps, subject to their conditions;
- adjusting function of the distributor;
- adjusting the mixture and the speed of idle operations, when necessary;
- replacing spark plugs and distributor leads, when necessary;
- replacing spark hoses and other minor items in the fuel system, electrical system and emissions control system, as necessary and subject to the allocated budget.

6.5 Exploring the Raw Data

This section reports on exploring the veracity of the raw data. It also reports on preparing the data for further statistical treatments. We first examined the data for any inappropriate values prior to using further applications. We then investigated the data to obtain some intuitions into the validity and consistency of the data.

Validity and Consistency Assessment

We undertake several steps to evaluate the validity of the data, and to establish the consistency of the data, as follows:

- (1) We excerpt comments from NISE report on creditability and suitability for each test and the recorded observations.
- (2) We seek and investigate obvious typing errors, of which were many, and examine almost every data field.
- (3) We identify the percentages of the missing data for each variable, and set missing values to -999, i.e., a missing data code.
- (4) We develop criteria for extracting relevant information from the raw database. We define the criteria based on our objective for testing emissions interdependencies between HC, CO, and NO_x emissions. Thus, we select the tests that contain less than 10 percent missing observations for the three emissions.
- (5) We determine the most significant variables to formulate models to investigate the hypothesis. We also select six tests that meet the criteria for testing the hypothesis of the thesis.

We tabulate test drive-cycles and percentages of missing observations for HC, CO, and NO_x, as shown in Table 6-7.

Table 6-7 Completeness of the Data

	% of missing data					
	Pre-tuning			Post-tuning		
	HC	CO	NO _x	HC	CO	NO _x
ADR 37/00						
Exhaust emissions						
Cold Start 505	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Transient 867	0.00%	0.00%	0.00%	0.00%	0.00%	0.185%
Hot 505	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Full Cycle	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Steady State Loaded (60km/h) [SS60]	0.37%	0.18%	0.37%	1.11%	0.18%	0.37%
IM240	0.55%	0.18%	0.37%	0.00%	0.00%	0.37%
ADR27	66.61%	66.61%	66.61%	66.61%	66.61%	66.61%
Acceleration Simulation Mode (ASM 2525)	8.67%	12.94%	19.40%	9.04%	14.39%	20.11%

The table illustrates the six tests selected to formulate models for estimating vehicle emissions interdependencies, as follows:

- **Test 1:** Federal Test Procedures, sub-cycle, Cold Start 505 “CS505”
- **Test 2:** Federal Test Procedures, sub-cycle, Transient 867 “T867”
- **Test 3:** Federal Test Procedures, sub-cycle, Hot Start 505 “H505”
- **Test 4:** Federal Test Procedures, full cycle total emissions, “ADR 37”
- **Test 5:** Steady State Loaded 60 km/h “SS60”
- **Test 6:** Inspection Maintenance 240 “IM240”

Preliminary Quality Assessment

The raw data were compiled by three testing facilities that are managed by different organisations, namely NSW EPA, EPA V, and Ford Motor Company. Existing literature reported several sources for variability in measurements of emissions (e.g., Millard and Neerchel, 2001), as follows:

- within a laboratory: from one day to another, from one machine to another, from one technician to another, etc.
- *among laboratories*: conditions of the local environment of various laboratories, such as temperature, humidity, barometric pressure, etc.

We find the data are of satisfactory quality despite being collected by three different laboratories. The main data was collected by several entities, namely a consultant who designed the sample, several contractors who tested the sample in three facilities, and another consultant at ANUTECH Pty Ltd., who analysed the data. We believe that minor differences might arise in the testing programme over time, because testing of the sample was undertaken over two years.

We take several steps as deemed necessary to correct any inconsistencies detected in the data. We find inconsistency in the documentation and the description of several variables in the data. In particular, we find some variations between the report of the designer of the sample, i.e., Foreman, 1993, and the report of Federal Office of Roads and Safety, i.e., FORS, 1996. Existing literature has reported several inherent errors associated with observations measured in laboratories, as follows:

- *Measurement errors*, such as human errors, misrepresentation of the sample (e.g., malfunctions, tampering), errors in equipments (e.g., conditions, calibration, and types of the instruments), and laboratory local environment (e.g., lab temperature, lab humidity).
- *Laboratory analytical errors*, such as data manipulations, e.g., human errors, statistical errors, and computer rounding off errors.
- *Data final reporting* such as data recordings, transfer errors, and rounding off significant digits.

6.6 Concluding Remarks

The raw data were of satisfactory quality, apart from some obvious recording errors. The raw data were compiled from the observations obtained by three testing

facilities. Duration of the testing programme over two years could have had effects on the quality of the data. The local environments of the facilities, such as temperature and humidity, might vary over time. The data might include some inherent problems, such as human errors, measuring equipment errors, e.g., instrument conditions, instrument calibration.

After preliminary cleaning and screening the data, we have a subset database that includes six tests, for each of pre and post tuning vehicles. The twelve tests have measurements of HC, CO, and NO_x emissions for more than 90 percent of all observations obtained, i.e., less than 10 percent missing observations. The raw data will not be described further, because the objective of this thesis is testing vehicle emissions interdependencies. We highlight the issue of the age of the data, and acknowledge that it is possible that the technological characteristic of the post-1991 fleet of vehicles is likely to differ from the sample analysed herein. The thesis sample consists of 542 gasoline-fuelled passenger vehicles, which belong to the technological group of vehicles of the model year range between 1980 and 1991. Over time, vehicles employ improved advanced technologies, such as advanced electronic management systems and on board computers, improved fuel delivery systems and air injection systems, and improved oxygen sensors (see Tables 8-1 through to 8-5 and also Appendix I, for details of the technologies used in the thesis sample). The sample consists of five vehicle makes, namely, Holden, Ford, Toyota, Mitsubishi and Nissan, and in turn each make consists of several models. It is also possible that more recent makes / models may have better designs and respond to more demanding design rules than the older makes / models that considered herein, especially with regards to fuel consumption, efficiency and durability of emission control systems. Appendix I presents the raw data as received and under preliminary coding. Chapter 8 describes the variables used to set up the models of vehicle emissions interdependencies. It also includes processing the data for the applications of the formal analysis.

Chapter Seven

Vehicle Emissions from Analytical Perspectives

Observations are generally influenced by three important factors (Branett and Lewis, 1994): (i) inherent variability, (ii) measuring equipments, and (iii) execution. Observations of vehicle emissions are particularly affected by five significant factors (Wenzel *et al.*, 2000): (i) inter- and intra- variability in vehicle emissions, (ii) measuring equipments (iii) the distributions of the observations, (iv) the sample selected to represent the fleet of vehicles and, (iv) the number of times testing is performed on a sub-set of the vehicle fleet.

This chapter represent the discussions on these five factors that are relevant to the observations obtained for this thesis. It discusses inherent variability in vehicle emissions, the differences between measuring methods and measuring equipments, nature of the distributions of observations on vehicle emissions, and extreme observations and outliers.

7.1 Inherent Variability in Vehicle Emissions

Vehicle emissions are naturally variable. The variability in emissions between vehicles or inter-variability in vehicle emissions is influenced by several factors (Wenzel *et al.*, 2000), as follows:

- **Vehicle technology:** emissions vary with various vehicle technologies, with all other things being equal.
- **Vehicle age:** vehicle emissions tend to increase as vehicles age. Vehicle design rules evolve over time, and consequently the performance of fuel consumption and production of emissions improve over time. For example in the US, older vehicle fleets of 10.8 years median age emit 63 percent more NO_x, 73 percent more CO, and 104 percent more VOC than younger vehicle fleets of 5.9 years median age (Miller *et al.*, 2002). Also, vehicle

emissions tend to increase with the accumulation of kilometres travelled. The failure or the degradation of emissions control systems over time play an important role in increasing emissions of older vehicles.

- **Vehicle model / make:** some makes have better designs than other makes, especially with regard to durability and efficiency of emissions control systems.
- **Maintenance-status:** remote sensing studies show that 20 percent of the on-road vehicles are responsible for 80 percent of the HC and CO emissions (Stedman, 2002; Lawson, cited in Singer and Harley, 1996). Various service practices create over time variability in emissions (Guenther *et al.*, 1994). In this regard, two main issues are important: (i) owners' willingness to service regularly their vehicles, and (ii) servicemen's abilities to provide the service according to original manufacturers' specifications. Moreover, tampering with vehicles, such as engine tuning-up, causes further inter-variability in emissions. Maintenance can generally influence the inter-variability in vehicle emissions, as follows (Wenzel *et al.*, 2000):
 - when repairs are not according to manufacturers' specifications, emissions are elevated, and also
 - when servicing is not according to manufacturers' schedules, it causes the engine and after-treatment systems to deteriorate sharply. Thus, emissions are elevated.
- **Driving behaviour:** driving behaviour affects significantly vehicle emissions (Chapter 3). Aggressive driving resulting of both events of enrichments, such as accelerations, and long driving under high power, e.g. pulling repeatedly loads uphill such as a caravan, generates enough heat to damage the catalytic converter, and hence increase emissions.
- **Inter-related malfunctions:** the malfunctions of various elements in one vehicle are inter-related, such as malfunctions of emission control systems. Inter-related malfunctions affect at the same time various emissions, but variably. For example, Wenzel and Ross (cited in Wenzel *et al.*, 2000)

observed that the malfunctioning vehicles that emit higher CO will emit higher HC, whereas those that emit higher NO_x will emit lower CO and HC.

- ***Socio-economics***: the average personal income in an area influence significantly the median vehicle age in the area. For example in the US, Miller *et al.* (2002) demonstrated that vehicle fleets were the oldest in counties with lowest income, and the median vehicle age was 10.8 years. They also found that vehicle fleets were younger in counties with highest income, and the median vehicle age was 5.9 years. Nonetheless, for identical age and vehicle technology the socio-economics of households affect strongly the levels of vehicle emissions (Wenzel *et al.*, 2000). Emissions from vehicles in low-income households are higher than emissions from vehicles in high-income households, because:
 - o high-income householders are more likely to sell vehicles that require frequent repairs, and these will end-up with low-income householders.
 - o high-income householders are more likely to spend more money on maintenance than low-income householders.
 - o high-income householders are more likely to sell vehicles that accumulated higher kilometres travelled, and will end-up with low-income householders.

Additionally, several factors are responsible for the variability in emissions within a vehicle or for intra-variability, as follows (Wenzel *et al.*, 2000):

- ***Intermittent emissions control failures***: malfunctions of emissions control systems, such as catalytic converters, on board computers, fuel delivery systems, and oxygen sensors, are intermittence. Failures in the emission control system, for example, may cause vehicles with partially degraded catalyst converters to emit low emissions under high engine loads.
- ***“Flipper” vehicles***: some vehicles could fail a test, and pass a second test without being repaired, and then could fail a third test. These are flipper vehicles that are often unpredictable, particularly for vehicles with

malfunctioning emission control systems (Wenzel *et al.*, 2004). In a US study in the state of California and Phoenix, Wenzel *et al.* (2004) found that 74 percent of the vehicles tested in Phoenix failed their initial I/M test, and then passed a retest.

- **Engine loads:** engine loads affect significantly the fuel delivered to the engine, and therefore affect vehicle emissions. For example, high engine loads, such as vehicles with air-conditioning, increase NO_x emissions.
- **Thermal conditions of the engine and the catalyst converter:** when the optimal operating temperature of the engine is below normal operating temperature, i.e., between 80 °C and 90 °C, a vehicle will run rich and emit more emissions. In addition, when the optimal operating temperature of the catalytic converter is below 300 °C, a vehicle will produce more emissions, because the catalytic converter will be less effective in converting emissions.
- **Ambient temperatures:** on the one hand, low ambient temperatures increase CO and HC emissions under starting and frequent short stop/starts. During both events, low ambient temperatures cool down the temperature of both the engine and catalytic converter, and thus increase emissions. On the other hand, high ambient temperatures play a secondary role in reducing emissions.
- **Fuel quality:** the chemical composition of fuels has substantial influences on both exhaust and evaporative emissions. The chemical composition of fuels varies generally in different seasons. Some regions specify reformulated fuel as a strategy to control pollution of vehicles.

7.2 Measuring Vehicle Emissions

Vehicle emissions are measured by several techniques. Laboratory-based methods employ test drive-cycles, which are mainly devised for testing light and heavy vehicles, but not motorcycles (Cloke *et al.*, 1998). The test drive cycles employed

do not represent adequately all modes of operations (Zachariadis and Samaras, 1997). Almost all procedures and instruments create inherent variability in the observations of vehicle emissions (Millard and Neerchal, 2001). We review Wenzel *et al.* (2000) and Cloke *et al.* (1998), and summarise briefly several methods for measuring vehicle emissions, as follows:

7.2.1 Tests for Type Approval and Production Conformity

Type approval and conformity of production tests are required by regulations to test all new vehicles. New models are designed to comply with legal limits of emissions (Cloke *et al.*, 1998). Vehicles during productions are tested for conformity, whereas in service vehicles are annually inspected for licensing.

For type approval and production conformity, sampling and analysis of HC, CO, and NO_x are according to two main methods:

- o constant volume sampler (CVS), by which constant proportions of diluted exhaust are collected in a bag of inert material. Then, in order to obtain average various emissions of the test drive-cycle, CO is analysed by infrared absorption, HC by flame ionisation, and NO_x by chemiluminescence; or
- o a sample is fed directly into analysers to read the concentrations of emissions in the exhaust.

Although that type approval tests are standardised, the readings obtained by them are not easily converted to actual emissions. Type approval tests do not also account for various external features of vehicles, such as body, weight, and design shape. Therefore, in order to measure emissions more accurately researchers have developed other methods, such as remote sensing and on-board measurements (7.2.5).

7.2.2 In-Service Inspections

Regulations in many countries require annual inspection for vehicles older than three years (Cloke *et al.*, 1998). In-service inspections, for catalyst-equipped vehicles, measure CO and HC under both idle and high idle test drive-cycles. In-service inspections do not represent adequately emissions from in-use vehicles, because the owners of vehicles service their vehicles only to get them pass the licensing tests once a year. Moreover, in-service tests use cheaper and less accurate equipments than the specialised equipments used in laboratory-based testing.

7.2.3 Laboratory-Based Testing

During laboratory-based testing, a vehicle is driven on power-absorbing apparatus called a chassis dynamometer, i.e., a treadmill for vehicles or an engine test-bed for heavy-duty diesel engines (Cloke *et al.*, 1998); for more details see Section 6.4. Several test drive-cycles are employed for testing emissions, e.g., Federal Test Procedure (FTP), Inspection Maintenance (IM240), Idle testing, and Acceleration Simulation Mode (ASM) (Section 6.4.1 in Chapter 6). Laboratory-based testing controls testing conditions better than other methods (Cloke *et al.*, 1998).

Samples are collected as the vehicle is driven under a standard test drive-cycle. The concentrations of the flow in the exhaust are measured, and therefore the mass emitted is calculated. Various countries use different testing settings, such as various speeds and distances of test drive-cycles, various pre-conditioning procedures, and various equipments (MacLean and Lave, 2003).

Testing vehicle emissions has been shifted from laboratory-based testing to measuring real-world emissions (Wenzel *et al.*, 2000). However, measurements of real-world emissions vary from those measured in a laboratory-based testing. Mensink *et al.* (2000), for example, compared emissions obtained from real-world measurements with those derived from laboratory chassis dynamometer testing, and found that laboratory-based testing overestimate NO_x and underestimate both CO and HC. On the one hand, laboratory-based testing is biased, and is often

undertaken on new or well-maintained vehicles that are only a sub-set of a fleet (Wenzel *et al.*, 2000). In the real world, however, vehicle fleets consist of new, aging, and out-of-state unregistered vehicles. For example, in several US counties, Younglove *et al.* (2004) found that between zero percent and 6.45 percent of the vehicles were unregistered. They found in most of the counties, the unregistered vehicles were less than 5 percent, and in about half of the counties between 2 percent and 4 percent. Also, they found in the State of California that 3.38 percent of light-duty vehicles were unregistered.

On the other hand, testing real-world emissions is a complex process. Several factors contribute to the complexity of testing real-world emissions, such as driving behaviours and the maintenance status of vehicles, in addition to the adequacy of measuring equipments that play a secondary role (Mensink *et al.*, 2000).

7.2.4 Remote Sensing

Remote sensing was developed in the late 1980s, by researchers at the University of Denver (Wenzel *et al.*, 2000). Remote sensing is a non-intrusive technique that remotely measures emissions from vehicles as driven, and without any assistance from the drivers (Stedman *et al.*, cited in Cloke *et al.*, 1998; Wenzel *et al.*, 2000). A study by Sjödin *et al.* (1997) showed that remote sensing could predict fairly accurately CO and HC, but not NO_x.

Nonetheless, remote sensing has several advantages over other testing methods (Stedman *et al.*, cited in Cloke *et al.*, 1998):

- o remote sensing can measure emissions from vehicles as driven on roads over a wide range of operating conditions;
- o it can monitor more than 1000 vehicles an hour a day (v h /day) for speeds between 2 km/h and 200 km/h; and
- o it is cheaper than other time-consuming techniques.

7.2.5 On-Board Diagnostics (OBD)

On-board diagnostics system was developed by several institutes, e.g., the Flemish Institute for Technological Research (VITO) (Lenaers and De Vileger, 1997), and Warren Spring Laboratory (Cloke *et al.*, 1998). The latter uses a sampler attached to the exhaust to measure emissions as vehicles are driven on roads. The sampler is called mini-CVS, because it is a smaller version of the CVS used in laboratory-based testing. Mini-CVS sampling is capable to sample vehicle emissions over a wide range of traffic flow conditions, such as urban, rural, and freeway conditions. Mini-CVS sampling grasps only a small fraction of the total exhaust by using an exhaust splitter. The latter is a passive device used to distribute the total exhaust into a number of identical tubes. Lenaers and De Vileger (1997) found that emissions measured by OBD devices were 10 percent lower than emissions measured by chassis dynamometer. Nonetheless, recent studies (e.g., EPA and Ross *et al.*, cited in Pickrell, 1999) demonstrated that OBD devices could be used to identify malfunctioning vehicles on roads. OBD systems can monitor electronically the performance of emission control systems, such as the efficiency of the catalyst, the response of the oxygen sensor, any evaporating leaks, and injection of fuel (The US National Research Council, cited in Mazzoleni *et al.*, 2004).

7.3 The Shapes of Distributions of Emissions

Inherent variability in vehicle emissions affects the shapes of distributions for the sample. Vehicle emissions are highly skewed even for large samples. Vehicle emissions tend to be positively skewed, similar to lognormal distribution (Millard and Neerchal, 2001). This is due to the fact that the majority of on-road vehicles have relatively low emissions, and a relatively small number of malfunctioning vehicles have extremely high emissions. Remote sensing studies show that 20 percent of the on-road vehicle fleet is responsible for 80 percent of the HC and CO emissions (Lawson, cited in Singer and Harley, 1996). Various emissions and samples do not follow necessarily identical distributions (Wenzel *et al.*, 2000). The distribution shape varies with emissions, vehicle types, and vehicle age.

Despite that, observations are bounded at the lower end by zero and skewed to the right, it does not necessarily imply that the lognormal distribution is the best shape to describe the distribution of vehicle emissions (Millard and Neerchal, 2001).

Several other distributions are skewed to the right and do not fall below zero, such as generalized extreme value, gamma, and weibull. These distributions are similar around the median, and different at the extreme end, i.e., above 90 percentile or 95 percentile. Nevertheless, it is difficult to determine the best shape for skewed observations, because the upper tail of the distribution requires large number of observations (Millard and Neerchal, 2001).

For a showcase, we use the distributions of HC, CO, and NO_x that are measured under the FTP test drive-cycle. The distributions of HC are shown in Figure 7-1 and Figure 7-2, for before and after vehicles were tuned, respectively. Similarly, the distributions of CO, are shown in Figure 7-3 and Figure 7-4, for before and after vehicles were tuned, respectively. Likewise, the distributions of NO_x are shown in Figure 7-5 and Figure 7-6, for before and after vehicles were tuned, respectively.

The figures show clearly that these distributions are not identical to Gaussian normal distribution. Also the figures show that in most cases the distributions are positively right skewed. The figures illustrate that larger number of vehicles have relatively lower emissions and smaller number have extremely higher emissions. This is very clear in the distributions of HC and CO shown in Figure 7-3 and Figure 7-4.

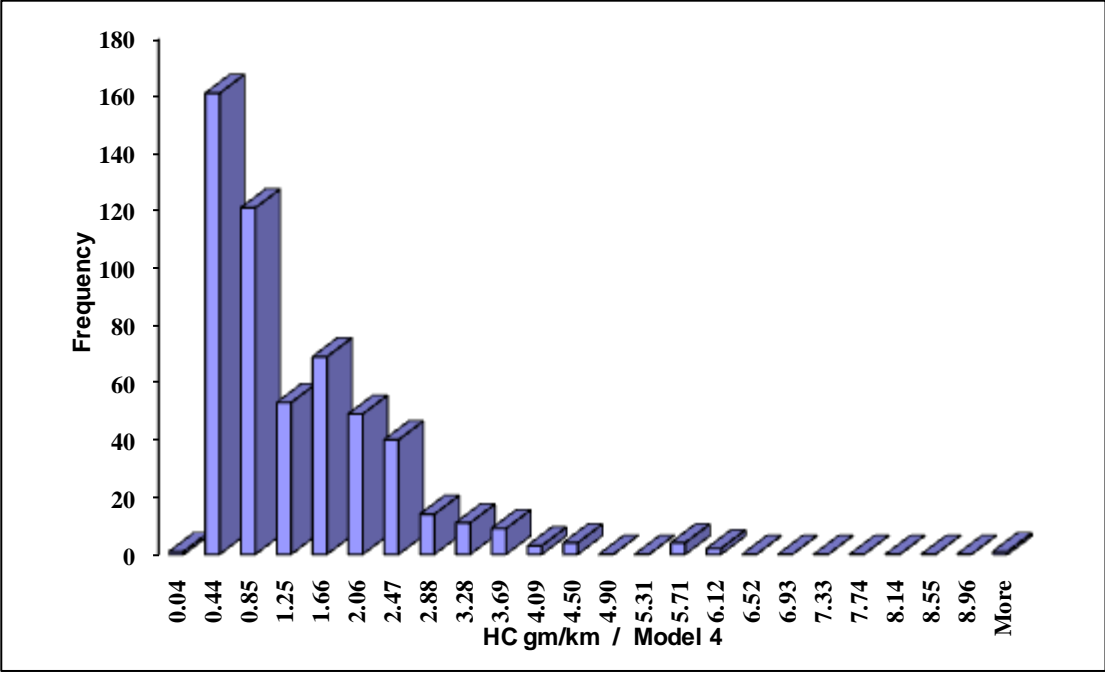


Figure 7-1 The Distribution of HC Measured under FTP Test Drive- cycle: Pre-Tuning

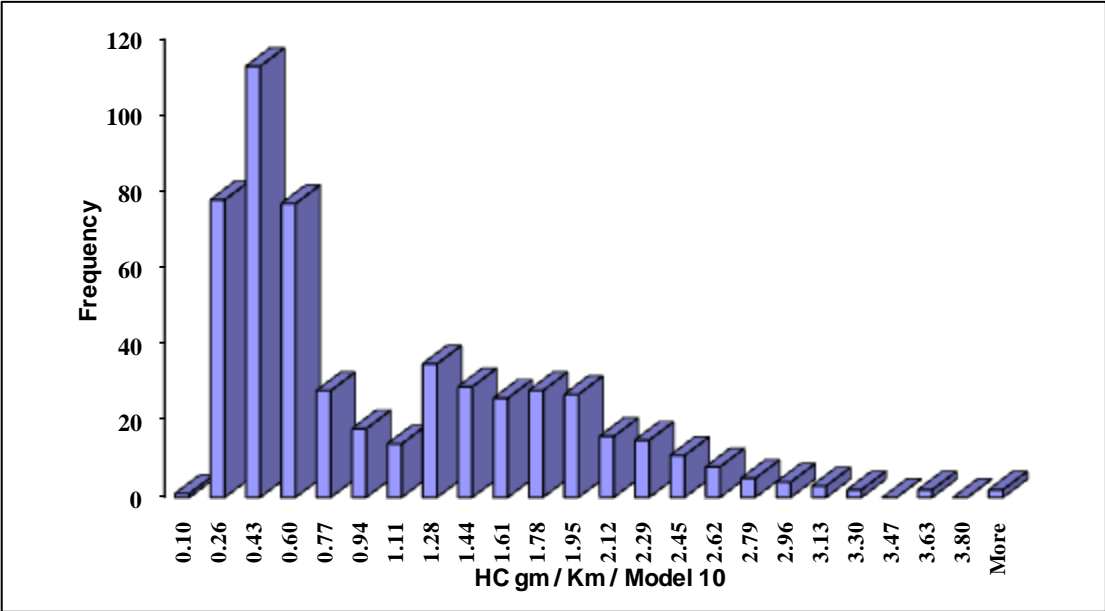


Figure 7-2 The Distribution of HC Measured under FTP Test Drive-Cycle: Post-Tuning

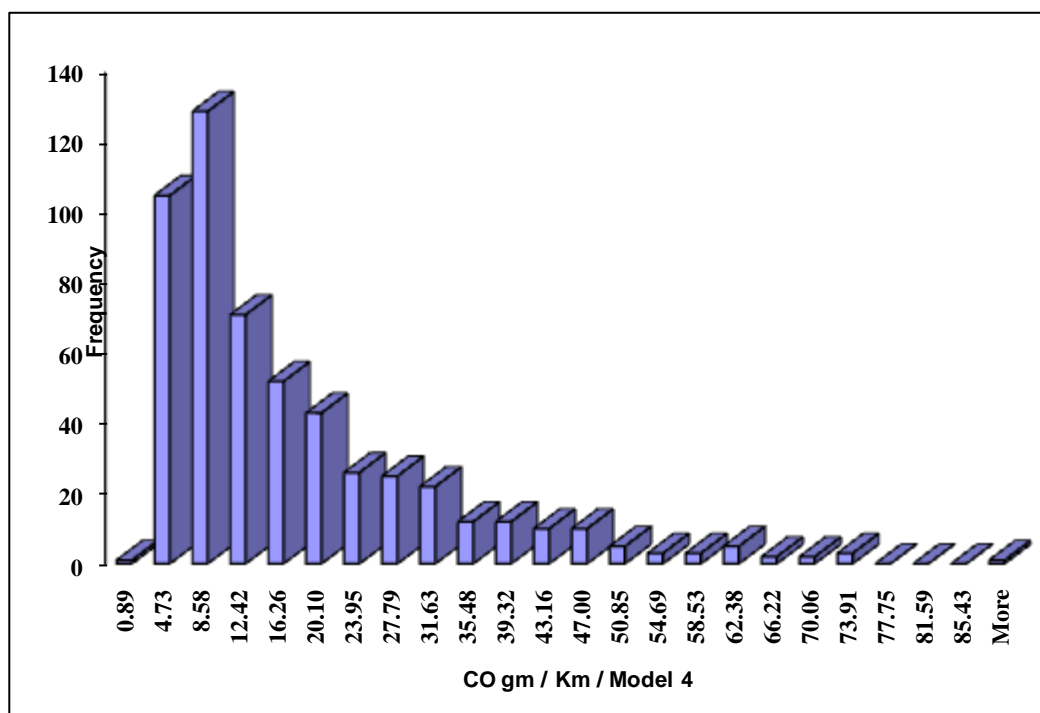


Figure 7-3 The Distribution of CO Measured under FTP Test Drive-Cycle: Pre-Tuning

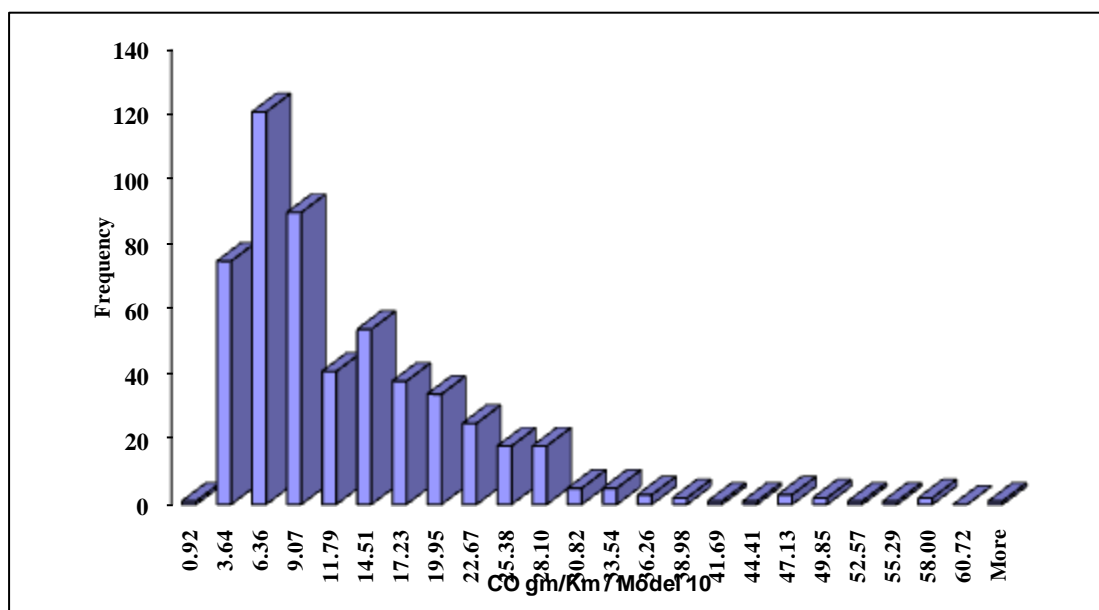


Figure 7-4 The Distribution of CO Measured under FTP Test Drive-Cycle: Post-Tuning

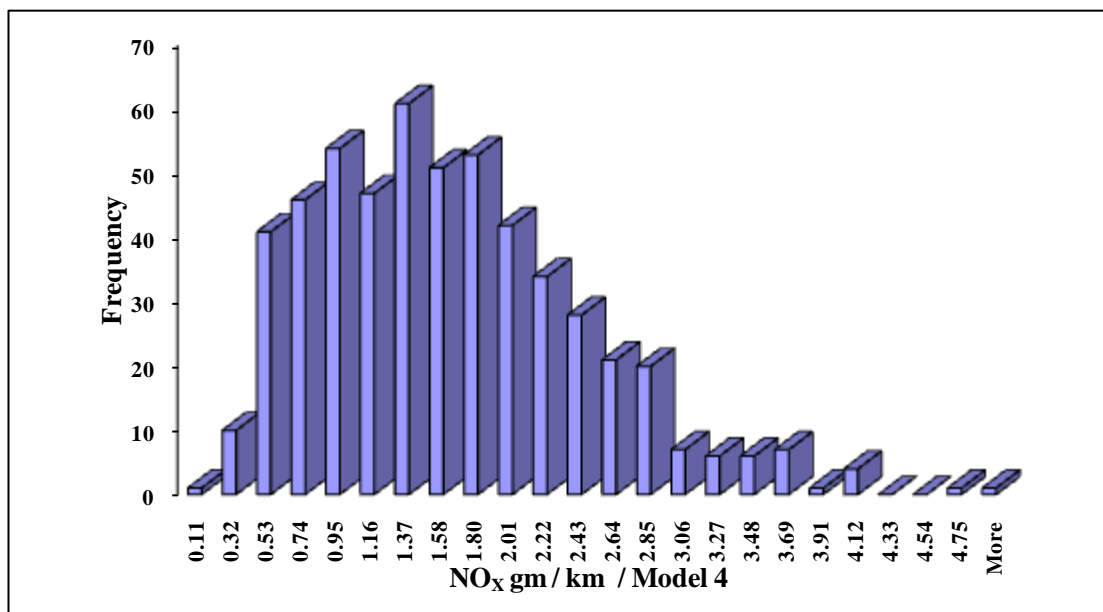


Figure 7-5 The Distribution of NO_x Measured under FTP Test Drive-Cycle: Pre-Tuning

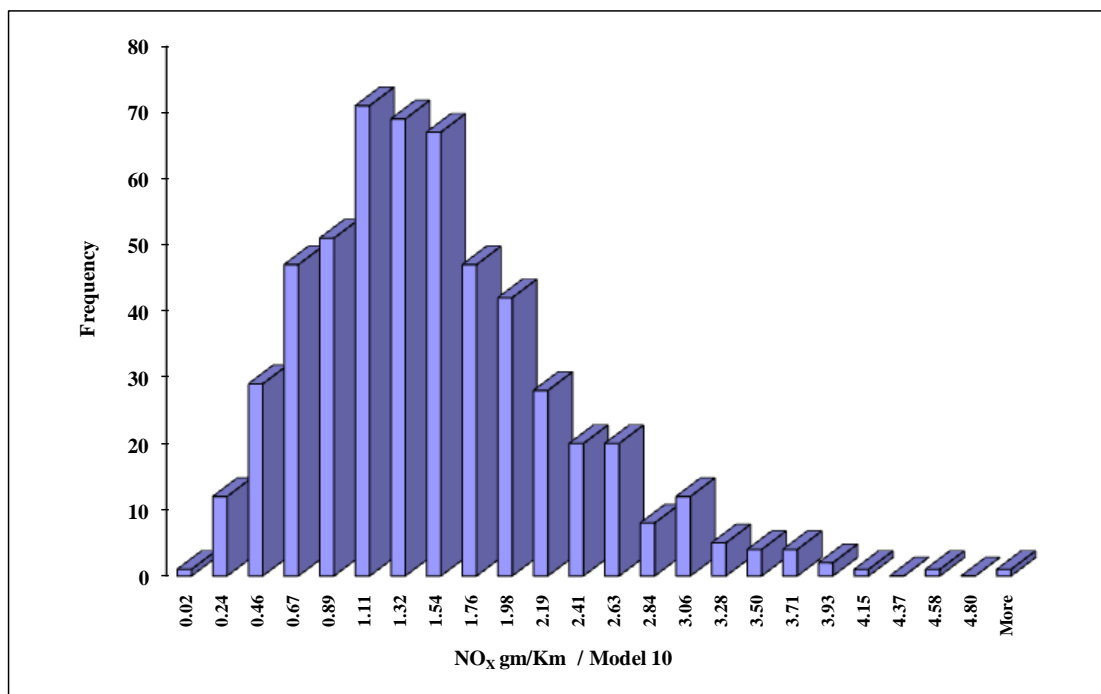


Figure 7-6 The Distribution of NO_x Measured under FTP Test Drive-Cycle: Post-Tuning

7.4 Extreme Observations and Outliers

Data often include unanticipated errors and outliers. Outliers are observations that are inconsistent with the rest of the data (Branett and Lewis, 1994). Outliers could be genuine observations but have extreme values that will distort the shape of the distribution. While outliers may or may not be contaminants, contaminants may or may not be outliers (Branett and Lewis, 1994). Both Millard and Neerchal (2001) and Branett and Lewis (1994) identified three sources of outliers in observations:

- **Deterministic:** outliers are not valid, but are measurements or coding errors.
- **Different Population:** outliers include non-representative observations. These are from different population than the rest of the observations.
- **Random:** outliers are valid, but represent either extreme values or rare event, e.g., ozone.

Table 7-1 Treatments of Outliers

Variation source	Outliers nature	Handling outliers	Actions taken
			Accommodate (in robust non-model-specific estimations or testing)
Inherent			
	Random		Incorporate (in a revised model)
Measurement		Test of discordantly (based on assumed initial distribution)	Identify (for a separate study)
			Reject (initial model inseparable)
	Deterministic (gross measurement or recording error)		
Execution	Observations of a different population		Reject
			Correct
			Repeat

Source: Branett and Lewis (1994)

Outliers are generally identified by several methods (see Barnett and Lewis, 1994). We investigate initially the following methods to determine the cut points of extreme observations for our data:

- **Using visual aids:**
 - o 2-D scatter plots: we plot two dimensional scatter plots, and then identify the cut points for the extreme observations of two emissions at the same time.
 - o histograms: we plot histograms for the emissions distribution to get insights into the approximate shape of the distribution. Also, we draw graphs of the sorted vehicles versus the measurements of emissions in order to obtain the inconsistent observations.

- **Box plots test:** we calculate $1 \cdot \text{IQR}$ and $1.5 \cdot \text{IQR}$ as in some statistical packages (Phipps and Quine, 2001).
 - o **Lower limits (LL):** $Q1 - \text{IQR}$, **Upper limits (UL):** $Q3 + \text{IQR}$
 - o **Lower limits (LL):** $Q1 - 1.5 \cdot \text{IQR}$ **Upper limits (UL):** $Q3 + 1.5 \cdot \text{IQR}$

- **Based on the normal distribution:** we identify the cut points for the extreme observations by using pre-defined percentiles based on the normal distribution of the observations. Previous studies, e.g., Wolf *et al.*, 1998, use 97.73 percentile, i.e., equivalent to the mean plus two standard deviations ($\text{mean} + 2 \cdot \text{Std.}$). Therefore, we exclude all observations that are greater than the ($\text{mean} + 2 \cdot \text{Std.}$).

- **In practice:** extreme observations are identified by judgment. They are impossible to be determined theoretically. The US EPA and CARB, for example, identify the cut points between normal and high emitters by multiplying the standards by a factor (Fomunung, 1999). The US EPA has used 5 times the standards for all emissions, while CARB has used various factors for normal, moderate, high, very high, and super emitters (Fomunung, 1999).

For a showcase, we illustrate the use of the aforementioned methods in two models, namely, Model No. 4 (Pre-Tuning ADR37 FTP test drive-cycle) and Model No. 10 (Post-Tuning ADR37 FTP test drive-cycle), as shown in Table 7-2.

Table 7-2 Comparison between Various Ways for Excluding Extreme Points

Model No.	Model name	Method used	HC	CO	NO _x	No. of Points cut	Remaining No. of points
4	ADR37 Pre-Tuning	visual Aids scale effect, no scale effect,	> 5.0 > 8.0	> 65.0 > 75.0	> 4.0 > 5.0	12 ± 1 2	530 ± 1 540
		Box Plots Q3 + IQR Q3 + 1.5*IQR	> 2.9 > 3.6	> 36.3 > 43.9	> 3.2 > 3.7	52+ 31+	490- 511-
		μ + 5S.d.	> 6.5	> 87.7	> 5.6	1	541
		μ + 2S.d.	> 3.28	> 44.45	> 3.16	23+	519-
10	ADR37 Post-Tuning	visual Aids	> 3.5	> 50.0	> 4.0	10 ± 1	532 ± 1
		Box Plots Q3 + IQR Q3 + 1.5*IQR	> 2.7 > 3.3	> 26.8 > 32.3	> 2.7 > 3.2	34+ 18+	508- 524-
		μ + 5S.d.	> 4.8	> 59.6	> 5.2	1	541
		μ + 2S.d.	> 2.52	> 30.87	> 2.94	22±	520±

The Table highlights the number of observations that are excluded from the sample using four different methods to identify the cut points of extreme observations. It shows, for each of the methods, the value above which an observation is excluded from the original sample, for each of HC, CO, and NO_x. The Table also, shows that the number of the excluded observations is relatively small compared to the original sample size of 542 vehicles. It shows for each of the methods the number of observations excluded and the remaining number of observations in the sample, in turn for each of HC, CO, and NO_x emissions. Table 7-2 calculates the four different methods, as follows:

- **Visual aids:**
 - based on the 2-D scatter plots in Figures 7-7 and 7-8, it identifies initial cut points for HC, CO, and NO_x emissions.
 - taking into account the scale effects of these plots, particularly, in the case of vehicles before were tuned, we map these initial cut points into graphs of sorted vehicles versus the measurements to obtain potential cut points that eliminates any scaling effects.
- **Box plots test:** calculates $1.0 * IQR$ (Interquartile Range) and $1.5 * IQR$.
- **In practice:** we calculate $(\text{mean} + 5 * \text{Std.})$.
- **Based on the normal distribution:** we calculates $(\text{mean} + 2 * \text{Std.})$.

After a close look at the four different methods that identify cut points of the extreme observations, and similar to other studies in the existing literature (e.g., Wolf *et al.*, 1998), we use extreme cut points equal to $(\text{mean} + 2 * \text{Std.})$. We acknowledge that high emitter vehicles are important in terms of urban air-quality, and for estimating total traffic pollution of the vehicle fleets. We consider, in the context of testing the hypothesis of this thesis, super high emitter vehicles are outliers, and therefore we exclude them from the thesis sample. However, the number of vehicles excluded from the sample with respect to the sample size is relatively small. 4.24 % and 4.05 % of vehicles are only excluded from 542 vehicles in the total thesis sample, after using two standard deviations as the cut point, for the two showcase models, namely Model No. 4 (Pre-Tuning ADR37FTP test drive-cycle) and Model No. 10 (Post-Tuning ADR37FTP test drive-cycle), i.e., 23 and 22 vehicles, respectively, (see Table 7-2). The exclusion of outliers concurs with Branett and Lewis (1994), who noted that outliers that are random in nature, can be either rejected or incorporated, especially when an initial distribution is assumed (see Table 7-1). Nonetheless, we also investigate whether the inclusion of outliers in the formal analysis of the data has influenced the results of the models (see Section 10.7 in Chapter 10).

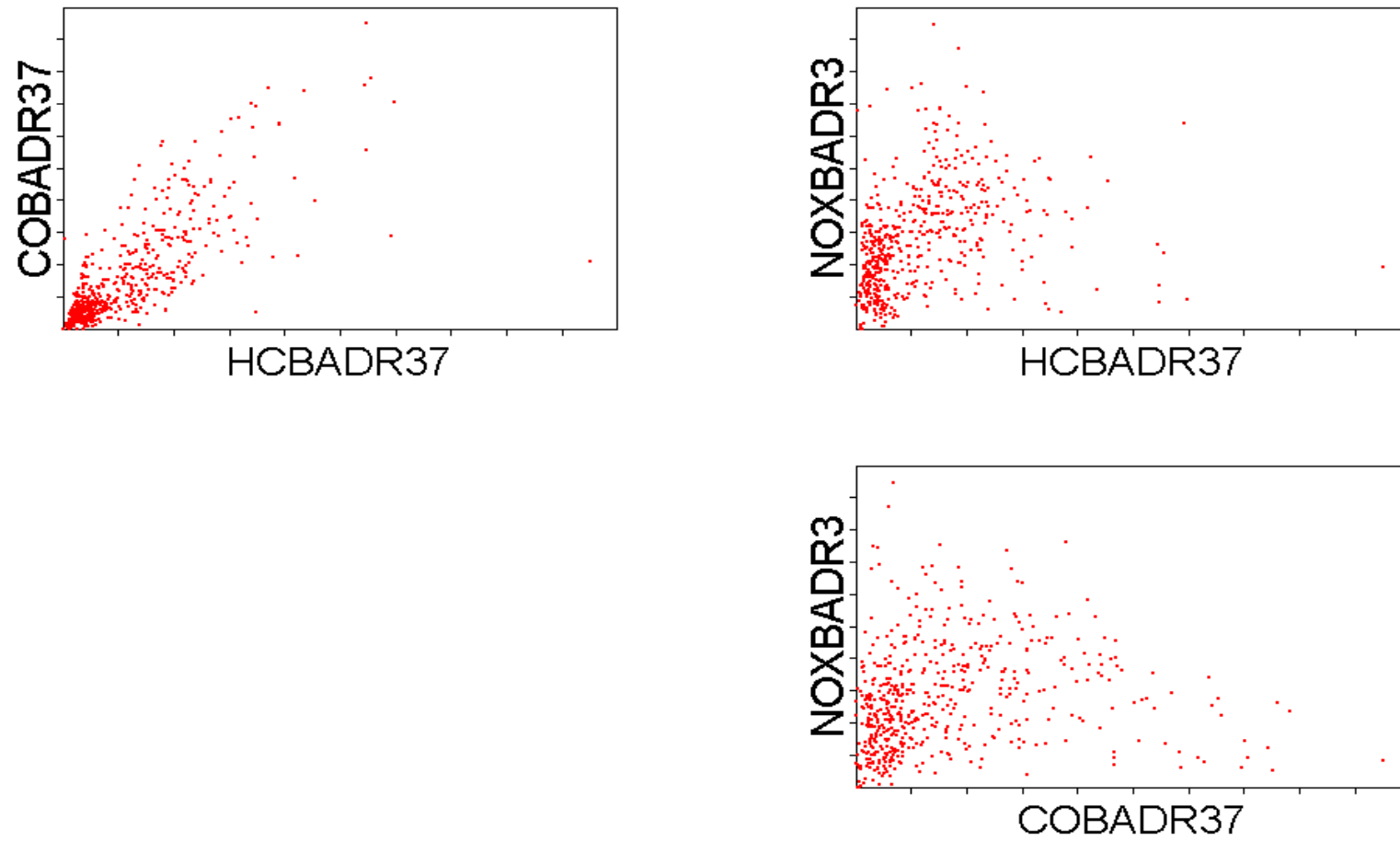


Figure 7-7 2-D Scatter Plot for HC, CO and NO_x under the FTP Test Drive-Cycle Pre-Tuning –M4

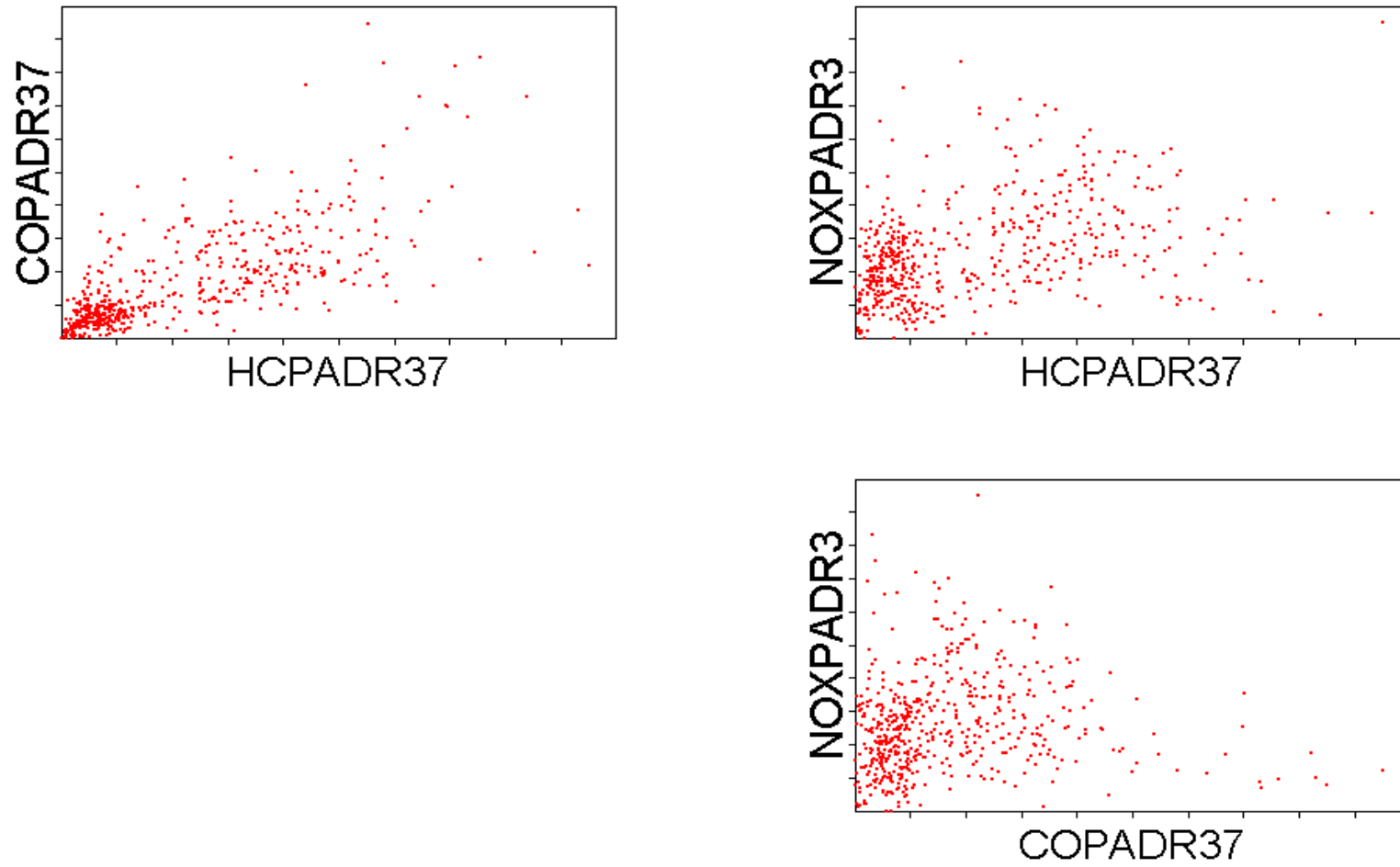


Figure 7-8 2-D Scatter Plot for HC, CO and NO_x under the FTP Test Drive-Cycle Pre-Tuning-M10

We use the normal distribution and original scale variables to screen out outliers, although CO and HC distributions are skewed. The well known central limit theorem (CLT) justifies the use of a normal distribution for large samples. CLT states that for larger n ($n > 25$), $\sum X_i$ is approximately normally distributed as $N(n\mu, \sigma^2)$.

7.5 Concluding Remarks

In this chapter, we review several techniques for testing vehicle emissions and present briefly their advantages and disadvantages. We investigate various methods to determine cut points in order to exclude the extreme observations from the data obtained. We identify the cut points for our observations equal to the mean plus 2 standard deviations (mean + 2 Std.). These cut points for the extreme observations of our data agree with Wolf *et al.* (1998). Observations that are larger than the mean plus 2 standard deviations (mean + 2 Std.) are excluded from the formal analysis of the data obtained. We do, however, investigate whether the inclusion of outliers in the formal analysis of the data has influenced the results of the models (see Section 10.7 in Chapter 10).

Additionally, we list the major points that affect laboratory-based testing (Zachariadis and Samaras, 1997; Samaras *et al.*, cited in Cloke *et al.*, 1998; Wenzel *et al.*, 2000), which is the method of measuring our observations, as follows:

- Vehicle emissions vary inherently among vehicles and within a vehicle.
- A few operating conditions are not represented adequately in the current standardised test drive-cycles (Zachariadis and Samaras, 1997).
- Laboratory-based testing incurs substantial costs. As a result, it uses relatively small samples to represent in-service vehicles. However, the sample size of our observations is relatively not small (Section 6.3 in Chapter 6).

- It is more likely that well-maintained vehicles are over represented in laboratory-based testing. However, our observations obtained are not biased in this sense (see Section 6.3 in Chapter 6).
- Emission measurements vary considerably among various laboratories (Samaras *et al.*, cited in Cloke *et al.*, 1998).
- Laboratory-based testing affects strongly the results of all emissions (Samaras *et al.*, cited in Cloke *et al.*, 1998).
- Laboratory-based testing controls the conditions of testing better than the other methods. The local testing conditions can almost be identically reproduced for various tests.

Chapter Eight

Data Processing and Preliminary Descriptive Analysis

8.1 Introduction

The raw data is processed in two phases. In the first phase, we use preliminary acronyms (Appendix I), which serve to examine the completeness and validity of the raw data. These acronyms are only used for the analysis of relative importance of the variables to predict each of HC, CO, and NO_x emissions (Chapter 9). In the second phase, we process the data prior to testing formally the hypothesis of the thesis (Chapter 8).

Chapter 8 presents the second phase of processing the data. It delineates three steps used to process the data. Also, it describes the coding schemes of the variables under six test-drive cycles, for each of before and after vehicles were tuned. The chapter demonstrates twelve sub-sets drawn from the raw data for the purpose of testing the hypothesis of the thesis. Then, it presents an overview on the descriptive analysis of the outcomes of the observations on HC, CO, and NO_x emissions for 542 vehicles under six test-drive cycles, for each of before and after vehicles were tuned. The chapter concludes with concluding remarks.

8.2 Processing the Raw Data

The raw data obtained is processed in two phases. The first phase was exploratory stage for assessing the validity and consistency of the data (Section 6.5 in Chapter 6). In the second stage, we use three steps in order to draw suitable sub-sets for testing the hypothesis of the thesis for vehicle emissions interdependencies. The three steps that we use concur with Wolf *et al.* (1998). These are as follows:

- (1) **Conversion:** converting the raw data obtained from its existing format to a structure that is suitable for the applications chosen to test the hypothesis of the thesis.

- (2) **Cleaning:** cleaning the raw data obtained, such as dealing with missing observations and using coding-schemes (see Section 8.3 and also see Section 10.2 of Chapter 10).
- (3) **Screening:** screening the raw data obtained for both test drive-cycles and variables that are suitable for testing the hypothesis of the thesis. We screen the data according to the pre-defined criteria in Section 6.5 of Chapter 6. These criteria are based on test drive-cycles, observations obtained, and percentage of non-missing observations.

8.3 Coding-Schemes of the Variables

We present the names, descriptions, and measuring units of the variables that are screened from the raw data, before and after vehicles were tuned respectively, as shown in Tables 8-1 and 8-2. We then tabulate the codes, number of levels, and measuring units of the variables selected, before and after vehicle were tuned, as shown in Tables 8-3 and 8-4 respectively. We also present dummy-codes of the variables before and after vehicles were tuned, as shown in Table 8-5 and Table 8-6 respectively.

We use the schemes of codes for about 50 variables, each of which before and after vehicles were tuned. We use three types of codes, namely variable-codes, dummy-codes and emissions-codes. The variable-codes are used for all the variables including 4 continuous variables, before and after vehicles were tuned. The dummy-codes are used for 20 and 13 categorical variables measured before and after vehicles were tuned respectively. The codes for HC, CO, and NO_x emissions, i.e., the three emissions used to testing the hypothesis of the thesis, vary with various test drive-cycles, as shown in Table 8-8.

Table 8-1 Names, Descriptions, and Types of the Variables: Pre-Tuning

No.	Variable Name	Description	Type
1	HC / Test dependent	HC / Test dependent	numeric
2	CO / Test dependent	CO / Test dependent	numeric
3	NO _x / Test dependent	NO _x / Test dependent	numeric

No.	Variable Name	Description	Type
4	LAB	Laboratory	alpha
5	ID_No	Vehicle allocated number	numeric (categorical)
6	ADR	Emission Standards	numeric (categorical)
7	YEAR	Compliance Data	numeric
8	MAKE	Vehicle Make	alpha
9	BODY	Body Type	alpha
10	ENG_DIS	Engine Displacement	numeric (continuous)
11	N_CYLIND	No. of Cylinders	numeric (categorical)
12	ENG_SIZE	Engine Size	alpha
13	MASS	Vehicle Mass (full tank)	numeric (continuous)
14	INERTIA	Inertia	numeric (continuous)
15	ODOMETER	Odometer	numeric (continuous)
16	ENG_CONF	Engine Configuration	alpha
17	TRANMISN	Transmission	alpha
18	N_GEAR	Number of Gears	numeric (categorical)
19	EEMS	Electronic Engine Management System	alpha
20	EEMS_OPR	Electronic Engine Management System operational	alpha
21	CHOKE	Choke	alpha
22	FUEL_SYS	Fuel System	alpha
23	A_IJ_SYS	Air Injection System Type	alpha
24	O2_SENS	O ₂ Sensor Fitted & Operational	alpha
25	AR_BH_F	Radiator Coolant Level	alpha
26	ENG_OIL	Battery Water Level	alpha
27	FLUID_LV	Fuel Filter	alpha
28	RD_CL_LV	Radiator Coolant Level	alpha
29	BAT_W_LV	Battery Water Level	alpha
30	FUEL_FLT	Fuel Filter	alpha
31	AIR_FLT	Air Filter	alpha
32	PROP_PRT	Fitted Proprietary Parts	alpha
33	AIR_COND	Air Conditioning	alpha
34	EXHAUST	Exhaust Comp Secure	alpha
35	CATALYST	Catalyst Present	alpha
36	CATAL_TS	Test for Catalyst Converter Rattle	alpha
37	EGR_OPER	Exhaust Gaseous Re-circulation	alpha
38	EVP_CANS	Evaporative Canister Fitted	alpha
39	V_HOS_CT	Vacuum Hose Conditions	alpha
40	SPAK_GAP	Spark plug conditions / gap	alpha
41	H_T_LEAD	High Tension Leads	alpha
42	PTS_CONT	Points Conditions	alpha
43	DIST_FUN	Distributor Functional	alpha
44	CAT_I_SH	Inlet to Catalyst Shrouded	alpha
45	CAT_O_SH	Outlet from Catalyst Shrouded	alpha
46	MODIFY	Modifications to Vehicle	alpha

Table 8-2 Names, Descriptions, and Types of the Variables: Post-Tuning

No.	Variable Name	Description	Type
1	HC / Test dependent	HC / Test dependent	numeric
2	CO / Test dependent	CO / Test dependent	numeric
3	NO_x / Test dependent	NO _x / Test dependent	numeric
4	LAB	Laboratory Name	alpha
5	ID_No	Vehicle allocated number	numeric (categorical)
6	ADR	Emission Standards	numeric (categorical)
7	YEAR	Compliance Data	numeric
8	MAKE	Vehicle Make	alpha
9	BODY	Body Type	alpha
10	ENG_DIS	Engine Displacement	numeric(continuous)
11	N_CYLIND	No. of Cylinders	numeric (categorical)
12	ENG_SIZE	Engine Size	alpha
13	MASS	Vehicle Mass (full tank)	numeric (continuous)
14	INERTIA	Inertia	numeric (continuous)
15	ODOMETER	Odometer	numeric (continuous)
16	ENG_CONF	Engine Configuration	alpha
17	TRANMISN	Transmission	alpha
18	N_GEAR	Number of Gears	numeric (categorical)
19	EEMS	Electronic Engine Management System	alpha
20	EEMS_OPR	Electronic Engine Management System operational	alpha
21	CHOKE	Choke	alpha
22	FUEL_SYS	Fuel System	alpha
23	A_IJ_SYS	Air Injection System Type	alpha
24	O2_SENST	O ₂ Sensor after replaced in tune up	alpha
25	AIR_BHT	Air before heat after replaced in tune up	alpha
26	OILT	Oil after replaced in tune up	alpha
27	OIL_FLTT	Oil filter after replaced in tune up	alpha
28	FLUD_LVT	Fluid level after topped in tune up	alpha
29	RD_CL_LV	Radiator Coolant Level	alpha
30	BAT_W_LV	Battery Water Level	alpha
31	FUL_FLTT	Fuel Filter after replaced in tune up	alpha
32	AIR_FLTT	Air Filter after replaced in tune up	alpha
33	PROP_PRT	Fitted Proprietary Parts	alpha
34	AIR_COND	Air Conditioning	alpha
35	EXHAUST	Exhaust after replaced in tune up	alpha
36	CATLYSTT	Catalyst present after tune up	alpha
37	EGRT	Exhaust Gas Re-circulation after replaced in tune up	alpha
38	EVP_CANT	Evaporative Canister after replaced in tune up	alpha
39	SPARKT	Spark plug conditions / gap after replaced in tune up	alpha

No.	Variable Name	Description	Type
40	H_LEADT	High Tension Leads replaced in tune up	alpha
41	POINTST	Points replaced in tune up	alpha
42	DISTFUNT	Distributor replaced in tune up	alpha
43	CAT_I_SH	Inlet to Catalyst Shrouded	alpha
44	CAT_O_SH	Outlet to Catalyst Shrouded	alpha
45	MODIFYCH	Vehicle modifications	alpha
46	PT_T COST	Parts Total cost	Currency (A\$)
47	P_ATCOST	Parts Adjusted Total Cost	Currency (A\$)

Table 8-3 Number of Levels and Measuring Units of the Variables: Pre-Tuning

No.	Variable Name	Units	# of Levels
1	HC / Test dependent	g	-
2	CO / Test dependent	g	-
3	NO _x / Test dependent	g	-
4	LAB	-	3
5	ID_No	random no.	-
6	ADR	-	2
7	YEAR	date	-
8	MAKE	-	5
9	BODY	-	2
10	ENG_DIS	litters	-
11	N_CYLIND	-	2
12	ENG_SIZE	-	3
13	MASS	kg	-
14	INERTIA	kg	-
15	ODOMETER	km	-
16	ENG_CONF	-	2
17	TRANMISN	-	2
18	N_GEAR	-	3
19	EEMS	-	2
20	EEMS_OPR	-	3
21	CHOKE	-	3
22	FUEL_SYS	-	2
23	A_IJ_SYS	-	2
24	O2_SENS	-	2
25	AR_BH_F	-	2
26	ENG_OIL	-	2
27	FLUID_LV	-	2
28	RD_CL_LV	-	2
29	BAT_W_LV	-	2
30	FUEL_FLT	-	2
31	AIR_FLT	-	2
32	PROP_PRT	-	2
33	AIR_COND	-	2
34	EXHAUST	-	2
35	CATALYST	-	2

No.	Variable Name	Units	# of Levels
36	CATAL_TS	-	3
37	EGR_OPER	-	3
38	EVP_CANS	-	2
39	V_HOS_CT	-	2
40	SPAK_GAP	-	2
41	H_T_LEAD	-	2
42	PTS_CONT	-	3
43	DIST_FUN	-	2
44	CAT_I_SH	-	3
45	CAT_O_SH	-	3
46	MODIFY	-	2

Table 8-4 Number of Levels and Measuring Units of the Variables: Post-Tuning

No.	Variable Name	Units	# of Levels
1	HC / Test dependent	g	-
2	CO / Test dependent	g	-
3	NO _x / Test dependent	g	-
4	LAB	-	3
5	ID_No	random no.	-
6	ADR	-	2
7	YEAR	date	-
8	MAKE	-	5
9	BODY	-	2
10	ENG_DIS	litters	-
11	N_CYLIND	-	2
12	ENG_SIZE	-	3
13	MASS	kg	-
14	INERTIA	kg	-
15	ODOMETER	km	-
16	ENG_CONF	-	2
17	TRANMISN	-	2
18	N_GEAR	-	3
19	EEMS	-	2
20	EEMS_OPR	-	3
21	CHOKE	-	3
22	FUEL_SYS	-	2
23	A_IJ_SYS	-	3
24	O2_SENST	-	2
25	AIR_BHT	-	3
26	OILT	-	1
27	OIL_FLTT	-	1
28	FLUD_LVT	-	1
29	RD_CL_LV	-	2
30	BAT_W_LV	-	2
31	FUL_FLTT	-	2

No.	Variable Name	Units	# of Levels
32	AIR_FLTT	-	1
33	PROP_PRT	-	2
34	AIR_COND	-	2
35	EXHAUST	-	2
36	CATLYSTT	-	3
37	EGRT	-	3
38	EVP_CANT	-	3
39	SPARKT	-	2
40	H_LEADT	-	2
41	POINTST	-	2
42	DISTFUNT	-	3
43	CAT_I_SH	-	3
44	CAT_O_SH	-	3
45	MODIFYCH	-	2
46	PT_TCOST	currency	-
47	P_ATCOST	currency	-

Table 8-5 Dummy-Codes of the Variables: Pre-Tuning

Variable Name	Description
	LAB
Lab1	1 if LAB is Ford , 0 otherwise
Lab2	1 if LAB is NSW, 0 otherwise
	MAKE
Make1	1 if MAKE is Ford, 0 otherwise
Make2	1 if MAKE is Toyota, 0 otherwise
Make3	1 if MAKE is Nissan, 0 otherwise
Make4	1 if MAKE is Holden, 0 otherwise
	ENG_SIZE
Size1	1 if ENG_SIZE is small, 0 otherwise
Size2	1 if ENG_SIZE is medium, 0 otherwise
	N_GEAR
Gear1	1 if number of gears is 3, 0 otherwise
Gear2	1 if number of gears is 4, 0 otherwise
	EEMS_OPR
Eems1	1 if No, 0 otherwise
Eems2	1 if Yes, 0 otherwise
	CHOKE
Choke1	1 if choke is Automatic, 0 otherwise
Choke2	1 if choke is Manual, 0 otherwise
	A_IJ_SYS
Air1	1 if Air injection system is AP , 0 otherwise

Variable Name	Description
Air2	1 if Air injection system is PA , 0 otherwise
	AR_BH_F
Preheat1	1 if air preheat fitted is No, 0 otherwise
Prehaet2	1 if air preheat fitted is Yes, 0 otherwise
	CATYST_TS
Ctest1	1 if test for catalyst convertor rattle is No, 0 otherwise
Ctest2	1 if test for catalyst convertor rattle is Yes, 0 otherwise
	EGR_OPR
Egr1	1 if EGR operational is No, 0 otherwise
Egr2	1 if EGR operational is Yes, 0 otherwise
	PTS_CONT
Point1	1 if points conditions is poor, 0 otherwise
Point2	1 if points conditions is OK, 0 otherwise
	CAT_I_SH
Shroudi1	1 if inlet catalyst shrouded = No, 0 otherwise
Shroudi2	1 if inlet catalyst shrouded = Yes , 0 otherwise
	CAT_O_SH
Shroudol1	1 if outlet catalyst shrouded = No, 0 otherwise
Shroudo2	1 if outlet catalyst shrouded = Yes, 0 otherwise

Table 8-6 Dummy-Codes of the Variables: Post-Tuning

Variable Name	Description
	LAB
Lab1	1 if LAB is Ford, 0 otherwise
Lab2	1 if LAB is NSW, 0 otherwise
	MAKE
Make1	1 if MAKE is Ford, 0 otherwise
Make2	1 if MAKE is Toyota, 0 otherwise
Make3	1 if MAKE is Nissan, 0 otherwise
Make4	1 if MAKE is Holden, 0 otherwise
	ENG_SIZE
Size1	1 if ENG_SIZE is small, 0 otherwise
Size2	1 if ENG_SIZE is medium, 0 otherwise
	N_GEAR
Gear1	1 if number of gears is 3, 0 otherwise
Gear2	1 if number of gears is 4, 0 otherwise
	EEMS_OPR
Eems1	1 if No, 0 otherwise
Eems2	1 if Yes, 0 otherwise

Variable Name	Description
	CHOKE
Choke1	1 if choke is Automatic, 0 otherwise
Choke2	1 if choke is Manual, 0 otherwise
	A_IJ_SYS
Air1	1 if Air injection system is AP, 0 otherwise
Air2	1 if Air injection system is PA, 0 otherwise
	AIR_BHT
Preheat1	1 if Air preheated is No, 0 otherwise
Preheat2	1 if Air preheated is Yes, 0 otherwise
	CATLYSTT
Ctaly1	1 if No, 0 otherwise
Ctaly2	1 if Yes, 0 otherwise
	EGRT
Egr1	1 if No, 0 otherwise
Egr2	1 if Yes, 0 otherwise
	EVP_CANT
Evapcan1	1 if Evaporative canister is NA , 0 otherwise
Evapcan2	1 if Evaporative canister is OK , 0 otherwise
	CAT_I_SH
Shroudi1	1 if inlet catalyst shrouded = No, 0 otherwise
Shroudi2	1 if inlet catalyst shrouded = Yes , 0 otherwise
	CAT_O_SH
Shroudo1	1 if outlet catalyst shrouded = No, 0 otherwise
Shroudo2	1 if outlet catalyst shrouded = Yes, 0 otherwise

8.4 Describing the Sub-Sets of the Data for the Twelve Models

We obtain after screening the data, twelve subsets, under six test drive cycles for each of before and after vehicles were tuned. The six test drive-cycles are FTP test drive-cycle, FTP test sub drive-cycles, namely cold, transient, and hot stabilised, inspection and maintenance test drive-cycle, and steady- state loaded test drive-cycle. We tabulate these together with the observations and measurement units of HC, CO, and NO_x emissions for each test drive-cycle before and after vehicles were tuned, as shown in Table 8-7.

Table 8-7 Sub-Sets Drawn from the Data: Twelve Models

No.	Acronym	Test Name	Emissions measured	Unit
Models Pre-tuning				
M1	CS505	Cold Start (505sec)	HC, CO, NO _x	g
M2	T867	Transient (867sec)	HC, CO, NO _x	g
M3	H505	Hot (505sec)	HC, CO, NO _x	g
M4	ADR37	Full Cycle (ADR37)	HC, CO, NO _x	g/km
M5	IM240	Inspection Maintenance (240 sec)	HC, CO, NO _x	g/km
M6	SSL60	Steady State Loaded (60 km/hr)	HC, CO, NO _x	g/min
Models Post-tuning				
M7	CS505	Cold Start (505sec)	HC, CO, NO _x	g
M8	T867	Transient (867sec)	HC, CO, NO _x	g
M9	H505	Hot (505sec)	HC, CO, NO _x	g
M10	ADR37	Full Cycle (ADR37)	HC, CO, NO _x	g/km
M11	IM240	Inspection Maintenance (240 sec)	HC, CO, NO _x	g/km
M12	SSL60	Steady State Loaded (60 km/hr)	HC, CO, NO _x	g/min

8.5 The Descriptive Analysis of HC, CO, and NO_x Observations

Section 8.5 demonstrates a summary of the descriptive statistics of the observations in our sample for testing the thesis hypothesis. The descriptive statistics is based on non-missing observations in the sample of 542 vehicles, for each of HC, CO, and NO_x emissions, as shown in Table 8-8.

Table 8-8 Summary Statistics of the Observations per Test Drive-Cycle

	Pre-Tuning			Post-Tuning		
	HCBCS505	COBCS505	NOXBCS55	HCPCS505	COPCS505	NOXPCS55
Test Drive-Cycle 1 (g)						
Mean	10.21	139.02	11.62	8.75	120.87	10.85
Std.Dev.	7.99	89.69	5.75	5.40	74.47	5.25
Skewness	3.99	1.22	0.83	1.89	1.19	0.70
Kurtosis	32.60	4.17	3.62	8.80	4.21	3.41
Minimum	0.83	19.44	1.25	0.92	8.00	0.19
Maximum	96.48	511.52	34.58	41.91	436.62	32.06
No.Cases	542	542	542	541	541	541

	Pre-Tuning			Post-Tuning		
Test Drive-Cycle2 (g)						
	HCBT867	COBT867	NOXBT867	HCPT867	COPT867	NOXPT867
Mean	6.46	90.13	6.99	5.18	59.95	6.38
Std.Dev.	7.32	106.91	4.32	5.04	64.89	4.24
Skewness	2.74	1.93	0.86	1.04	2.03	1.18
Kurtosis	16.95	7.16	3.74	3.51	8.78	4.97
Minimum	0.04	0.11	0.09	0.07	0.03	0.04
Maximum	70.01	682.22	24.61	27.10	452.73	26.73
No.Cases	542	542	542	542	542	541
Test Drive-Cycle 3 (g)						
	HCBH505	COBH505	NOXBH505	HCPH505	COPH505	NOXPH505
Mean	5.53	65.64	11.00	4.75	49.40	10.07
Std.Dev.	5.18	66.51	6.12	4.18	49.76	5.66
Skewness	1.77	1.85	0.69	1.03	2.54	0.78
Kurtosis	8.18	6.59	3.46	3.36	11.81	3.66
Minimum	0.08	0.52	0.55	0.09	0.15	0.03
Maximum	40.88	362.87	36.65	21.78	330.15	34.09
No.Cases	542	542	542	541	541	541
Test Drive-Cycle 4 (g/km)						
	HCBADR37	COBADR37	NOXBADR37	HCPADR37	COPADR37	NOXPADR37
Mean	1.16	15.63	1.52	0.97	11.71	1.40
Std.Dev.	1.06	14.41	0.82	0.77	9.59	0.77
Skewness	2.20	1.76	0.79	1.00	1.86	0.95
Kurtosis	11.73	6.36	3.64	3.36	7.82	4.32
Minimum	0.04	0.89	0.11	0.10	0.92	0.02
Maximum	9.36	89.28	4.96	3.97	63.44	5.02
No.Cases	542	542	542	541	541	541
Test Drive-Cycle 5 (g/km)						
	HCBIM240	COBIM240	NOXBIM240	HCPIM240	COPIM240	NOXPIM240
Mean	0.81	10.96	1.88	0.72	8.80	1.72
Std.Dev.	0.79	10.67	1.09	0.72	8.79	1.07
Skewness	1.88	1.77	0.70	2.50	2.47	0.64
Kurtosis	9.01	6.32	3.29	19.31	12.53	3.33
Minimum	0.01	0.01	0.01	0.01	0.01	0.00
Maximum	6.19	62.98	5.88	7.79	75.25	5.00
No.Cases	539	541	540	541	541	539
Test Drive-Cycle 6 (g/min)						
	HCBSS60	COBSS60	NOXBSS60	HCPSS60	COPSS60	NOXPSS60
Mean	0.44	6.80	0.85	0.40	5.24	0.83
Std.Dev.	0.55	9.41	0.76	0.51	7.19	0.86
Skewness	3.11	2.13	2.68	2.95	2.02	3.38
Kurtosis	21.30	8.20	17.81	19.29	7.64	23.96
Minimum	0.00	0.00	0.01	0.00	0.00	0.00
Maximum	5.15	55.16	7.85	4.96	45.19	9.03
No.Cases	540	541	539	541	541	541

We examine closely the descriptive statistics of the observations in the sample for testing the hypothesis of the thesis. We examine, particularly, variations in the observations of HC, CO, and NO_x emissions under the screened test drive-cycles (Table 8-7), for each of before and after vehicles were tuned. We compare, firstly, the means, minimum, and maximum of the observations of HC, CO, and NO_x emissions, for each of the test drive-cycles before and after vehicles were tuned (Table 8-8). We expect, according to Section 3.3.4.4 of Chapter 3, the mean, minimum, and maximum observations of HC, CO, and NO_x emissions after vehicles were tuned are less than those before vehicles were tuned, except for NO_x emissions.

However, we note that the mean, minimum, and maximum observations of HC, CO, and NO_x emissions after vehicles were tuned are less than those before vehicles were tuned under all the six test drive-cycles except for the observations obtained under IM240 test drive-cycle (see Table 8-8). We find, under IM240 test drive-cycle, that on the one hand the maximum observation of each of HC, CO, and NO_x emissions, after vehicles were tuned is greater than those before vehicles were tuned (see Table 8-8). We find, on the other hand, that the mean and minimum observations of each of HC, CO, and NO_x emissions after vehicles were tuned are less than those before vehicles were tuned (see Table 8-8).

We then, examine whether the mean observations of HC, CO, and NO_x emissions of a vehicle, especially those observations that have similar units of measurements, are of equal magnitude under all the six test drive-cycles, for each of before and after vehicles were tuned. We note that the mean observations of each of HC, CO, and NO_x emissions under CS505, T867, and H505 test drive-cycles, after vehicles were tuned is less than each of those before vehicle were tuned (see Figure 8-1). Similarly, we note that the mean observations of each of HC, CO, and NO_x emissions under ADR37 and IM240 test drive-cycles, after vehicles were tuned is less than the mean observations of each of HC, CO, and NO_x emissions before vehicles were tuned (see Figure 8-2).

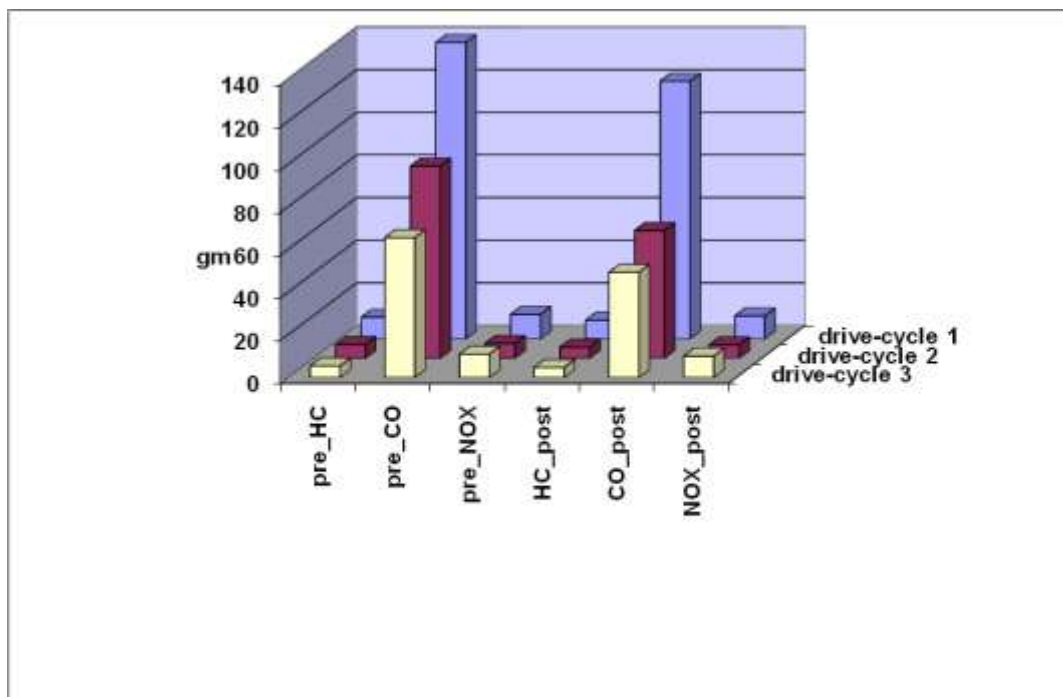


Figure 8-1 The mean of HC, CO, and NO_x Emissions in grams, for each of Pre- and Post-Tuning of Vehicles

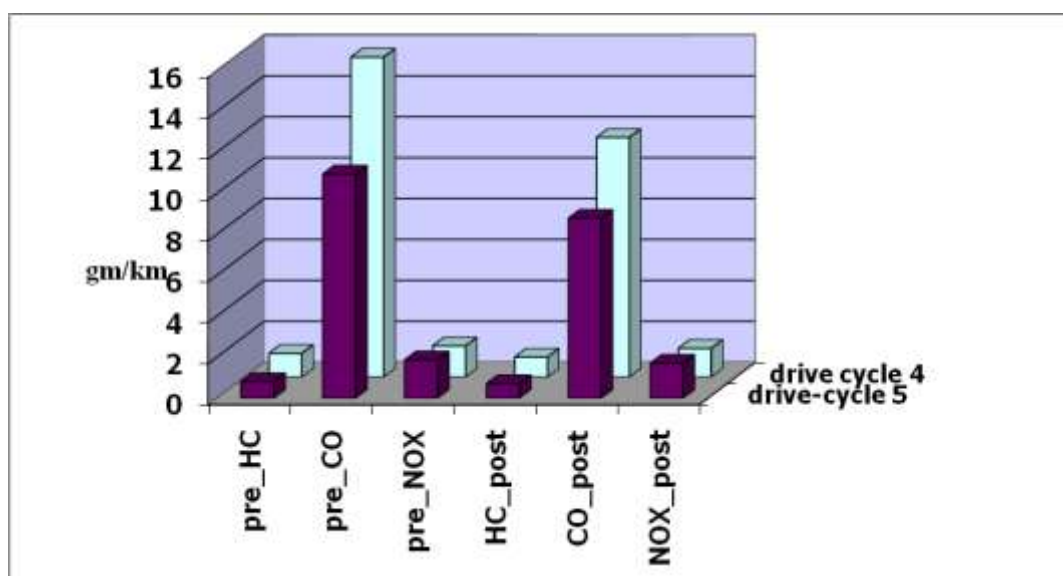


Figure 8-2 The Mean of HC, CO, and NO_x Emissions in grams, for each of Pre- and Post-Tuning of Vehicles

Additionally, we examine whether the identification number (ID) of the vehicle, which exhibits the maximum or the minimum observation of each of HC, CO and NO_x emissions, is the same ID for each of before and after vehicles were tuned (Tables 8-9 and 8-10). We find that it is not necessarily always true, and that the

ID of those vehicles varies with the test drive-cycle employed (Table 8-9 and Table 8-10).

Table 8-9 The Minimum and Maximum of the Observations: Pre-Tuning

Max observation		Data subset 1	
HCB _{CS505}	96.48	24.42	13.83
CO _{bCS505}	175.67	511.52	43.11
NOX _{bCS55}	11.24	3.73	34.58
Vehicle ID	212	1753	215
Vehicle Make	Ford	Ford	Holden

Min observation		Data subset 1	
HCB _{CS505}	0.83	2.03	1.44
CO _{bCS505}	20.38	19.44	49.81
NOX _{bCS55}	5.33	12.10	1.25
Vehicle ID	2256	1669	3489
Vehicle Make	Toyota	Nissan	Ford

Max observation		Data subset 2	
HCB _{T867}	70.01	43.69	8.54
CO _{bT867}	67.82	682.22	32.86
NOX _{bT867}	3.62	2.03	24.61
Vehicle ID	1928	6161	2465
Vehicle Make	Holden	Ford	Holden

Min observation		Data subset 2	
HCB _{T867}	0.04	0.15	0.13
CO _{bT867}	1.10	0.11	0.71
NOX _{bT867}	1.81	3.59	0.09
Vehicle ID	2256	966	1242
Vehicle Make	Toyota	Toyota	Toyota

Max observation		Data subset 3	
HCB _{H505}	40.88	18.97	7.88
CO _{bH505}	73.62	362.87	32.87
NOX _{bH505}	6.83	2.80	36.65
Vehicle ID	1928	1753	2465
Vehicle Make	Holden	Ford	Holden

Min Observation		Data-subset 3	
HCB _{H505}	0.08	0.18	0.35
CO _{bH505}	0.55	0.52	1.68
NOX _{bH505}	1.82	2.94	0.55
Vehicle ID	12055	966	3287
Vehicle Make	Ford	Toyota	Toyota

Max Observation		Data subset 4	
HCB _{ADR37}	9.36	5.39	1.43
CO _{bADR37}	20.78	89.28	7.30
NOX _{bADR3}	1.10	0.53	4.96
Vehicle ID	1928	6161	2465
Vehicle Make	Holden	Ford	Holden

Min Observation		Data subset 4	
HCB _{ADR37}	0.04	0.15	0.13
CO _{bADR37}	0.93	0.89	1.43
NOX _{bADR3}	0.49	1.49	0.11
Vehicle ID	2256	1669	3287
Vehicle Make	Toyota	Nissan	Toyota

Max Observation		Data subset 5	
HCB _{IM240}	6.19	3.82	1.23
CO _{bIM240}	18.26	62.98	8.78
NOX _{bIM24}	1.18	1.08	5.88
Vehicle ID	1928	6204	2465
Vehicle Make	Holden	Ford	Holden

Min Observation		Data subset 5	
HCB _{IM240}	0.01	0.02	0.01
CO _{bIM240}	13.99	0.01	0.04
NOX _{bIM24}	1.61	0.49	0.01
Vehicle ID	214	966	2256
Vehicle Make	Ford	Toyota	Toyota

Max Observation		Data subset 6	
HCB _{SS60}	5.15	5.15	2.50
CO _{bSS60}	55.16	55.16	22.97
NOX _{bSS60}	4.58	4.58	7.84
Vehicle ID	633	633	630
Vehicle Make	Nissan	Nissan	Nissan

Min Observation		Data subset 6	
HCB _{ADR37}	0.00	0.02	0.13
CO _{bADR37}	0.35	0.00	0.61
NOX _{bADR3}	0.02	0.89	0.01
Vehicle ID	2730	2654	6002
Vehicle Make	Ford	Nissan	Ford

Table 8-10 The Minimum and Maximum of all Observations: Post-Tuning

Max observation		Data subset 7	
HCpCS505	41.91	21.68	32.08
COpCS505	279.71	436.62	165.81
NOXpCS55	2.84	7.66	32.06
Vehicle ID	1492	3694	6675
Vehicle Make	Ford	Mitsubishi	Nissan

Min observation		Data subset 7	
HCpCS505	0.92	0.92	2.83
COpCS505	8	8.00	64.96
NOXpCS55	13.23	13.23	0.19
Vehicle ID	6135	6135	8881
Vehicle Make	Toyota	Toyota	Ford

Max observation		Data subset 8	
HCp_T867	27.10	15.35	22.81
COp_T867	172.38	452.73	73.88
NOXp T867	15.18	2.9	26.73
Vehicle ID	6805	1962	6675
Vehicle Make	Ford	Ford	Nissan

Min observation		Data subset 8	
HCp_T867	0.07	0.15	0.09
COp_T867	0.18	0.03	1.00
NOXp T867	0.46	3.6	0.04
Vehicle ID	12055	966	1242
Vehicle Make	Ford	Toyota	Toyota

Max observation		Data subset 9	
HCp_H505	21.78	13.27	19.06
COp_H505	318.31	330.15	70.29
NOXpH505	12.23	3.97	34.09
Vehicle ID	2410	334	6675
Vehicle Make	Ford	Nissan	Nissan

Min Observation		Data subset 9	
HCp_H505	0.09	0.17	0.86
COp_H505	11.09	0.15	19.77
NOXpH505	3.07	3.18	0.03
Vehicle ID	10825	966	8881
Vehicle Make	Ford	Toyota	Ford

Max Observation		Data subset 10	
HCpADR37	3.97	2.35	3.97
COpADR37	15.5	63.44	15.5
NOX pADR3	5.02	0.68	5.02
Vehicle ID	6675	1962	6675
Vehicle Make	Nissan	Ford	Nissan

Min Observation		Data subset 10	
HCpADR37	0.10	0.1	0.17
COpADR37	0.92	0.92	4.63
NOX pADR3	0.83	0.83	0.02
Vehicle ID	7262	7262	8881
Vehicle Make	Holden	Holden	Ford

Max Observation		Data subset 11	
HCpIM240	7.79	7.79	0.16
COpIM240	75.25	75.25	0.72
NOXpIM24	2.48	2.48	5.42
Vehicle ID	1261	1261	1446
Vehicle Make	Holden	Holden	Toyota

Min Observation		Data subset 11	
HCpIM240	0.01	0.02	0.87
COpIM240	0.26	0.01	20.90
NOXpIM24	0.15	0.54	0.01
Vehicle ID	2078	966	458
Vehicle Make	Ford	Toyota	Ford

Max Observation		Data subset 12	
HCp_SS60	4.96	1.66	3.37
COp_SS60	26.81	45.19	21.28
NOXpSS60	4.46	0.27	9.03
Vehicle ID	633	1352	2329
Vehicle Make	Nissan	Ford	Mitsubishi

Min Observation		Data subset 12	
HCpADR37	0.005	0.02	0.15
COp_ADR37	0.002	0.00	2.80
NOX pADR3	0.53	1.3	0.0003
Vehicle ID	2256	17103	8881
Vehicle Make	Toyota	Toyota	Ford

8.6 Concluding Remarks

Chapter 8 presents detailed documentations of processing the obtained raw data, in order to get them ready for testing the hypothesis of the thesis. We use three steps for processing the data, namely conversion, cleaning, and screening. We demonstrate in details the cleaning and screening of the raw data obtained, including detailed coding-schemes of the variables and descriptions of the screened data obtained of twelve proposed models.

The Chapter also presents a preliminary descriptive analysis of the observations. It discusses briefly the observations of our obtained sample under six test-drive cycles employed in measuring HC, CO, and NO_x emissions of the sample. We examine, particularly, variations in the observations of each of HC, CO, and NO_x emissions under the six test drive-cycles, for each of before and after vehicles were tuned. We note that the mean, minimum, and maximum observations for each of HC, CO, and NO_x emissions after vehicles were tuned are less than the mean, minimum, and maximum observations for each of HC, CO, and NO_x emissions before vehicles were tuned. We find that it is true under all test drive-cycles, except under IM240 test drive-cycle. On the one hand, the maximum observations for each of HC, CO, and NO_x emissions after vehicles were tuned are greater than the maximum observations for each of HC, CO, and NO_x emissions before vehicles were tuned. On the other hand, the mean and minimum observations after vehicles were tuned are less than those before vehicles were tuned. Moreover, we investigate whether the mean observations of each of HC, CO, and NO_x emissions of a vehicle, which are of similar units of measurements, are of equal magnitude under all six test drive-cycles, for each of before and after vehicles were tuned. We note that this is not necessarily always true under all test drive-cycles.

Chapter Nine

Analysis of Relative Importance of the Variables Using Classification and Regression Trees (CART)

9.1 Introduction

Chapter 8 reveals that we have more than 40 explanatory variables to estimate each of HC, CO, and NO_x emissions, for each of the proposed twelve models. Therefore, we need to identify, in advance, the variables that have the most explanatory power on each of HC, CO, and NO_x emissions under six test drive-cycles, for each of before and after vehicles were tuned. Tree-structured rules are useful in this context, and they serve to narrow down these variables to the most significant ones in determining each of the emissions.

Chapter 9 uses Classification and Regression Trees (CART) to gain insights into the structure of the data. It also, determines the relative importance of the variables in explaining each of the emissions. The relative importance of the variables assists further in the evaluation of the quality of the data. The Chapter investigates relative importance of the variables in predicting each of HC, CO, and NO_x emissions under six test drive-cycles, for each of before and after vehicles were tuned. It presents the results of the exploratory analysis using CART. At the beginning, we summarise briefly what makes CART an appealing-algorithm. We then present brief discussions on decision trees and the algorithm of CART. After that, we outline the preparation of the data for CART. The chapter concludes with discussions on the main objective of using CART in this thesis.

9.2 CART

Classification and Regression Trees (CART) has been used increasingly by many disciplines. Transport, for example, uses CART in several classification problems, such as, suitability of fuel efficiency in vehicle classifications (Ton and Wang, 1999), and the organisational change of the bus industry (Brewer and Hensher, 1998).

Breiman *et al.* (1984) integrated classification trees into a monograph on classification and regression trees. They included briefly a historical overview on the use of classification and regression trees. They reported that structured trees in regression were first used early 1960s by Morgan and Sonquist in the Automatic Interaction Detection (AID) program. They also mentioned that the concept of classification was introduced in the 1970s by Morgan and Messenger in the THAID program. However, they also added that not until the 1973 when Breiman and Friedman used trees for classification.

This thesis uses CART to identify the relative importance of various variables in influencing HC, CO, and NO_x under six test drive-cycles, for each of before and after vehicles were tuned. The thesis uses CART algorithm, because of its several appealing features (Breiman *et al.*, 1984; Steinberg *et al.* 1995), such as:

- it can be used for any data structure;
- it makes use of conditional information in handling non-homogenous relationships;
- it handles both continuous and categorical variables;
- the algorithm selects automatically the best variables to predict a target variable;
- it estimates classification and misclassification;
- it is invariant under all monotone transformations and robust to outliers and missing observations;
- it displays the final results in the form of a decision tree that is easily interpreted; and
- it can be used for linear and logistic regressions.

9.3 Classification Trees in CART

CART classifies or predicts records in databases (Breiman. *et al.*, 1984; Berry *et al.*, 1997; Steinberg *et al.*, 1995). Each record in a database moves along a path of branches, the flow direction of which is determined by a series of conditional

questions until it reaches a terminal node. We explain classification trees and summarise briefly the technique of CART (Brieman *et al.*, 1984; Berry *et al.*, 1997; and Steinberg and Colla, 1998), as follows:

- (1) **Building the decision tree:** decision trees are grown through binary recursive partitioning. The process dictates that parent nodes are split into two child nodes and the children are further split into two nodes. When a node (t) is split into a left node (t_L) and a right node (t_R), each of the nodes is then searched for the most significant split. After that, CART algorithm chooses the split that separates the data into two partitions based on *YES / NO* responses to conditional questions, such as whether *the condition is less than or equal to a numeric*. There are at most N splits for one continuous variable in a sample of N size, and 2^{L-1} splits for one categorical variable that has L levels.

- (2) **Finding the initial split:** CART carries on a comprehensive search and considers every variable as the best splitter. The best split reduces impurity in the node and has the minimum diversity index (Equation 9-4). Equations 9-1 through to Equation 9-4 demonstrate three common impurity functions, namely Minimum, Gini, and Entropy (Steinberg, 2001). The Gini index tends to favour splits that separate the largest number of cases in a class. While, the entropy index tends to favour balanced splits (Berry *et al.*, 1997). These impurity functions are defined, as follows:

$$i(t) = \text{Minimum } (p_i) \quad (9-1)$$

$$\text{Gini index } i(t) = \sum_i 1 - p_i^2 \quad (9-2)$$

$$\text{Entropy function } i(t) = \sum_i p_i * \log_2 * p_i \quad (9-3)$$

$$\Delta (t,s) = i(t) - p_L * i(t_L) - P_R * i(t_R) \quad (9-4)$$

where: p_L = probability of a class going left,
 p_R = probability of a class going right
 t = node, t_R = right node, t_L = left node
 s = splitting rule

- (3) **Growing the full tree:** CART grows decision trees to the maximum tree using splitting rules and a stopping criterion. CART keeps on looking for the best split until further splitting is impossible because either: (i) there is only one case in the node, or (ii) all the cases are exact copies of each other in the node, and or (iii) there is a few number of cases in the node (< 10 cases). CART classifies the cases in the terminal node according to the rule of plurality, which says that the largest number of cases determine the class of the node.
- (4) **Pruning the tree:** Decision trees are normally grown larger than required. Then, they are pruned back selectively, especially for large trees in order to reduce the linear combination of both accuracy and penalty. The misclassification cost $R(T)$ is calculated according to Equation 9-5:

$$R_{\alpha}(T) = R(T) + \alpha * |\bar{T}| \quad (9-5)$$

where: $\alpha = \text{complexity parameter}$
 $\bar{T} = \text{number of terminal nodes}$

- (5) **Trees testing:** CART divides the sample into learning and test sub-samples, in order to testing the generated trees, provided that there is sufficient data. Alternatively, CART uses the cross validation method to test the generated trees.
- (6) **Building effective predictive models:** the best model is the model that predicts well any new data. Also, it is not necessarily the model with the highest lift of the curve. The model is better, the larger is the area between the curve of the model and the diagonal line (see Section 9.5).

9.4 The Data Preparation for the Application

Although that CART reads and discovers missing and inconsistent records, we investigate the data prior to using CART. We undertake several other measures (see Section 6.5 in Chapter 6) to prepare the data for the applications, as follows:

- (1) We use 8-character acronym, which is consistent, simple, and readable.
- (2) We re-organise the data into 12 sub-sets, six of which were before vehicles were tuned and the other six were after vehicles were tuned.
- (3) We classify HC, CO, and NO_x into four categories. The classifications results are better the fewer are the number of classes. While, more classes causes the variables under considerations to split on every single numeric, and therefore leads to a very bushy tree that runs out of values quickly (Berry *et al.*, 1997).
- (4) We ignore the variables with more than 10 percent missing observations, and only focus on non-missing observations.
- (5) We use the initial results of running CART to obtain insights into the quality of the data, and to fix the data when necessary.
- (6) The initial results of CART serve as a guide to check the raw data for the following: (i) 8-character acronyms; (ii) the levels of categorical variables; (iii) observations with invalid records, such as, (*..0*), *1141..7*, *A to A4*, *RECO to RECONNECTED*, “*Y*” *without the leading space*, *n to N instead*.

9.5 The Analysis of Relative Importance of the Variables

We use CART in the exploratory analyses of the dataset under six test drive-cycles, each of which before and after vehicles were tuned. Then, we investigate the results of the relative importance of the variables in explaining HC, CO, and NO_x emissions. For a showcase, we present the results of using CART for studying HC emissions that is measured under the FTP hot-stabilised sub-drive cycle before vehicles were tuned, namely HC (H505) “CATHCBH5\$”.

CART grows the classification trees of HC under hot stabilised drive-cycle, namely HC (H505) “CATHCBH5\$”, based on the input data of 542 observations and 35 predictors. A typical classification tree is shown in Figure 9-1. The Figure illustrates a scheme of branches and nodes that represent two types of nodes, i.e., splitting and terminal nodes, for the CATHCBH5\$ model. The splitting nodes are shown as filled-in rectangular, and the terminal nodes are shown as a clear

diamond shape. CART examines all possible splits for the input data of 542 observations and 35 predictors (see Table 9-1).

Table 9-1 35 Variables for Predicting HC under FTP Hot (505)

Series Number	Variable Acronym*	Series Number	Variable Acronym
1	MASS	18	ENG_OIL\$
2	ODOMETER	19	FLUID_LV\$
3	ENG_DIS	20	RD_CL_LV\$
4	INERTIA	21	BAT_W_LV\$
5	MAKE\$	22	FUEL_FLT\$
6	MODEL\$	23	AIR_FLT\$
7	BODY\$	24	DIST_FUN\$
8	ENG_SYS\$	25	CATYST_TS\$
9	A_IJ_SYS\$	26	EGR_OPER\$
10	N_CYLIND	27	EVP_CANS\$
11	ENG_CONF\$	28	V_HOS_CT\$
12	GEAR_TYP\$	29	O2_SENS\$
13	FUEL_SYS\$	30	AR_BH_F\$
14	CHOKES\$	31	EEMS_OPR\$
15	CATALYST\$	32	H_T_LEAD\$
16	AIR_COND\$	33	PTS_CONT\$
17	EXHAUST\$	34	MODIFY\$
		35	PROP_PRT\$

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variables is categorical

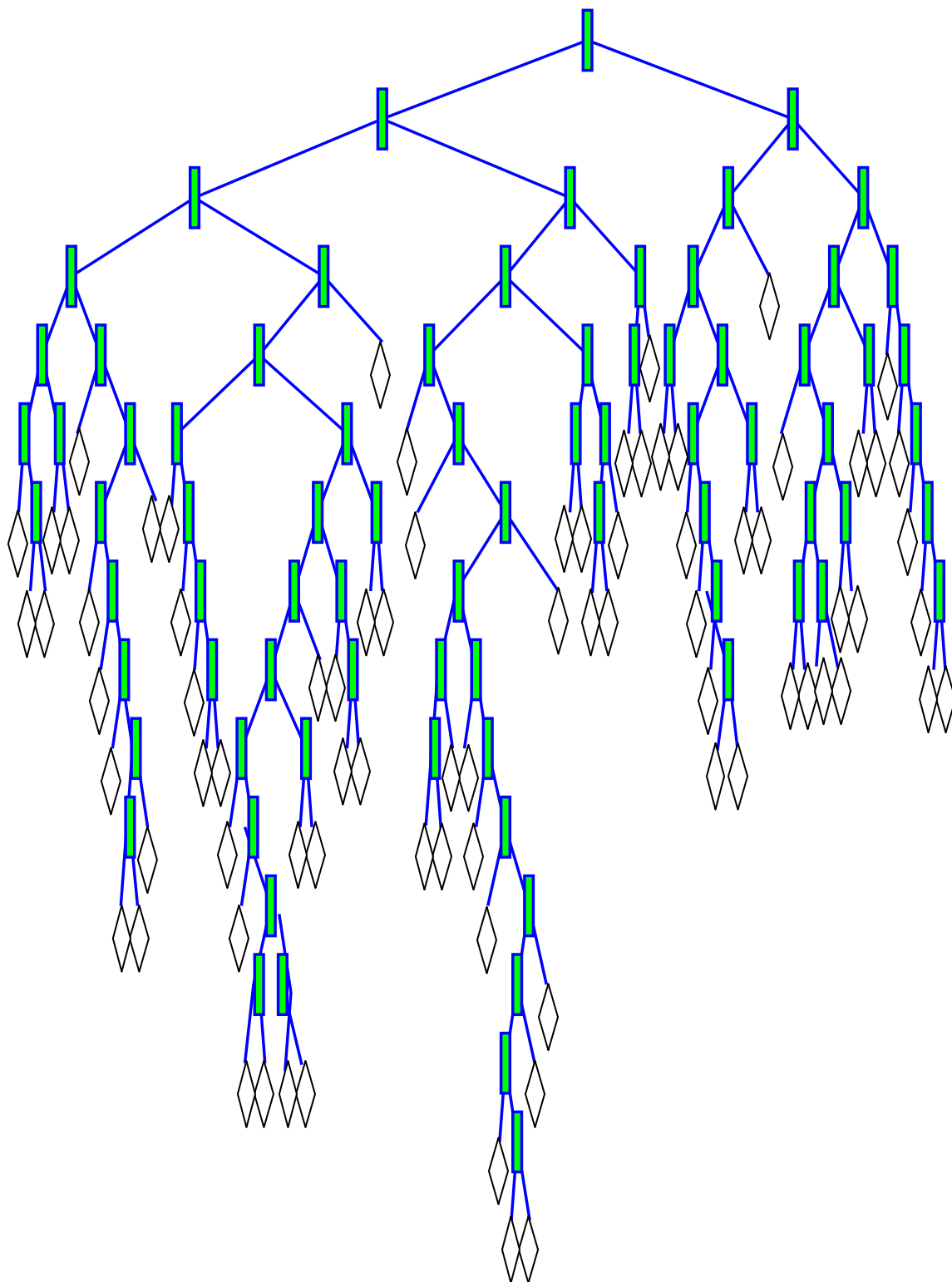


Figure 9-1 Branches and Nodes Scheme for the Classification Tree of HC “CATHCBH5S”

The performance of classification trees is best checked by a prediction success index introduced by McFadden (1979). We use, as a showcase, the chart of cumulative gains for (H505) “CATHCBH5\$”, where the horizontal axis represents the observations. We include in the model (CATHCBH5\$) the variables that yield the larger area between the curve of the model and the diagonal line, as shown in Figure 9-2.

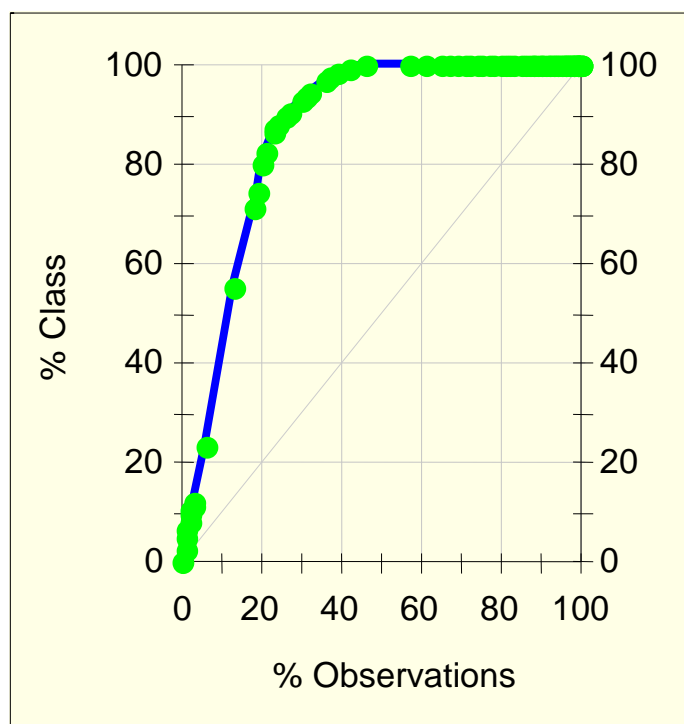


Figure 9-2 Chart of Cumulative Gains for HC (H505) “CATHCBH5\$”

9.6 The Results of Relative Importance of the Variables

Each variable in the classification tree has a score. The score is based on how often and significant a variable is served as a primary or surrogate splitter. The scores of the relative importance of the variables for HC under the FTP hot-stabilised drive-sub cycle before vehicles were tuned are shown in Table 9-2. These reflect the contributions of each variable in predicting HC. The results are the contributions of both the role of the variable in primary splits and its role as a surrogate splitter.

When a primary split is missing, the first surrogate is used instead. If the first top surrogate is also missing, then the second best surrogate is used, etc. The surrogate reduces the mismatch between primary and surrogate splits relative to a primary mismatch. Surrogates are arranged in the order of association, as shown in Equation 9-6 (Steinberg, 2001):

$$\text{Association} = \frac{(\text{Default mismatch} - \text{Surrogate mismatch})}{\text{Default mismatch}} \quad (9-6)$$

Table 9-3 through to Table 9-5 illustrate the scores of relative importance of the variables for HC, CO, and NO_x under the FTP hot stabilised drive-sub cycle before vehicles were tuned. Also, Table 9-6 through to Table 9-9 illustrate the scores of relative importance of the variables for HC, CO, and NO_x under the FTP hot stabilised drive-sub cycle after vehicles were tuned.

Table 9- 2 Relative Importance of the Variables for HC: Pre-Tuning M3

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
1	ODOMETER	100.00	18	FUEL_FLT\$	10.57
2	MODEL\$	96.95	19	O2_SENS\$	9.99
3	CATYST_TS\$	96.50	20	N_CYLIND	9.47
4	CATALYST\$	87.48	21	AIR_FLT\$	6.91
5	EGR_OPER\$	72.82	22	DIST_FUN\$	6.59
6	ENG_DIS	48.78	23	PROP_PRT\$	5.78
7	MASS	47.22	24	H_T_LEAD\$	5.40
8	PTS_CONT\$	47.20	25	ENG_OIL\$	4.66
9	INERTIA	35.47	26	ENG_CONF\$	4.59
10	GEAR_TYP\$	32.11	27	RD_CL_LV\$	4.36
11	EEMS_OPR\$	24.54	28	BODY\$	3.18
12	FUEL_SYSS\$	24.50	29	EVP_CANS\$	3.06
13	ENG_SYSS\$	22.87	30	BAT_W_LV\$	2.82
14	MAKE\$	21.17	31	FLUID_LV\$	2.24
15	A_IJ_SYSS\$	19.95	32	AIR_COND\$	2.03
16	CHOKES\$	12.56	33	MODIFY\$	1.53
17	AR_BH_F\$	12.34	34	EXHAUST\$	1.03
			35	V_HOS_CT\$	0.00

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variables is categorical

Table 9-3 Relative Importance of the Variables for CO: Pre-Tuning M3

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
1	MODEL\$	100.00	18	CATYST_TS\$	13.73
2	MASS	81.50	19	CATALYST\$	13.36
3	EEMS_OPR\$	64.64	20	ENG_OIL\$	12.33
4	ODOMETER	64.25	21	AIR_FLT\$	11.79
5	FUEL_SYSS\$	60.38	22	H_T_LEAD\$	8.85
6	ENG_SYSS\$	57.65	23	ENG_CONF\$	7.88
7	O2_SENS\$	53.40	24	BAT_W_LV\$	6.82
8	ENG_DIS	49.31	25	FLUID_LV\$	6.69
9	CHOKE\$	48.12	26	V_HOS_CT\$	6.59
10	AR_BH_F\$	46.03	27	EXHAUST\$	6.40
11	INERTIA	45.22	28	DIST_FUN\$	3.18
12	N_CYLIND	29.49	29	EVP_CANS\$	2.78
13	MAKE\$	27.39	30	BODY\$	2.76
14	EGR_OPER\$	25.88	31	FUEL_FLT\$	2.69
15	PTS_CONT\$	19.99	32	PROP_PRT\$	2.67
16	A_IJ_SYSS\$	16.36	33	AIR_COND\$	2.15
17	GEAR_TYP\$	16.05	34	RD_CL_LV\$	1.91

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variable is categorical

Table 9-4 Relative Importance of the Variables for NO_x: Pre-Tuning M3

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
1	MODEL\$	100.00	18	EEMS_OPR\$	10.31
2	ODOMETER	73.86	19	EVP_CANS\$	10.21
3	CATALYST\$	71.84	20	FUEL_FLT\$	7.86
4	MASS	71.56	21	PROP_PRT\$	7.78
5	CATYST_TS\$	69.18	22	N_CYLIND	7.64
6	EGR_OPER\$	59.73	23	BODY\$	7.57
7	ENG_DIS	45.18	24	PTS_CONT\$	7.02
8	INERTIA	36.25	25	AIR_COND\$	5.67
9	MAKE\$	19.71	26	V_HOS_CT\$	4.98
10	GEAR_TYP\$	19.66	27	EXHAUST\$	3.71
11	O2_SENS\$	16.73	28	ENG_OIL\$	3.61
12	A_IJ_SYSS\$	15.72	29	BAT_W_LV\$	3.31
13	CHOKE\$	14.84	30	MODIFY\$	3.30

14	FUEL_SYSS\$	14.08	31	AIR_FLT\$	3.25
15	AR_BH_F\$	13.11	32	DIST_FUN\$	2.42
16	H_T_LEAD\$	12.10	33	FLUID_LV\$	2.14
17	ENG_SYSS\$	10.67	34	RD_CL_LV\$	0.78
			35	ENG_CONF\$	0.05

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variables is categorical

Table 9-5 Relative Importance of the Variables for HC: Post-Tuning M9

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
1	MODEL\$	100.00	25	H_T_LEAD\$	9.56
2	CATALYST\$	91.15	26	DCAP_C_T\$	9.04
3	CATYST_TS\$	86.61	27	BODY\$	8.90
4	MASS	76.28	28	PTS_CONT\$	8.45
5	ODOMETER	70.35	29	ENG_OIL\$	7.19
6	EEMS_OPR\$	60.45	30	FCAP_C_T\$	6.70
7	FUEL_SYSS\$	58.88	31	DIST_FUN\$	5.21
8	PTS_CH_T\$	51.20	32	PROP_PRT\$	5.16
9	O2_SENS\$	50.42	33	CTALS_C_T\$	5.08
10	ENG_DIS	34.16	34	EXHAUST\$	4.92
11	INERTIA	30.34	35	AIR_FLT\$	4.65
12	MAKE\$	28.75	36	RBUT_C_T\$	4.60
13	GEAR_TYP\$	25.75	37	AR_BH_AC\$	4.41
14	ENG_SYSS\$	21.46	38	O2SN_C_T\$	3.95
15	EGR_OPER\$	19.52	39	PLG_CH_T\$	3.31
16	HT_LDS_T\$	16.27	40	FLUID_LV\$	3.04
17	EGR_ACT\$	15.59	41	BAT_W_LV\$	1.66
18	FUEL_FLT\$	15.34	42	RD_CL_LV\$	1.45
19	CHOKES\$	14.20	43	ENG_CONF\$	0.90
20	CANS_ACT\$	13.08	44	MODIFY\$	0.78
21	AR_BH_F\$	11.38	45	OLF_CH_T\$	0.00
22	N_CYLIND	11.31	46	ARF_CH_T\$	0.00
23	A_IJ_SYSS\$	11.02	47	AIR_COND\$	0.00
24	EVP_CANS\$	10.99	48	OIL_CH_T\$	0.00

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variables is categorical

Table 9-6 Relative Importance of the Variables for CO: Post-Tuning M9

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
1	ODOMETER	100.00	25	MODIFY\$	8.97
2	MODEL\$	93.67	26	H_T_LEAD\$	8.02
3	MASS	83.72	27	ENG_OIL\$	7.91
4	O2_SENS\$	67.93	28	FUF_CH_T\$	7.87
5	EEMS_OPR\$	62.42	29	EXHAUST\$	7.73
6	CATYST_TS\$	52.61	30	PTS_CONT\$	7.44
7	CATALYST\$	48.49	31	CANS_ACT\$	6.20
8	INERTIA	40.29	32	DIST_FUN\$	5.91
9	ENG_DIS	35.30	33	HT_LDS_T\$	5.69
10	EGR_OPER\$	34.42	34	PLG_CH_T\$	4.75
11	MAKE\$	33.56	35	PROP_PRT\$	4.64
12	PTS_CH_T\$	33.33	36	RBUT_C_T\$	4.39
13	A_IJ_SYSS\$	24.48	37	DCAP_C_T\$	4.11
14	GEAR_TYP\$	24.19	38	FUEL_FLT\$	3.01
15	CHOKES\$	23.06	39	RD_CL_LV\$	2.91
16	ENG_SYSS\$	21.59	40	AR_BH_F\$	2.71
17	FUEL_SYSS\$	17.10	41	AIR_COND\$	2.57
18	BODY\$	16.15	42	CTALS_C_T\$	2.49
19	EGR_ACT\$	13.64	43	FLUID_LV\$	2.41
20	N_CYLIND	13.21	44	FCAP_C_T\$	2.14
21	AR_BH_AC\$	11.26	45	EVP_CANS\$	1.44
22	BAT_W_LV\$	10.52	46	ENG_CONF\$	1.40
23	AIR_FLT\$	10.27	47	OIL_CH_T\$	0.00
24	O2SN_C_T\$	9.51	48	ARF_CH_T\$	0.00
			49	OLF_CH_T\$	0.00

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variable is categorical

Table 9-7 Relative Importance of the Variables for NO_x: Post-Tuning M9

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
1	MODEL\$	100.00	25	ENG_OIL\$	9.83
2	ODOMETER	71.34	26	BAT_W_LV\$	9.13
3	MASS	71.33	27	H_T_LEAD\$	9.02
4	INERTIA	43.79	28	EXHAUST\$	8.67
5	CATYST_TS\$	42.66	29	RD_CL_LV\$	8.43
6	FUEL_SYSS\$	42.40	30	PTS_CONT\$	8.13

Series Number	Variable Name*	Relative Importance	Series Number	Variable Name	Relative Importance
7	EGR_OPER\$	39.71	31	HT_LDS_T\$	8.13
8	O2_SENS\$	36.14	32	BODY\$	8.00
9	CATALYST\$	35.89	33	FCAP_C_T\$	7.68
10	ENG_DIS	35.46	34	PLG_CH_T\$	7.45
11	MAKE\$	34.51	35	RBUT_C_T\$	7.06
12	GEAR_TYP\$	32.76	36	N_CYLIND	6.68
13	PTS_CH_T\$	31.99	37	ENG_CONF\$	6.32
14	AIR_COND\$	30.74	38	AR_BH_AC\$	6.16
15	AIR_FLT\$	24.80	39	O2SN_C_T\$	6.14
16	EEMS_OPR\$	22.14	40	DCAP_C_T\$	5.19
17	AR_BH_F\$	20.99	41	FLUID_LV\$	5.12
18	EGR_ACT\$	19.61	42	PROP_PRT\$	4.50
19	A_IJ_SYSS\$	17.30	43	EVP_CANS\$	4.07
20	CHOKES\$	13.94	44	CTALS_C_T\$	2.54
21	FUF_CH_T\$	13.21	45	CANS_ACT\$	2.24
22	DIST_FUN\$	13.08	46	MODIFY\$	0.95
23	ENG_SYSS\$	12.77	47	OLF_CH_T\$	0.00
24	FUEL_FLT\$	12.08	48	ARF_CH_T\$	0.00
			49	OIL_CH_T\$	0.00

* See Appendix I for variable descriptions

\$ at the end of the acronym indicates the variable is categorical

The findings of the exploratory analysis show that odometer-reading, vehicle model, vehicle mass, fuel system, vehicle make, type of the gear, engine displacement and the number of cylinders all play a significant role in influencing vehicle emissions. We conclude that the variables that have important explanatory power in determining HC also have relatively important explanatory power on both CO and NO_x, but with variable scores. The findings suggest that the factors that have explanatory powers on HC, CO, and NO_x that are closely related.

9.7 Conclusions: Beyond CART

In this chapter, we investigate the relative importance of the variables in explaining each of the three emissions under six test drive-cycles, for each of before and after vehicles were tuned. A bottom-up or a theoretical approach is a

logical initial starting points for determining the input variables into the thesis models, because of the complex effects of the variables on the emissions considered. The use of the theoretical approach concurs with Fomunung *et al.*, (1999). Nonetheless, a theoretical approach is a very complex approach, especially because variables of the vehicles are inter-related. Therefore, CART is used to narrow down the number of input variables to the models formulated for testing the hypothesis of the thesis. CART is used as an exploratory tool to identify the relative importance of the variables in influencing each emission. Variables that scored more than 15 percent are initially used for testing the thesis hypothesis (Chapter 10).

Classification trees are illuminating for exploring the data, and are flexible nonparametric tools for analysing the data (Breiman *et al.*, 1984). CART has shed more light on the structure of the data and its complexity, especially since CART is robust in the presence of missing data, and because the data was compiled from a large number of laboratory-based testing under six test drive-cycles, for each of before and after vehicles were tuned. However, CART is not used to the exclusion of other methods.

Hierarchical tree-based (HTRB) regression has several benefits over other methods (Washington *et al.*, 1997): (i) it is more adept at treating interactions and monotonic transformations on independent variables, (ii) it is better at handling categorical independent variables with more than two levels, (iii) it is not affected adversely by multi-collinearity, and (iv) it is appealing in capturing non-additive behaviour across a range of independent variables. However, Washington *et al.* (1997) added that HTBR theory is less developed than other regression theories. Also some of the parameters, such as efficiency, unbiasedness, and consistency, still need to be developed further. Chapter 10 uses 3SLS regression to test the hypothesis of the thesis of emissions interdependencies for twelve models, six of which are before and six are after vehicles were tuned.

Chapter Ten

Testing Vehicle Emissions Interdependencies

10.1 Introduction

Chapter 10 illustrates the formal analysis of testing the hypothesis of the thesis for the interdependencies of HC, CO, and NO_x emissions. It demonstrates the formulations of a system of simultaneous-equations under six test drive-cycles, for each of before and after vehicles were tuned. The chapter includes the synthesis of the estimations results of the twelve models. The chapter also derives indicators of the responses of emissions to changes in the other emissions. Then, it presents the interpretations for the indicators of responses of one emission to the changes in the levels of other emissions. Furthermore, it investigates the responses of the emissions to one percent increase in the other emissions.

In summary, this chapter investigates based on the empirical framework in Chapter 5 the following:

- (1) The form of relations that relate HC, CO, NO_x emissions to vehicle characteristics and the other emissions.
- (2) The variables that will have significant impacts on various emissions under six test drive-cycles, for each of before and after vehicles were tuned.
- (3) The responses of the emissions to changes with respect to changes in the other emissions.

Table 10-1 The Twelve Sub-Sets: Twelve Models

Subset Name	Description	Pollutants
Pre-Tuning		
M1	Model 1- data for cold start test cycle	HCbCS505, CObCS505, NOXbCS55
M2	Model 2- data transient test cycle	HCbT867, CObT867, NOXbT867
M3	Model 3- data for hot start test cycle	HCbH505, CObH505, NOXbH505
M4	Model 4- data for FTP test cycle	HCbADR37, CObADR37, NOXbADR3
M5	Model 5- data for IM240 test cycle	HCbIM240, CObIM240, NOXbIM24
M6	Model 6- data for SS60 test cycle	HCbSS60, CObSS60, NOXbSS60
Post-Tuning		
M7	Model 7- data for cold start test cycle	HCpCS505, COpCS505, NOXpCS55
M8	Model 8- data for transient test cycle	HCpT867, COpT867, NOXpT867
M9	Model 9- data for hot start test cycle	HCpH505, COpH505, NOXpH505
M10	Model 10- data for FTP test cycle	HCpADR37, COpADR37, NOXpADR3
M11	Model 11- data for IM240 test cycle	HCpIM240, COpIM240, NOXpIM24
M12	Model 12- data for SS60 test cycle	HCpSS60, COpSS60, NOXpSS60

10.2 Data Preparation for the Computer Application

Prior to estimating the models, we undertake several measures, in order to test the hypothesis of the thesis for the interdependencies of HC, CO, and NO_x emissions, as follows:

- (1) We use the scheme of codes in Chapter 8 developed for continuous and categorical variables, as shown in Table 8-3 and Table 8-4.
- (2) We transform the categorical variables into dummy-variables, especially for variables with more than two levels, as shown in Table 8-5 and Table 8-6.
- (3) We use -999 as a numeric code to fill in the missing data, so that the computer application will ignore the unobserved records of data.

10.3 The Formulation of the Models for Testing the Hypothesis of the Thesis

We use three-stage least squares (3SLS) regression to estimate the twelve models formulated for testing the hypothesis of the thesis. We use initial candidates to estimate the models of simultaneous-equations system. The initial candidates used are selected from the variables that scored greater than or equal to 15 percent in the analysis of the relative importance of the variables (Chapter 9). Accordingly, we formulate thirty-six equations in twelve models, for each of a system of three simultaneous-equations. We then estimate each model by using the 3SLS module of the computer application (Green, 1998). We present herein, the 3SLS module that we formulate to estimate the first model (Model 1_CS505_pre-tuning), which is used to test the hypothesis of the thesis for the observations measured under cold start test drive-cycle before vehicles were tuned, as follows:

3SLS

Endogenous Lhs variables=HCbCS505, CObCS505, NOXbCS55

- (1) **HCbCS505=one, CObCS505, NOXbCS55,
CATALYST, eems1,O2_SENS, size2,EEMS,
ODOMETER, MASS, egr1,egr2, make1,make2,
make3, make4, TRANMISN,choke2,air1,air2**
- (2) **CObCS505=one, HCbCS505, NOXbCS55,
size1, size2, make1,make2,make3,make4,
ODOMETER,O2_SENS,FUEL_SYS,eems1,
preheat1, choke2,egr1,egr2,TRANMISN,gear2,
ctest1, ctest2, EXHAUST, FUEL_FLT,
BAT_W_LV, air1, ENG_OIL**
- (3) **NOXbCS55=one, HCbCS505, CObCS505,
size1, size2, ODOMETER,ctest1,ctest2,
egr1, egr2, CATALYST,TRANMISN,gear2,
make1, make2, make3,make4,air1,air2,
point1, point2, eems1,preheat1,preheat2,
BODY, BAT_W_LV**

Exogenous variables=make1, make2, make3, make4, BODY, ENG_DIS, size2, ODOMETER , ENG_CONF , TRANMISN, gear2, EEMS, eems1, choke2, FUEL_SYS, air1, preheat1, ENG_OIL, FLUID_LV, RD_CL_LV,BAT_W_LV, FUEL_FLT, AIR_FLT,PROP_PRT, AIR_COND, EXHAUST, CATALYST,ctest2,egr1,egr2, EVP_CANS, SPAK_GAP, H_T_LEAD, point1,point2, DIST_FUN,MODIFY

Where:

(1) represents solving for HC on the Lhs and a list of variables that influences HC are on the Rhs.

(2) represents solving for CO on the Lhs, with a list of variables that influencing CO are on the Rhs.

(3) represents solving for NO_x on the Lhs, with a list of variables influencing NO_x are on the Rhs.

- a list of all endogenous variables are in the first row
- a complete list of all exogenous variables are at the end
- One indicates an equation constant.
- For complete descriptions of variables in capital letters refer to Table 10-2 and for the dummy variables in small letters refer to Table 10-3

Table 10-2 2 Level-variables only (model 1_CS505_ pre-tuning): 3SLS Module

No.	Variable Name	Description	Data Type
1	BODY	Body Type	alpha
2	ENG_DIS	Engine Displacement	numeric (continuous)
3	MASS	Vehicle Mass (full tank)	numeric (continuous)
4	ODOMETER	Odometer	numeric (continuous)
5	ENG_CONF	Engine Configuration	alpha
6	TRANMISN	Transmission	alpha
7	EEMS	Electronic Engine Management System	alpha
8	FUEL_SYS	Fuel System	alpha
9	O2_SENS	O ₂ Sensor Fitted & Operational	alpha
10	ENG_OIL	Battery Water Level	alpha
11	FLUID_LV	Fuel Filter	alpha
12	RD_CL_LV	Radiator Coolant Level	alpha
13	BAT_W_LV	Battery Water Level	alpha
14	FUEL_FLT	Fuel Filter	alpha
15	AIR_FLT	Air Filter	alpha

No.	Variable Name	Description	Data Type
16	PROP_PRT	Fitted Proprietary Parts	alpha
17	AIR_COND	Air Conditioning	alpha
18	EXHAUST	Exhaust Comp Secure	alpha
19	CATALYST	Catalyst Present	alpha
20	EGR_OPER	Exhaust Gaseous Re-circulation	alpha
21	EVP_CANS	Evaporative Canister Fitted	alpha
22	SPAK_GAP	Spark plug conditions / gap	alpha
23	H_T_LEAD	High Tension Leads	alpha
24	DIST_FUN	Distributor Functional	alpha
25	MODIFY	Modifications to Vehicle	alpha

Table 10-3 Dummy-Variables with more than 2 Levels for (model 1_CS505_ pre-tuning): 3SLS module

Variable name	Description
	MAKE
make1	1 if MAKE is Ford, 0 otherwise
make2	1 if MAKE is Toyota, 0 otherwise
make3	1 if MAKE is Nissan, 0 otherwise
make4	1 if MAKE is Holden, 0 otherwise
	ENG_SIZE
size1	1 if ENG_SIZE is small, 0 otherwise
size2	1 if ENG_SIZE is medium, 0 otherwise
	N_GEAR
gear1	1 if number of gears is 3, 0 otherwise
gear2	1 if number of gears is 4, 0 otherwise
	EEMS_OPR
eems1	1 if No, 0 otherwise
eems2	1 if Yes, 0 otherwise
	CHOKE
choke1	1 if choke is Automatic, 0 otherwise
choke2	1 if choke is Manual, 0 otherwise
	A_IJ_SYS
air1	1 if Air injection system is AP , 0 otherwise
air2	1 if Air injection system is PA , 0 otherwise
	AR_BH_F
preheat1	1 if air preheat fitted is No, 0 otherwise
prehaet2	1 if air preheat fitted is Yes, 0 otherwise

Variable name	Description
	CATYST_TS
ctest1	1 if test for catalyst converter rattle is No, 0 otherwise
ctest2	1 if test for catalyst converter rattle is Yes, 0 otherwise
	EGR_OPR
egr1	1 if EGR operational is No, 0 otherwise
egr2	1 if EGR operational is Yes, 0 otherwise
	PTS_CONT
point1	1 if points conditions is poor, 0 otherwise
point2	1 if points conditions is OK, 0 otherwise

Additionally, we use the initial results of running the computer application of the 3SLS module, for cleaning further the input data. Particularly, we use the descriptive statistics of the model and the correlation matrices, as follows:

- to detect any errors in the schemes of the codes;
- to discover any missing observations;
- to assess the quality of the results for descriptive statistics;
- to rejoin levels together, especially for a few cases in a level and when it is logically possible.
- to classify the categories of input variables; and
- to re-code the variables that show highly correlated dummies.

We eliminate the variables that have high levels of multi-collinearity and retained only the variables with absolute correlation factor less than 0.50 for two variables in the correlation matrix of the model. We concur with similar studies in the literature, e.g., Fomunung *et al.* (1999), who used a factor equal to 0.50 to eliminate correlated variables. We present in this chapter and only as a show case the correlation matrix for the input variables into the simulations-equations system for model 1 for before vehicles were tuned (Table 10-4).

Table 10-4 Correlation Matrix for Pre-Tuning Variables: Model 1

	ENG_DIS	N_CYLIND	SIZE1	SIZE2	MASS	INERTIA	TRANMISN	GEAR1	GEAR2	EEMS	EEMS2	CHOKE1	FUEL_SYS	AIR2	O2_SENS	PREHEAT2	CATALYST	CTEST1	SHROUDI1	SHROUDI2	SHROUDO1	SHROUDO2	
ENG_DIS	1.00																						
N_CYLIND	0.91	1.00																					
SIZE1	-0.74	-0.59	1.00																				
SIZE2	-0.12	-0.39	-0.52	1.00																			
MASS	0.85	0.72	-0.78	0.12	1.00																		
INERTIA	0.91	0.79	-0.81	0.09	0.94	1.00																	
TRANMISN	-0.42	-0.34	0.42	-0.12	-0.49	-0.48	1.00																
GEAR1	0.11	0.11	-0.05	-0.07	0.10	0.08	-0.55	1.00															
GEAR2	0.20	0.13	-0.23	0.13	0.25	0.26	-0.20	-0.59	1.00														
EEMS	0.38	0.35	-0.43	0.13	0.51	0.52	-0.28	-0.20	0.38	1.00													
EEMS2	0.31	0.27	-0.33	0.10	0.44	0.43	-0.21	-0.21	0.34	0.84	1.00												
CHOKE1	-0.24	-0.24	0.32	-0.11	-0.34	-0.35	0.13	0.25	-0.31	-0.75	-0.66	1.00											
FUEL_SYS	0.38	0.34	-0.44	0.14	0.52	0.52	-0.30	-0.21	0.39	0.95	0.81	-0.78	1.00										
AIR2	-0.31	-0.29	0.37	-0.11	-0.41	-0.40	0.26	0.00	-0.28	-0.54	-0.46	0.44	-0.57	1.00									
O2_SENS	0.37	0.35	-0.39	0.08	0.48	0.49	-0.29	-0.23	0.39	0.83	0.70	-0.67	0.86	-0.47	1.00								
PREHEAT2	-0.23	-0.18	0.35	-0.21	-0.34	-0.33	0.18	0.18	-0.32	-0.65	-0.60	0.54	-0.64	0.42	-0.58	1.00							
CATALYST	0.10	0.09	-0.11	0.03	0.21	0.21	-0.21	-0.13	0.14	0.46	0.40	-0.25	0.49	0.11	0.51	-0.24	1.00						
CTEST1	0.05	0.02	-0.07	0.06	0.14	0.15	-0.19	-0.08	0.13	0.36	0.28	-0.16	0.36	0.13	0.39	-0.16	0.80	1.00					
SHROUDI1	0.02	0.00	0.02	-0.03	0.02	0.03	0.00	-0.17	0.12	0.15	0.14	-0.03	0.17	0.10	0.20	-0.04	0.38	0.35	1.00				
SHROUDI2	0.09	0.07	-0.13	0.08	0.19	0.18	-0.18	0.03	0.03	0.27	0.22	-0.18	0.27	0.00	0.27	-0.16	0.50	0.38	-0.56	1.00			
SHROUDO1	0.03	0.00	0.00	-0.01	0.07	0.07	-0.01	-0.17	0.12	0.19	0.19	-0.07	0.20	0.11	0.23	-0.07	0.45	0.34	0.82	-0.35	1.00		
SHROUDO2	0.08	0.08	-0.11	0.05	0.15	0.15	-0.17	0.04	0.02	0.25	0.18	-0.14	0.25	-0.01	0.25	-0.14	0.45	0.41	-0.44	0.84	-0.56	1.00	

We remove all observations for HC, CO, and NO_x emissions that are greater than the mean of HC, CO, and NO_x emissions respectively plus two standard deviations, in other words, $\mu+2*\text{Std}$, (see Chapter 7). We demonstrate size of the observations used for testing the hypothesis of the thesis in three different ways, as shown in Table (10-5): (i) based on non-missing observations; (ii) based on the size of the sample after removing observations greater than $\mu+2*\text{Std}$; and (iii) based on the refined size of the sample.

Table 10-5 Size of the Sample

No.	Model name	Number of all observations	Number of Observations < (Mean + 2 Std.)			Estimations based on non-missing observations
			HC	CO	NO _x	
Pre-Tuning						
M1	Model1_CS505	542	524	508	519	475
M2	Model2_T867	542	520	514	522	483
M3	Model3_H505	542	519	511	520	482
M4	Model4_ADR37	542	519	516	519	484
M5	Model5_IM240	540	521	510	522	487
M6	Model6_SS60	537	520	512	511	475
Post-Tuning						
M7	Model7_CS505	542	520	512	518	474
M8	Model8_T867	541	517	518	520	484
M9	Model9_H505	542	519	523	518	486
M10	Model0_ADR37	542	523	520	516	509
M11	Model1_IM240	540	523	516	515	475
M12	Model2_SS60	542	525	511	524	488

10.4 Three Stage Least-Squares (3SLS) Regression

A few studies in the literature, such as (Washburn *et al.*, 2001), have questioned the validity of using ordinary least-squares (OLS) regression for estimating vehicle emissions. OLS does not account for simultaneous relations among emissions, particularly when the right hand side endogenous variables are included in estimating the relations between emission and exogenous variables of the vehicles (Chapter 5). Therefore, an alternative technique that recognises better the simultaneous relations among emissions is necessary.

Several alternative techniques are suggested in the literature, such as 3SLS and full information maximum likelihood (FIML). These methods are similar, but the

3SLS method with no constraints imposed converges to the maximum likelihood estimator (Greene, 1998). The 3SLS method is proposed in this thesis to solve the system of equations for the estimators, provided that the unobserved error terms are normally distributed. The coefficients are inconsistent if the statistical assumptions on the error terms are not valid. The 3SLS method accounts for the simultaneous correlation of error terms when solving for coefficients in the system of equations in order to give asymptotically efficient coefficient estimates (Zellner and Theil, 1962).

In summary, the 3SLS method provided that error terms are normally distributed, has the following advantages (Zellner and Theil, 1962; Green, 1997):

- (1) It gives unbiased and efficient coefficient estimates.
- (2) It accounts for the simultaneous correlation of error terms.
- (3) It produces a unique set of coefficient estimates.
- (4) It gives the least sums of the residuals squared.
- (5) It converges to the maximum likelihood estimator.
- (6) It is asymptotically more efficient compared to other methods, because it incorporates information on the error term covariance into the estimation procedure.

10.5 Specifications and Estimations of Emissions Interdependencies Models

Formally,

$$HC_n = \alpha + \delta_i X_{in} + \lambda_{ij} CO_n + \lambda_{ik} NO_{X_n} + \varepsilon_{in}$$

$$CO_n = \beta + \delta_j X_{jn} + \lambda_{ji} HC_n + \lambda_{jk} NO_{X_n} + \varepsilon_{jn}$$

$$NO_{X_n} = \gamma + \delta_k X_{kn} + \lambda_{ki} HC_n + \lambda_{kj} CO_n + \varepsilon_{kn}$$

(10-1)

Where:

HC_n = hydrocarbons (i emission) for the n^{th} observation
 CO_n = carbon monoxide (j emission) for the n^{th} observation
 NO_{X_n} = oxides of nitrogen (k emission) for the n^{th} observation

$\delta_{in}, \delta_{jn}, \delta_{kn}$ = vectors of variables influencing *HC*, *CO* and *NO_x* emissions, respectively, for the n^{th} observation

α, β, γ = constant terms for *HC*, *CO* and *NO_x* equations respectively, for the n^{th} observation

$\varepsilon_{in}, \varepsilon_{jn}, \varepsilon_{kn}$ = disturbance terms for *HC*, *CO* and *NO_x* equations respectively, for the n^{th} observation

$\lambda_{ij}, \lambda_{ik}$ = coefficients for *CO* and *NO_x* respectively in the *HC* equation

$\lambda_{ji}, \lambda_{jk}$ = coefficients for *HC* and *NO_x* respectively in the *CO* equation

$\lambda_{ki}, \lambda_{kj}$ = coefficients for *HC* and *CO* respectively in the *NO_x* equation

Twelve models and a total of thirty-six equations were estimated (Table 10-1). The models are estimated under six drive-cycles, for each before and after vehicles were tuned, as shown in Table 10-6.

Table 10-6 The Test Drive-Cycles Employed: Six test Drive- Cycles

N	Test	Acronym	Emissions measured	Unit
1	Cold Start (505)	CS505	HC, CO, NO _x	g
2	Transient (867)	T867	HC, CO, NO _x	g
3	Hot Stabilised (505)	H505	HC, CO, NO _x	g
4	Full cycle (ADR37)	ADR37	HC, CO, NO _x	g/km
6	Steady State Loaded 60 km/hr	SSL60	HC, CO, NO _x	g/min

A model that relates each of the three emissions as a dependent variable, to other emissions and explanatory variables that scored greater than or equal to 15 percent relative importance of the variables in CART. Detailed variable descriptions are given in Table 8-3 through to Table 8-6 in Chapter 8. The estimates of modelling twelve models are provided in Section 10.6, and also the detailed estimations of the models are shown in Appendix II.

The key focus in model estimation is to test the hypotheses set out in previous chapters; and not on predicting levels of pollution. The general findings on the extent of interdependency between the three air pollutants of interest, has higher

relevance than the specifics of the functional form of models. This is in large part due to the constraints on the quality of the data, including measurement issues in respect of the set of endogenous variables. This results in a degree of caution about how far one can investigate non-linear treatments of the exogenous and endogenous effects. The linear specification of the 3SLS system of equations is the base model; however given that the theoretical studies (Chapter 4 and Appendix III) suggest non-linear behavioural forms for HC, CO, and NO_x emissions, we use the log_e function to transform variables in one model. The results of running the model with log_e function transformed variables did not improve the overall statistical efficiency of the initial base model. The transformed model converged to approximately the same log likelihood value as the base model.

10.5.1 Post-Tuning ADR37 Model

In this section, we present as a showcase post-tuning ADR37 model to illustrate the estimations of the models formulated. Table 10-7 gives the 3SLS estimation results of HC (g/km) under the ADR37 test drive-cycle post-tuning. The table shows all the significant variables indicated by t-statistics for level of significance equals to 0.05 ($\alpha = 0.05$); the diagnostic log likelihood for estimating HC is – 265.115. The Table shows that an increase in NO_x (g/km) and a slight increase in CO (g/km) will increase HC (g/km). The results show that HC is more likely to increase as NO_x (g/km) increases, and that HC (g/km) will increase slightly as CO (g/km) increases.

The Table shows that the larger is the engine capacity, the higher HC is. Large engines have larger crevices that produce HC significantly (Stone, 1992). The table shows that the larger are the number of kilometres accumulated, the higher HC emissions are (g/km).

Table 10-7 Estimation Results: HC from the ADR37 Test Drive-Cycle Post Tuning -M10

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			-0.010	-0.052	
COPADR37	CO Post-Tuning (ADR37)	g/km	0.037	6.011	10.229
NOXPADR3	NO_x Post-Tuning (ADR37)	g/km	0.548	12.129	1.407
ODOMETER	Odo Readings	km	.128590D-05	4.194	115365.155
ENG_CONF	Engine Configuration V-shape, Inline	0,1	-0.165	-2.448	0.919
ENG_DIS	Engine Displacement Engine Capacity	Liters	0.078	4.359	2.493
POINTST	Points condition after points replaced in Tune-up NA, OK	0,1	-0.288	-3.079	1.851
TRANMISN	Transmission Automatic, Manual	0,1	0.231	5.645	0.316
Diagnostic: Log-L = -265.1151		Restricted (b=0) Log-L = -506.798			
HCPADR37		Mean=0.869725		S.D.= 0.6555495	

Table 10-8 presents the results of the 3SLS for estimating CO emissions. The Table shows all the significant variables. It shows that CO (g/km) is more likely to increase as HC (g/km) increases. Also it shows that CO decreases as NO_x increases, although it is insignificant (t-statistic = -0.218) for determining CO (g/km) under the FTP test drive-cycle after vehicles were tuned.

Table 10-8 Estimation Results: CO in the ADR37 Post-Tuning- M10

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			5.993	7.155	
HCPADR37	HC Post-Tuning ADR37	g/km	6.355	9.634	0.870
NOXPADR3	NO_x Post-Tuning ADR37	g/km	-0.149	-0.218	1.407
EEMS1	NO	1,0	-3.988	-5.423	0.067
EEMS_OPR	Electronic Engine Management System Operational? N, Y, NA				
EEMS2	YES	1,0	-4.387	-7.458	0.363
EEMS_OPR	Electronic Engine Management System Operational? N, Y, NA				
AIR_COND	Air Conditioning No, Yes	0,1	1.041	2.274	0.749
Diagnostic: Log-L = -1480.162		Restricted (b=0) Log-L = -1711.579			
COPADR37		Mean=10.229		S.D.= 6.991	

Table 10-9 presents the results of 3SLS for estimating NO_x (g/km) under the FTP test drive-cycle after vehicles were tuned. The Table shows all the significant variables. It shows that NO_x is more likely to increase as HC (g/km) increases. Also, it shows that CO (g/km) is not significant (t-statistic of -0.806) in determining NO_x ; however, the higher are CO (g/km) emissions, the less (g/km) NO_x is. The Table shows that NO_x (g/km) and CO (g/km) are negatively correlated: NO_x (g/km) decreases as CO (g/km) increases.

Table 10-9 Estimation Results: NO_x in the ADR37 Post Tuning-M10

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			0.482	4.286	
HCPADR37	HC Post-Tuning ADR37	g/km	1.084	10.466	0.870
COPADR37	CO Post-Tuning ADR37	g/km	-0.010	-0.806	10.229
ODOMETER	Odo Meter	km	-.172662D-05	-3.089	115365.155
TRANMISN	Transmission Automatic, Manual	0,1	-0.333	-5.104	0.316
ENG_CONF	Engine Configuration V-shape, Inline	0,1	0.418	3.737	0.919
Diagnostic: Log-L = -515.150		Restricted (b=0) Log-L = -580.701			
NOXPADR3		Mean=1.407	S.D.= 0.758		

To present a more intuitive picture of the model, the estimations of HC, CO and NO_x are as shown in Equations 10-2:

$$\begin{aligned}
 HC &= -0.010 + 0.037 * CO + 0.58 * NO_x + 0.129 * 10^{-5} * ODOMETER \\
 &\quad - 0.165 * ENG_CONF + 0.078 * ENG_DIS - 0.288 * POINTSTS \\
 &\quad + 0.231 * TRANMISN \\
 CO &= 5.993 + 6.355 * HC - 0.149 * NO_x - 3.988 * EEMS1 \\
 &\quad - 4.387 * EEMS2 + 1.041 * AIR_COND \\
 NO_x &= 0.482 + 1.084 * HC - 0.010 * CO - 0.173 * 10^{-5} * ODOMETER \\
 &\quad - 0.333 * TRANMISN + 0.418 * ENG_CONF
 \end{aligned}$$

(10-2)

10.6 Synthesis of the Results of Estimations

In this section, we synthesise the estimation results of testing the hypothesis of the thesis. The detailed results of estimating twelve models for testing the hypothesis of the thesis are presented in Appendix II. Moreover, a summary of the key findings of estimating the thesis models for testing the hypothesis for emissions interdependencies are shown in Table 11-1 and Table 11-2. We also, present discussions on the findings of the models estimated for testing the thesis hypothesis.

The thesis does not provide predictive vehicle emissions models, nor does it investigate any other related issues that prediction models require. We recognise that the theoretical behaviour of the relationships amongst CO, HC, and NO_x are complex within the theoretical range of fuel to air ratio. However, examining Figure 4-19 of Chapter 4, for example, demonstrates that NO and CO are negatively related over the whole range of the practical fuel-air ratio, though the relationship is clearly not perfectly linear.

Inspecting the fuel-rich side diagrams of Figure 4-11 of Chapter 4 indicates that within the practical rich fuel-air ratio, considering a linear approximation selected in the current chapter does not deviate noticeably from the curves shown in Figure 4-19. Nonetheless, we considered transformed log_e function models, but still the results converge to approximately the same log likelihood as the initial models (Section 10.5).

Model 1 estimation results (see Equations 10-3, Tables 10-10, 10-11 and 10-12) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase as NO_x increases. On the other hand, as CO increases HC slightly increases.
- HC and NO_x are both significant emissions influencing CO. CO is more likely to increase as HC increases. On the other hand, as NO_x increases CO will increase.
- HC is the only significant influence on NO_x. NO_x is more likely to increase as HC increases. On the other hand, although CO is insignificant in determining NO_x, the higher are the levels, the lower is the levels of NO_x.

$$\begin{aligned}
 HC = & -7.138 + 0.069*CO + 0.784*NO_X + 1.956*MAKE1 \\
 & + 2.719*MAKE2 + 1.338*MAKE3 + 3.085*MAKE4 \\
 & - 0.989*ENG_DIS - 3.128*ENG_CONF \\
 & + 2.608*TRANMISN + 4.268*FUEL_SYS
 \end{aligned}$$

$$\begin{aligned}
 CO = & 108.628 + 4.464*HC + 2.296*NO_X - 39.583*MAKE2 \\
 & - 18.033*MAKE3 - 15.329*MAKE4 + 3.085*MAKE4 \\
 & - 0.989*ENG_DIS - 63.123*FUEL_SYS - 15.928*TRANMISN
 \end{aligned}$$

$$\begin{aligned}
 NO_X = & -0.295 + 0.738*HC - 0.001*CO - 1.626*TRANMISN \\
 & - 2.033*MAKE1 - 2.119*MAKE4 + 1.059*ENG_DIS \\
 & + 3.350*ENG_CONF + 1.406*AIR_COND
 \end{aligned}$$

(10-3)

Table 10-10 Estimation Results: HC in M1

Variable	Variable Definition	Units	Coefficient	t-value	Variable Mean
Constant			-7.138	-5.527	
COBCS505	CO Pre-Tuning (CS505)	grams	0.069	10.721	122.528
NOXBCS55	NO _x Pre-Tuning (CS505)	grams	0.784	10.934	10.973
MAKE1	Ford	1,0	1.956	4.221	0.324
MAKE2	Toyota	1,0	2.719	6.676	0.253
MAKE3	Nissan	1,0	1.338	2.820	0.097
MAKE4	Holden	1,0	3.085	5.965	0.208
ENG_DIS	Engine Displacement	Liters	-0.989	-3.587	2.460
ENG_CONF	Engine Configuration	0,1	-3.128	-3.840	0.909
TRANMISN	Transmission	0,1	2.608	6.732	0.343
FUEL_SYS	Fuel System	0,1	4.268	8.486	0.465

Diagnostic: Log-L = -1264.156
 Restricted (b=0) Log-L = -1419.614
 Mean= 8.638 S.D.= 4.810
 HCBCS505

Table 10-11 Estimation Results: CO in M1

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			108.628	10.707	
HCBCS505	HC Pre-Tuning (CS505)	grams	4.464	4.092	8.638
NOXBCS55	NO _x Pre-Tuning (CS505)	grams	2.296	2.141	10.973
MAKE2	Toyota	1,0	-39.583	-7.781	0.253
MAKE3	Nissan	1,0	-18.033	-2.646	0.097
MAKE4	Holden	1,0	-15.329	-2.471	0.208
FUEL_SYS	Fuel System	0,1	-63.123	-11.125	0.465
TRANMISN	Transmission	0,1	-15.928	-2.943	0.343

Diagnostic: Log-L = -2492.039
 Restricted (b=0) Log-L = 2685.322
 COBCS505 Mean=122.528 S.D.=69.091

Table 10-12 Estimation Results: NO_x in M1

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			-0.295	-0.215	
HCBCS505	HC Pre-Tuning (CS505)	grams	0.738	9.237	8.638
COBCS505	CO Pre-Tuning (CS505)	grams	-0.001	-0.199	122.528
TRANMISN	Transmission	0,1	-1.626	-3.124	0.343
MAKE1	Ford	1,0	-2.033	-4.219	0.324
MAKE4	Holden	1,0	-2.119	-3.558	0.208
ENG_DIS	Engine Displacement	Liters	1.059	3.650	2.460
ENG_CONF	Engine Configuration	0,1	3.350	3.845	0.909
AIR_COND	Air Conditioning	0,1	1.406	3.226	0.733

Diagnostic: Log-L = -1384.066
 Restricted (b=0) Log-L = -1427.493
 NO_xBCS55 Mean=10.973 S.D.= 4.891

Model 2 estimation results (see Equations 10-4, Tables 10-13, 10-14 and 10-15) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase slightly as CO increases. Similarly, as NO_x increases an increase in HC results.
- HC and NO_x are both significant influences on CO. CO is more likely to increase as HC increases, however, the higher the levels of NO_x, the lower the levels of CO are.
- HC and CO are both significant influences on NO_x. NO_x is more likely to increase as HC increases. On the other hand, the higher the levels of CO the lower NO_x is, NO_x and CO are negatively correlated.

$$HC = -3.076 + 0.060 * CO + 0.704 * NO_X - 1.880 * ENG_CONF \\ + 1.393 * TRANMISN - 1.194 * AIR_COND + 3.176 * EEMS$$

$$CO = 45.400 + 15.677 * HC - 9.541 * NO_X - 48.105 * EEMS1 \\ - 51.046 * EEMS2 - 21.577 * TRANMISN + 18.464 * AIR_COND \\ + 26.890 * ENG_CONF$$

$$NO_X = -0.105 + 1.132 * HC - 0.063 * CO + 0.634 * EGRI - \\ 1.565 * TRANMISN + 2.669 * ENG_CONF + 3.982 * CHOKE1 \\ + 3.834 * CHOKE2 + 1.295 * AIR_COND$$

(10-4)

Table 10-13 Estimation Results: HC M2

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			-3.076	-4.964	
COBT867	CO Pre-Tuning (T867)	grams	0.060	22.725	69.288
NOXBT867	NO _x Pre-Tuning (T867)	grams	0.704	10.393	6.568
ENG_CONF	Engine Configuration	0,1	-1.880	-4.469	0.909
TRANMISN	Transmission	0,1	1.393	5.366	0.332
AIR_COND	Air Conditioning	0,1	-1.194	-4.099	0.737
EEMS	Engine Electronic Management System	0,1	3.176	9.542	0.446
Diagnostic: Log-L = -1135.557		Restricted (b=0) Log-L = -1434.889			
HCBT867		Mean=4.983	S.D.=4.754		

Table 10-14 Estimation Results: CO M2

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			45.400	4.441	
HCBT867	HC Pre-Tuning (T867)	grams	15.677	23.007	4.983
NOXBT867	NO _x Pre-Tuning (T867)	grams	-9.541	-6.643	6.568
EEMS1	EEMS operational NO	1,0	-48.105	-6.310	0.068
EEMS2	EEMS Operational YES	1,0	-51.046	-9.519	0.373
TRANMISN	Transmission	0,1	-21.577	-5.145	0.332
AIR_COND	Air Conditioning	0,1	18.464	4.091	0.737
ENG_CONF	Engine Configuration	0,1	26.890	3.953	0.909
Diagnostic: Log-L = -2461.762		Restricted (b=0) Log-L = -2753.516			
COBT867		Mean=69.288	S.D.=73.317		

Table 10-15 Estimation Results: NO_x M2

Variable	Variable Description	Units	Coefficient	t-value	Variable mean
Constant			-0.105	-0.166	
HCBT867	HC Pre-Tuning (T867)	grams	1.132	12.013	4.983
COBT867	CO Pre-Tuning (T867)	grams	-0.063	-7.582	69.288
EGR1	EGR operational NO	1, 0	0.634	2.495	0.199
TRANMISN	Transmission	0, 1	-1.565	-4.830	0.332
ENG_CONF	Engine Configuration	0, 1	2.669	5.370	0.909
CHOKE1	Automatic	1, 0	3.982	8.211	0.548
CHOKE2	Manual	1, 0	3.834	4.472	0.056
AIR_COND	Air Conditioning	0, 1	1.295	3.657	0.737
Diagnostic: Log-L = -1232.212		Restricted (b=0) Log-L = -1315.301			
NOXBT867		Mean=6.568	S.D.=3.710		

Model 3 estimation results (see Equations 10-5, Tables 10-16, 10-17 and 10-18) suggest:

- CO is the only significant influence on HC. HC is more likely to increase as CO increased. Although NO_x is insignificant in determining HC, a slight increase in NO_x increases HC.
- HC and NO_x are both significant influences on CO. CO is more likely to increase as HC increases, similarly it is more likely to increase as NO_x increases.
- CO is the only significant influence on NO_x. NO_x is more likely to increase slightly as CO increases. On the other hand, HC is insignificant in determining NO_x; however, the higher the levels of HC are, the lower the levels of NO_x are.

$$HC = 1.895 + 0.079 * CO + 0.001 * NO_X + 1.506 * TRANMISN \\ - 4.807 * AIR2 - 1.714 * O2_SENS$$

$$CO = -46.321 + 9.087 * HC + 3.430 * NO_X + 23.617 * O2_SENS \\ + 61.082 * AIR2 - 12.833 * TRANMISN$$

$$NO_X = 8.689 - 0.166 * HC + 0.097 * CO - 2.559 * O2_SENS \\ - 5.834 * AIR2$$

(10-5)

Table 10-16 Estimation Results: HC M3

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			1.895	2.648	
COBH505	CO Pre-Tuning (H505)	grams	0.079	14.001	52.445
NOXBH505	NO _x Pre-Tuning (H505)	grams	0.001	0.015	10.354
TRANMISN	Transmission	0,1	1.506	6.815	0.340
AIR2	PA	1,0	-4.807	-9.277	0.276
O2_SENS	O ₂ Sensor	0,1	-1.714	-4.086	0.415
Diagnostic: Log-L = -1133.716 HCBH505		Restricted (b=0) Log-L = -1327.563 Mean=4.519 S.D.= 3.805			

Table 10-17 Estimation Results: CO M3

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			-46.321	-5.420	
HCBH505	HC Pre-Tuning (H505)	grams	9.087	13.859	4.519
NOXBH505	NO _x Pre-Tuning (H505)	grams	3.430	6.595	10.354
O2_SENS	O ₂ Sensor				
	Fitted & Operational	0,1	23.617	4.060	0.415
AIR2	PA	1,0	61.082	8.757	0.276
TRANMISN	Transmission	0,1	-12.833	-6.013	0.340
Diagnostic: Log-L = -2415.285 COBH505		Restricted (b=0) Log-L = -2517.308 Mean=52.445 S.D.= 44.913			

Table 10-18 Estimation Results: NO_x M3

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			8.689	7.411	
HCBH505	HC Pre-Tuning (H505)	grams	-0.166	-0.958	4.519
COBH505	CO Pre-Tuning (H505)	grams	0.097	6.832	52.445
O2_SENS	O ₂ Sensor				
	Fitted & Operational	0,1	-2.559	-2.623	0.415
AIR2	PA	1,0	-5.834	-4.715	0.276
Diagnostic: Log-L = -1496.373 NOXBH505		Restricted (b=0) Log-L = -1482.913 Mean=10.354 S.D.= 5.252			

Model 4 estimation results (see Equations 10-6, Tables 10-19, 10-20 and 10-21) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase as NO_x increases; similarly an increase in CO will increase HC.
- HC and NO_x are both significant influences on CO. CO is more likely to increase as HC increases. Similarly, the higher the levels of NO_x are, the higher the levels of CO are.
- HC and CO are both significant influences on NO_x. NO_x is more likely to increase slightly as CO increases. The higher are the levels of HC the higher the levels of NO_x are.

$$\begin{aligned}
 HC = & 0.137 + 0.041 * CO + 0.222 * NO_X + 0.066 * ENG_DIS \\
 & - 0.464 * CATALYST + 0.104 * MAKE2 + 0.198 * MAKE4 \\
 & + 0.211 * TRANMISN
 \end{aligned}$$

$$\begin{aligned}
 CO = & -9.04 + 14.58 * HC + 5.08 * NO_X - 1.09 * ENG_DIS \\
 & + 1.38 * MAKE1 - 1.71 * MAKE2 - 3.15 * MAKE4 \\
 & - 3.40 * TRANMISN + 7.47 * CATALYST
 \end{aligned}$$

$$NO_X = 0.799 + 0.186 * HC + 0.038 * CO - 0.151 * MAKE1$$

(10-6)

Table 10-19 Estimation Results: HC M4

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			0.137	1.146	
COBADR37	COPre-Tuning (ADR37)	g/km	0.041	12.432	13.144
NOXBADR3	NO _x Pre-Tuning (ADR37)	g/km	0.222	3.216	1.430
ENG_DIS	Engine Displacement	Liters	0.066	3.340	2.455
CATALYST	Catalyst Present	0,1	-0.464	-8.035	0.719
MAKE2	Toyota	1,0	0.104	2.530	0.248
MAKE4	Holden	1,0	0.198	4.940	0.211
TRANMISN	Transmission	1,0	0.211	5.843	0.333
Diagnostic: Log-L = -135.908		Restricted (b=0) Log-L = -541.317			
HCBADR37		Mean =0.961		S.D.= 0.741	

Table 10-20 Estimation Results: CO M4

Variable	Variable definition	Units	Coefficient	value	Variable mean
Constant			-9.04	-4.37	
HCBADR37	HC Pre-Tuning (ADR37)	g/km	14.58	17.04	0.96
NOXBADR3	NO _x Pre-Tuning (ADR37)	g/km	5.08	4.34	1.43
ENG_DIS	Engine Displacement	Liters	-1.09	-3.24	2.45
MAKE1	Ford	1,0	1.38	2.31	0.30
MAKE2	Toyota	1,0	-1.71	-2.47	0.25
MAKE4	Holden	1,0	-3.15	-4.50	0.21
TRANMISN	Transmission	0,1	-3.40	-5.41	0.33
CATALYST	Catalyst Present	0,1	7.47	7.25	0.72
Diagnostic: Log-L = -1660.737		Restricted (b=0) Log-L = -1826.502			
COBADR37		Mean =13.144		S.D.= 10.547	

Table 10-21 Estimation Results: NO_x M4

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			0.799	14.378	
HCBADR37	HC Pre-Tuning (ADR37)	g/km	0.186	2.123	0.961
COBADR37	CO Pre-Tuning (ADR37)	g/km	0.038	5.848	13.144
MAKE1	Ford	1,0	-0.151	-2.316	0.304
Diagnostic: Log-L = -481.046		Restricted (b=0) Log-L = -508.801			
NOXBADR3		Mean =1.430		S.D.= 0.693	

Model 5 estimation results (see Equations 10-7, Tables 10-22, 10-23 and 10-24) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase slightly as CO increases. The higher are the levels of NO_x, the higher the levels of HC are.
- HC is the only significant influence on CO. CO is more likely to increase as HC increases. Although, NO_x is insignificant in influencing CO, as NO_x increased CO is reduced.
- CO is the only significant influence on NO_x. CO is more likely to increase slightly as NO_x increases. Also, HC is insignificant in determining NO_x, but the higher are the levels of HC the higher the levels of NO_x are.

$$\begin{aligned}
 HC = & 1.668 + 0.078 * CO + 0.275 * NO_X + 1.234 * MAKE1 \\
 & + 0.259 * POINT2 + .157 * TRAMISN + 0.362 * EEMS1 \\
 & + 0.343 * EEMS2
 \end{aligned}$$

$$\begin{aligned}
 CO = & 2.913 + 10.348 * HC - 0.227 * NO_X + 1.634 * CATALYST \\
 & - 2.902 * POINT2 - 1.763 * TRANMISN \\
 & - 4.155 * EEMS1 - 3.976 * EEMS2
 \end{aligned}$$

$$\begin{aligned}
 NO_X = & 1.669 + 0.318 * HC + 0.032 * CO - 0.566 * CATALYST \\
 & + 0.112 * EGR1
 \end{aligned}$$

(10-7)

Table 10-22 Estimation Results: HC M5

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			-0.668	-9.415	
COBIM240	CO Pre-Tuning (IM240)	g/km	0.078	16.924	8.884
NOXBIM24	NO _x Pre-Tuning (IM240)	g/km	0.275	7.683	1.786
MAKE1	Ford	1,0	-0.234	-6.485	0.312
POINT2	Points Conditions OK	1,0	0.259	4.068	0.076
TRANMISN	Transmission	0,1	0.157	4.332	0.341
EEMS1	EEMS operational No	1,0	0.362	5.062	0.070
EEMS2	EEMS Operational Yes	1,0	0.343	7.059	0.372
Diagnostic: Log-L = -181.484		Restricted (b=0) Log-L = -429.259			
HCBIM240		Mean = 0.672		S.D. = 0.588	

Table 10-23 Estimation Results: CO M5

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			2.913	2.689	
HCBIM240	HC Pre-Tuning (IM240)	g/km	10.348	13.780	0.672
NOXBIM24	NO _x Pre-Tuning (IM240)	g/km	-0.227	-0.513	1.786
CATALYST	Catalyst Present	0,1	1.634	2.993	0.715
MAKE1	Ford	1,0	2.694	6.555	0.312
POINT2	Points Conditions OK	1,0	-2.902	-3.939	0.076
TRANMISN	Transmission	0,1	-1.763	-4.193	0.341
EEMS1	EEMS Operational No	1,0	-4.155	-5.135	0.070
EEMS2	EEMS Operational Yes	1,0	-3.976	-7.701	0.372
Diagnostic: Log-L = -1421.245		Restricted (b=0) Log-L = -1650.412			
COBIM240		Mean = 8.884		S.D. = 7.330	

Table 10-24 Estimation Results: NO_x M5

variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			1.669	7.772	
HCBIM240	HC Pre-Tuning (IM240)	g/km	0.318	1.532	0.672
COBIM240	CO Pre-Tuning (IM240)	g/km	0.032	2.496	8.884
CATALYST	Catalyst Present	0,1	-0.566	-3.435	0.715
EGR1	EGR Operational=NO	1,0	0.112	2.039	0.202
Diagnostic: Log-L = -577.434		Restricted (b=0) Log-L = -663.666			
NOXBIM24		Mean = 1.786		S.D. = 0.954	

Model 6 estimation results (see Equations 10-8, Tables 10-25, 10-26 and 10-27) suggest:

- CO is the only significant influence on HC. HC is more likely to increase as CO increases, although NO_x is insignificant in influencing HC, as NO_x increases HC increases.
- HC and NO_x are both significant influences on CO. CO is more likely to increase as HC increased, similarly the higher the levels of NO_x are, the higher the levels of CO are.
- CO is the only significant emission influencing NO_x. NO_x is more likely to increase slightly as CO increases. On the other hand HC is insignificant in influencing NO_x; however, the higher are the levels of HC, the lower are the levels of NO_x.

$$HC = 0.065 + 0.046 * CO + 0.091 * NO_X + 0.040 * ENG_DIS \\ - 0.224 * CATALYST + 0.081 * FUEL_SYS$$

$$CO = -2.051 + 11.440 * HC + 3.178 * NO_X + 3.562 * AIR2$$

$$NO_X = 0.779 + 0.009 * HC + 0.029 * NO_X - 0.270 * CATALYST$$

(10-8)

Table 10-25 Estimation Results: HC M6

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			0.065	0.939	
COBSS60	CO Pre-Tuning (SS60)	g/min	0.046	10.721	5.282
NOXBSS60	NO _x Pre-Tuning (SS60)	g/min	0.091	1.883	0.743
ENG_DIS	Engine Displacement	Liters	0.040	4.638	2.471
CATALYST	Catalyst present	0,1	-0.224	-6.856	0.709
FUEL_SYS	Fuel System	0,1	0.081	2.589	0.443
Diagnostic: Log-L =95.173 HCBSS60		Restricted (b=0) Log-L =-203.046 Mean = 0.350 S.D.=0.369			

Table 10-26 Estimation Results: CO M6

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			-2.051	-3.783	
HCBSS60	HC Pre-Tuning (SS60)	g/min	11.440	12.069	0.350
NOXBSS60	NO _x Pre-Tuning (SS60)	g/min	3.178	3.607	0.743
AIR2	PA	1,0	3.562	7.442	0.274
Diagnostic: Log-L =-1403.134 COBSS60		Restricted (b=0) Log-L =-1580.338 Mean =5.281534 S.D.=6.473			

Table 10-27 Estimation Results: NO_x M6

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			0.779	6.441	
HCBSS60	HC Pre-Tuning (SS60)	g/min	0.009	0.044	0.350
COBSS60	CO Pre-Tuning (SS60)	g/min	0.029	3.042	5.282
CATALYST	Catalyst present	0,1	-0.270	-2.852	0.709
Diagnostic: Log-L =-344.462 NOXBSS60		Restricted (b=0) Log-L =-363.118 Mean = 0.743 S.D.=0.515			

Model 7 estimation results (see Equations 10-9, Tables 10-28, 10-29 and 10-30) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase as NO_x increases; also as CO increases slightly HC will increase.
- HC and NO_x are both significant influences on CO. CO is more likely to increase as HC increases. On the other hand, the higher are the levels of NO_x the lower the levels of CO are.
- HC and CO are both significant influences on NO_x. NO_x is more likely to increase when HC increases; however, as CO increases slightly NO_x will decrease.

$$\begin{aligned}
 HC = & -2.646 + 0.042 * CO + 0.634 * NO_X - 1.628 * ENG_CONF \\
 & + 2.075 * TRANMISN + 0.384 * MAKE4
 \end{aligned}$$

$$\begin{aligned}
 CO = & 75.2012 + 9.454 * HC - 2.126 * NO_X - 31.897 * EEMS \\
 & - 12.310 * TRANMISN
 \end{aligned}$$

$$\begin{aligned}
 NO_X = & 0.034 + 1.054 * HC - 0.024 * CO \\
 & - 2.529 * TRANMISN + 3.354 * ENG_CONF \\
 & - 0.002 * P_ATCOST
 \end{aligned}$$

(10-9)

Table 10-28 Estimation Results: HC M7

Variable	Variable description	Units	Coefficient	t-value	Variable mean
Constant			-2.646	-4.353	
COPCS505	CO POST (CS505)	grams	0.042	10.135	106.626
NOXPCS55	NOX POST (CS505)	grams	0.634	13.314	10.223
ENG_CONF	Engine Configuration	0,1	-1.628	-3.796	0.909
TRANMISN	Transmission	0,1	2.075	7.262	0.335
MAKE4	Holden	1,0	0.384	2.055	0.209
Diagnostic: Log-L = -1184.674 HCPCS505		Restricted (b=0) Log-L = -1299.991 Mean = 7.617 S.D. = 3.761			

Table 10-29 Estimation Results: CO M7

Variable	Variable description	Units	Coefficient	t-value	Variable Mean
Constant			75.012	7.535	
HCPCS505	HC POST (CS505)	grams	9.454	9.107	7.617
NOXPCS55	NO _x POST (CS505)	grams	-2.126	-2.012	10.223
EEMS	Electronic Engine Management System	0,1	-31.897	-7.248	0.456
TRANMISN	Transmission	0,1	-12.310	-2.486	0.335
Diagnostic: Log-L = -2430.713 COPCS505		Restricted (b=0) Log-L = -2586.441 Mean = 106.6259 S.D. = 56.75507			

Table 10-30 Estimation Results: NO_x M7

Variable	Variable Description	Units	Coefficient	t-value	Variable Mean
Constant			0.034	0.025	
HCPCS505	HC POST (CS505)	grams	1.054	12.160	7.617
COPCS505	CO POST (CS505)	grams	-0.024	-3.140	106.626
MASS	Vehicle Mass	Kg	0.002	3.100	1231.507
TRANMISN	Transmission	0,1	-2.529	-5.810	0.335
ENG_CONF	Engine Configuration	0,1	3.354	5.093	0.909
P_ATCOST	Adjusted Total Parts Cost Replaced in Tune-up	\$	-0.002	-1.990	202.568
Diagnostic: Log-L = -1332.597 NOXPCS55		Restricted (b=0) Log-L = -1383.442 Mean = 10.22268 S.D. = 4.485144			

Model 8 estimation results (see Equations 10-10, Tables 10-25, 10-26 and 10-27) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase as NO_x increases; similarly, as CO increases HC will increase slightly.
- HC is only significant influence on CO. CO is more likely to increase as HC increases. Although NO_x is insignificant in determining CO, the higher NO_x is resulted in a reduced CO.
- CO and HC are both significant emissions influencing NO_x. NO_x is more likely to increase as HC increases. On the other hand, the higher are the levels of CO NO_x will slightly increase.

$$\begin{aligned}
 HC = & -5.90 + 0.061 * CO + 0.843 * NO_X + 0.957 * EEMS \\
 & + 1.067 * TRANMISN + 1.622 * N_CYLIND \\
 & + 0.004 * P_ATCOST + 0.726 * MAKE3 + 0.870 * MAKE4
 \end{aligned}$$

$$CO = 36.234 + 7.492 * HC - 1.397 * NO_X - 25.758 * EEMS$$

$$\begin{aligned}
 NO_X = & 5.753 + 0.912 * HC - 0.030 * CO - 1.349 * TRANMISN \\
 & - 2.049 * N_CYLIND - 0.005 * P_ATCOST - 0.917 * MAKE3 \\
 & - 1.098 * MAKE4
 \end{aligned}$$

(10-10)

Table 10-31 Estimation Results: HC M8

Variable	Variable description	Units	Coefficient	t-value	Variable mean
Constant			-5.900	-15.101	
COPT867	CO Post-Tuning (T867)	grams	0.061	13.514	48.744
NOXPT867	NO _x Post-Tuning (T867)	grams	0.843	18.150	5.854
EEMS	Engine Electronic Management System	0,1	0.957	6.131	0.445
TRANMISN	Transmission	0,1	1.067	4.124	0.315
N_CYLIND	No. of cylinders	0,1	1.622	5.909	0.337
P_ATCOST	Adjusted Total Parts Cost Replaced in Tune-up	\$	0.004	4.037	201.863
MAKE3	Nissan	1,0	0.726	1.965	0.091
MAKE4	Holden	1,0	0.870	3.056	0.213
Diagnostic: Log-L = -1135.934 HCPT867			Restricted (b=0) Log-L = -1370.818 Mean =4.293 S.D.=4.138		

Table 10-32 Estimation Results: CO M8

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			36.234	5.643	
HCPT867	HC Post-Tuning (T867)	grams	7.492	11.111	4.293
NOXPT867	NO _x Post-Tuning (T867)	grams	-1.397	-1.219	5.854
EEMS	Engine Electronic Management System	0,1	-25.758	-6.529	0.445
Diagnostic: Log-L = -2302.559 COPT867			Restricted (b=0) Log-L = -2538.394 Mean =48.744 S.D.=46.413		

Table 10-33 Estimation Results: NO_x M8

Variable	Variable description	Units	Coefficient	t-value	Variable Mean
Constant			5.753	15.090	
HCPT867	HC Post-Tuning (T867)	grams	0.912	22.751	4.293
COPT867	HC Post-Tuning (T867)	grams	-0.030	-4.996	48.744
TRANMISN	Transmission	0,1	-1.349	-4.161	0.315
N_CYLIND	No. of cylinders	0,1	-2.049	-5.983	0.337
P_ATCOST	Adjusted Total Parts Cost Replaced in Tune-up	\$	-0.005	-4.053	201.863
MAKE3	Nissan	1,0	-0.917	-1.971	0.091
MAKE4	Holden	1,0	-1.098	-3.051	0.213
Diagnostic: Log-L = -1184.811 COPT867			Restricted (b=0) Log-L = -1283.857 Mean =5.853727 S.D.= 3.456256		

Model 9 estimation results (see Equations 10-11, Tables 10-34, 10-35 and 10-36) suggest:

- CO and NO_x are both significant influences on HC. HC is more likely to increase slightly as CO increases. NO_x is more likely to increase as HC increases.
- HC and NO_x are both significant influences on CO. HC is more likely to increase as CO increases. However, NO_x and CO are negatively correlated; NO_x increases with a decrease in CO.
- Both HC and CO are significant emissions influencing NO_x. HC is more likely to increase with the increase in NO_x. Also, as CO increases NO_x will decrease slightly.

$$HC = -5.666 + 0.085 * CO + 0.564 * NO_X + 0.404 * TRANMISN \\ + 0.908 * MAKE2 + 0.610 * MAKE3 + 2.260 * MAKE4$$

$$CO = 44.843 + 8.832 * HC - 3.267 * NO_X - 12.949 * MAKE2 \\ + 0.908 * MAKE2 + 0.610 * MAKE3 + 2.260 * MAKE4$$

$$NO_X = 7.532 + 1.137 * HC - 0.046 * CO - 2.146 * MAKE4 \\ - 1.210 * TRANMISN$$

(10-11)

Table 10-34 Estimation Results: HC M9

Variable	Variable description	Units	Coefficient	t-value	Variable Mean
Constant			-5.666	-14.871	
COPH505	CO Post (CS505)	grams	0.085	16.744	41.223
NOXPH505	NO _x Post (CS505)	grams	0.564	13.678	9.399
TRANMISN	Transmission	0,1	0.404	2.906	0.331
MAKE2	Toyota	1,0	0.908	4.796	0.241
MAKE3	Nissan	1,0	0.610	2.286	0.099
MAKE4	Holden	1,0	2.260	8.234	0.210
Diagnostic: Log-L =-1145.653 HCPH505		Restricted (b=0) Log-L =-1290.223 Mean =4.039 S.D.= 3.445			

Table 10-35 Estimation Results: CO M9

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			44.843	9.067	
HCPH505	HC Post (CS505)	grams	8.832	18.980	4.039
NOXPH505	NO _x Post (CS505)	grams	-3.267	-5.591	9.399
MAKE2	Toyota	1,0	-12.949	-4.986	0.241
MAKE3	Nissan	1,0	-8.702	-2.358	0.099
MAKE4	Holden	1,0	-21.977	-7.540	0.210
Diagnostic: Log-L =-2219.566 COPH505		Restricted (b=0) Log-L =-2385.496 Mean =41.223 S.D.= 32.803			

Table 10-36 Estimation Results: NO_x M9

Acronym	Variable definition	Units	Coefficient	t-value	Mean of X
Constant			7.532	16.892	
HCPH505	HC Post (CS505)	grams	1.137	11.884	4.039
COPH505	CO Post (CS505)	grams	-0.046	-3.061	41.223
MAKE4	Holden	1,0	-2.146	-4.537	0.210
TRANMISN	Transmission	0,1	-1.210	-3.055	0.331
Diagnostic: Log-L =-1346.678 NOXPH505		Restricted (b=0) Log-L =-1448.231 Mean =9.399 S.D.= 4.768			

Model 10 estimation results (see Equations 10-12, Tables 10-37, 10-38 and 10-39) suggest:

- Both CO and NO_x are significant influences on HC. HC is more likely to increase as NO_x increases. CO increases slightly as HC increases.
- HC is the only significant influence on CO. HC is more likely to increase with increasing CO. Also, CO decreases with increasing NO_x, although NO_x is insignificant in determining CO.
- HC is the only significant emission influencing NO_x. CO is more likely to increase as NO_x increases. However, CO will increase slightly with decreasing NO_x.

$$\begin{aligned}
 HC = & -0.010 + 0.037 * CO + 0.548 * NO_X - .129 * 10^{-5} * ODOMETER \\
 & - 0.165 * ENG_CONF + 0.078 * ENG_DIS - 0.288 * POINTST \\
 & + 0.231 * TRANMISN
 \end{aligned}$$

$$\begin{aligned}
 CO = & 5.993 + 6.355 * HC - 0.149 * NO_X - 3.988 * EEMS1 \\
 & - 4.387 * EEMS2 + 1.041 * AIR_COND
 \end{aligned}$$

$$\begin{aligned}
 NO_X = & 0.482 + 1.084 * HC - 0.010 * CO - 0.173 * 10^{-5} * ODOMETER \\
 & - 0.333 * TRANMISN + 0.418 * ENG_CONF
 \end{aligned}$$

(10-12)

Table 10-37 Estimation Results: HC M10

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			-0.010	-0.052	
COPADR37	CO Post-Tuning (ADR37)	g/km	0.037	6.011	10.229
NOXPADR3	NO _x Post-Tuning (ADR37)	g/km	0.548	12.129	1.407
ODOMETER	Odo Readings	Km	.128590D-05	4.194	115365.155
ENG_CONF	Engine Configuration	0,1	-0.165	-2.448	0.919
ENG_DIS	Engine Displacement	litre	0.078	4.359	2.493
POINTST	Points condition after points replaced in Tune-up	0,1	-0.288	-3.079	1.851
TRANMISN	Transmission	0,1	0.231	5.645	0.316
Diagnostic: Log-L = -265.1151 HCPADR37		Restricted (b=0) Log-L = -506.798 Mean =0.869725 S.D.= 0.6555495			

Table 10-38 Estimation Results: CO M10

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			5.993	7.155	
HCPADR37	HC Post-Tuning ADR37	g/km	6.355	9.634	0.870
NOXPADR3	NO _x Post-Tuning ADR37	g/km	-0.149	-0.218	1.407
EEMS1	EEMS= NO	1,0	-3.988	-5.423	0.067
EEMS2	EEMS= YES	1,0	-4.387	-7.458	0.363
AIR_COND	Air Conditioning	0,1	1.041	2.274	0.749
Diagnostic: Log-L = -1480.162 COPADR37		Restricted (b=0) Log-L = -1711.579 Mean =10.229 S.D.=6.991			

Table 10-39 Estimation Results: NO_x M10

Variable	Variable Description	Units	Coefficient	t-value	Variable Mean
Constant			0.482	4.286	
HCPADR37	HC Post-Tuning ADR37	g/km	1.084	10.466	0.870
COPADR37	CO Post-Tuning ADR37	g/km	-0.010	-0.806	10.229
ODOMETER	Odo Meter	Km	-.172662D-05	-3.089	115365.155
TRANMISN	Transmission	0,1	-0.333	-5.104	0.316
ENG_CONF	Engine Configuration	0,1	0.418	3.737	0.919
Diagnostic: Log-L = -515.150 NOXPADR3		Restricted (b=0) Log-L = -580.701 Mean =1.407 S.D.= 0.758			

Model 11 estimation results (see Equations 10-13, Tables 10-40, 10-41 and 10-42) suggest:

- Both CO and NO_x are significant influences on HC. CO increases slightly with increasing HC, and NO_x increases with increasing HC.
- Both HC and NO_x are significant influences on CO. The levels of HC are more likely to increase with the increase in CO. NO_x increases as CO decreases.
- Both HC and CO are significant influences on NO_x. NO_x is more likely to increase as HC increases. However, as CO increases NO_x decreases slightly.

$$\begin{aligned}
 HC = & -0.584 + 0.048 * CO + 0.393 * NO_X + 0.062 * ENG_DIS \\
 & + 0.102 * 10^{-5} * ODOMETER + 0.271 * POINTST \\
 & + 0.117 * TRANMISN - 0.148 * ENG_CONF
 \end{aligned}$$

$$CO = 8.918 + 6.173 * HC - 2.257 * NO_X + 4.112 * O2_SENST$$

$$\begin{aligned}
 NO_X = & 0.819 + 1.537 * HC - 0.052 * CO - .177 * 10^{-5} * ODOMETER \\
 & - 0.198 * TRANMISN + 0.525 * ENG_CONF
 \end{aligned}$$

(10-13)

Table 10-40 Estimation Results: HC M11

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			-0.584	-7.069	
COPIIM240	CO Post-Tuning (IM240)	g/km	0.048	8.365	7.261
NOXPIM24	NO _x Post-Tuning (IM240)	g/km	0.393	7.770	1.556
ENG_DIS	Engine Displacement	litre	0.062	3.315	2.493
ODOMETER	Odo Readings	km	.101592D-05	3.906	112777.419
POINTST	Points condition after points replaced in Tune-up	0,1	0.271	2.470	0.139
TRANMISN	Transmission	0,1	0.117	3.362	0.328
ENG_CONF	Engine Configuration	0,1	-0.148	-2.431	0.914
Diagnostic: Log-L = -170.637 HCPIM240		Restricted (b=0) Log-L = -376.596 Mean =0.584 S.D.= 0.535			

Table 10-41 Estimation Results: CO M11

Variable	Variable definition	Units	Coefficient	t-value	Variable mean
Constant			8.918	8.352	
HCPIM240	HC Post-Tuning (IM240)	g/km	6.173	7.464	0.584
NOXPIM24	NO _x Post-Tuning (IM240)	g/km	-2.257	-3.234	1.556
O2_SENST	O ₂ Sensor fitted & Operational after replaced in Tune-Up	0,1	-4.112	-7.587	0.425
Diagnostic: Log-L = -1345.218 COPIIM240		Restricted (b=0) Log-L = -1510.77 Mean =7.261 S.D.= 5.828			

Table 10-42 Estimation Results: NO_x M11

Variable	Variable Description	Units	Coefficient	t-value	Variable Mean
Constant			0.819	6.467	
HCPIM240	CO Post-Tuning (IM240)	g/km	1.537	10.211	0.584
COPIIM240	CO Post-Tuning (IM240)	g/km	-0.052	-3.201	7.261
ODOMETER	Odo Readings	Km	-.176962D-05	-2.704	112777.419
TRANMISN	Transmission	0,1	-0.198	-2.539	0.328
ENG_CONF	Engine Configuration	0,1	0.525	4.150	0.914
Diagnostic: Log-L = -529.816 NOXPIM24		Restricted (b=0) Log-L = -610.307 Mean =1.55 6 S.D.= 0.875			

Model 12 estimation results (see Equations 10-14, Tables 10-43, 10-44 and 10-45) suggest:

- Both CO and NO_x are significant influences on HC. HC is more likely to increase slightly as CO increases. NO_x increases with the increase in HC.
- Both HC and NO_x are significant influences on CO. HC is more likely to increase with the increase in CO. However, NO_x and CO are correlated negatively, so that as NO_x increases CO decreases.
- Both HC and CO are significant emissions influencing NO_x. HC is more likely to increase with the increase in NO_x. However, CO increases slightly with the decrease in NO_x.

$$HC = -0.432 + 0.065 * CO + 0.348 * NO_X + 0.101 * ENG_DIS \\ + 0.142 * POINTST - 0.074 * TRAMISN$$

$$CO = 4.594 + 12.635 * HC - 2.48 * NO_X - 1.209 * ENG_DIS \\ + 1.412 * TRANMISN - 2.561 * POINTST$$

$$NO_X = 0.877 + 1.504 * HC - 0.058 * CO - 0.166 * ENG_DIS$$

(10-14)

Table 10-43 Estimation Results: HC M12

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			-0.432	-9.838	
COPSS60	CO Post-Tuning (SS60)	g/min	0.065	17.560	3.903
NOXPSS60	NO _x Post-Tuning (SS60)	g/min	0.348	9.005	0.713
ENG_DIS	Engine Displacement	liters	0.101	8.262	2.499
POINTST	Points condition after replaced in Tune-up	0,1	0.142	2.172	0.142
TRANMISN	Transmission	0,1	-0.074	-3.360	0.320
Diagnostic: Log-L = -17.120		Restricted (b=0) Log-L = -169.661			
HCPSS60		Mean = 0.317 S.D.= 0.343			

Table 10-44 Estimation Results: CO M12

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			4.594	6.364	
HCPSS60	HC Post-Tuning (SS60)	g/min	12.635	16.990	0.317
NOXPSS60	NO _x Post-Tuning (SS60)	g/min	-2.480	-3.521	0.713
ENG_DIS	Engine Displacement	liters	-1.209	-5.975	2.499
TRANMISN	Transmission	0,1	1.412	3.757	0.320
POINTST	Points condition after replaced in Tune-up	0,1	-2.561	-2.194	0.142
Diagnostic: Log-L = -1278.741		Restricted (b=0) Log-L = -1450.856			
COPSS60		Mean = 3.903 S.D.=4.765			

Table 10-45 Estimation Results: NO_x M12

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			0.877	10.496	
HCPSS60	HC Post-Tuning (SS60)	g/min	1.504	10.284	0.317
COPSS60	CO Post-Tuning (SS60)	g/min	-0.058	-4.137	3.903
ENG_DIS	Engine Displacement	Liters	-0.166	-6.212	2.499
Diagnostic: Log-L = -356.697		Restricted (b=0) Log-L = -408.58			
NOXPSS60		Mean = 0.713 S.D.= 0.560			

10.7 Measures of Emissions Responses to Changes with respect to Changes in the other Emissions

In this section, we quantify emissions responses to changes with respect to other emissions. We use the model specified in Equation 10-15. We define the indicators of responses to changes in i emission with respect to changes in j emission by percentages of changes in the mean of the i emission (Y_i) to changes in the mean of the j emission (Y_j), when the k emission is maintained at a given level (Y_k), as follows:

$$Y_i = \alpha + \delta_i X_i + \lambda_{ij} Y_j + \lambda_{ik} Y_k + \text{error}_i$$

$$\varepsilon_J^i = \lambda_{ij} * \frac{Y_j}{Y_i} \quad (10-15)$$

where: ε_J^i is elasticity of the i emission with respect to the j emission

We then derive the indicators of emission responses to changes with respect to changes in the other emissions, for each of HC, CO, and NO_x emissions in the twelve formulated models. These are presented in Table 10-46 and Table 10-47.

Table 10-46 Indicators of Changes in one Emission with respect to the Other Emissions: Pre Tuning

Model	Test	Indicators of HC		Indicators of CO		Indicators of NO _x	
		ε_{CO}^{HC}	ε_{NOX}^{HC}	ε_{HC}^{CO}	ε_{NOX}^{CO}	ε_{HC}^{NOX}	ε_{CO}^{NOX}
1	Pre-Tuning (CS505)	0.979	0.996	0.315	0.206	0.581	-0.014
2	Pre-Tuning (T867)	0.831	0.928	1.127	-0.904	0.859	-0.662
3	Pre-Tuning (H505)	0.914	0.002*	0.783	0.677	-0.073*	0.491
4	Pre-Tuning (ADR37)	0.562	0.331	1.067	0.552	0.125	0.348
5	Pre-Tuning (IM240)	1.034	0.730	0.783	-0.046*	0.120*	0.161
6	Pre-Tuning (SS60)	0.693	0.194*	0.758	0.447	0.006*	0.296

* indicates insignificant relations

Table 10-47 Indicators of Changes in one Emission with respect to the Other Emissions: Post Tuning

Model	Test	Indicators of HC		Indicators of CO		Indicators of NO _x	
		ϵ_{CO}^{HC}	ϵ_{NOX}^{HC}	ϵ_{HC}^{CO}	ϵ_{NOX}^{CO}	ϵ_{HC}^{NOX}	ϵ_{CO}^{NOX}
7	Post-Tuning (CS505)	0.589	0.851	0.675	-0.204	0.785	-0.250
8	Post-Tuning (T867)	0.691	1.150	0.660	-0.168*	0.668	-0.249
9	Post-Tuning (H505)	0.872	1.311	0.865	-0.745	0.489	-0.200
10	Post-Tuning (ADR37)	0.433	0.887	0.540	-0.020*	0.670	-0.069*
11	Post-Tuning (IM240)	0.594	1.047	0.496	-0.483	0.577	-0.241
12	Post-Tuning (SS60)	0.798	0.783	1.027	-0.453	0.669	-0.316

* indicates insignificant relations

We also investigate whether keeping outliers in the data influences the results of the models. We derive the indicators of emission responses to changes in the other emissions, for each of HC, CO, and NO_x emissions in the twelve models, based on the total sample size including outliers. These results are presented in Tables 10-48 and 10-49 and they indicate that outliers influence some results of the pre-tuning models.

Figure 10-48 Indicators of Changes in One Emission with respect to the Other Emissions: Pre Tuning including Outliers

Model	Test	Indicators of HC		Indicators of CO		Indicators of NO _x	
		ϵ_{CO}^{HC}	ϵ_{NOX}^{HC}	ϵ_{HC}^{CO}	ϵ_{NOX}^{CO}	ϵ_{HC}^{NOX}	ϵ_{CO}^{NOX}
1	Pre-Tuning (CS505)	1.227	1.068	0.496	-0.132	0.485	-0.374
2	Pre-Tuning (T867)	0.964	0.873	1.015	-0.840	0.953	-0.899
3	Pre-Tuning (H505)	0.836	0.094	0.946	0.525	-0.076	0.406
4	Pre-Tuning (ADR37)	0.739	0.023	0.886	0.687	-0.056	0.530
5	Pre-Tuning (IM240)	1.147	0.349	0.742	0.239	0.031	0.197
6	Pre-Tuning (SS60)	0.785	0.587	0.974	-0.212	0.722	-0.499

Figure 10-49 Indicators of Changes in one Emission with respect to the Other Emissions: Post Tuning including Outliers

Model	Test	Indicators of HC		Indicators of CO		Indicators of NO _x	
		ϵ_{CO}^{HC}	ϵ_{NOX}^{HC}	ϵ_{HC}^{CO}	ϵ_{NOX}^{CO}	ϵ_{HC}^{NOX}	ϵ_{CO}^{NOX}
7	Post-Tuning (CS505)	0.492	0.748	0.664	-0.254	0.616	-0.356
8	Post-Tuning (T867)	0.854	0.744	0.837	-0.253	0.822	-0.407
9	Post-Tuning (H505)	0.876	0.755	0.914	-0.353	0.580	-0.181
10	Post-Tuning (ADR37)	0.452	0.872	0.696	-0.160	0.673	-0.119
11	Post-Tuning (IM240)	0.518	0.946	0.386*	-0.099	0.634	-0.160
12	Post-Tuning (SS60)	0.782	0.533	1.170	-0.447	0.783	-0.413

* indicates insignificant relations

We conclude that outliers influence some of the results of pre-tuning models. We find obvious sign discrepancies between the results of the models that exclude outliers and the results of the models that include outliers, particularly in model 1, model 5, and model 6 (Tables 10-46 and 10-48). There exists particularly, sign discrepancies in the indicators for NO_x and CO. On the other hand, we find that outliers do not have any effects on the results of the post-tuning models. There are not any sign discrepancies between the results of the post tuning models that include outliers and those that exclude them.

Nevertheless, we do not discuss any further the results of the models that include outliers. Sections 10.8 and 10.9, thereafter, elaborate on the results of the models that exclude outliers, and discuss the hypothesis of the thesis in the view of the results of models that exclude outliers. Also, Chapter 11 concludes in view of the results of the models that exclude outliers.

We graph the relationships between indicators of responses to changes in HC, CO, and NO_x respectively to changes in the other emissions under six test drive-cycles, for each before and after vehicles were tuned. These are shown in Figures 10-1 and 10-2.

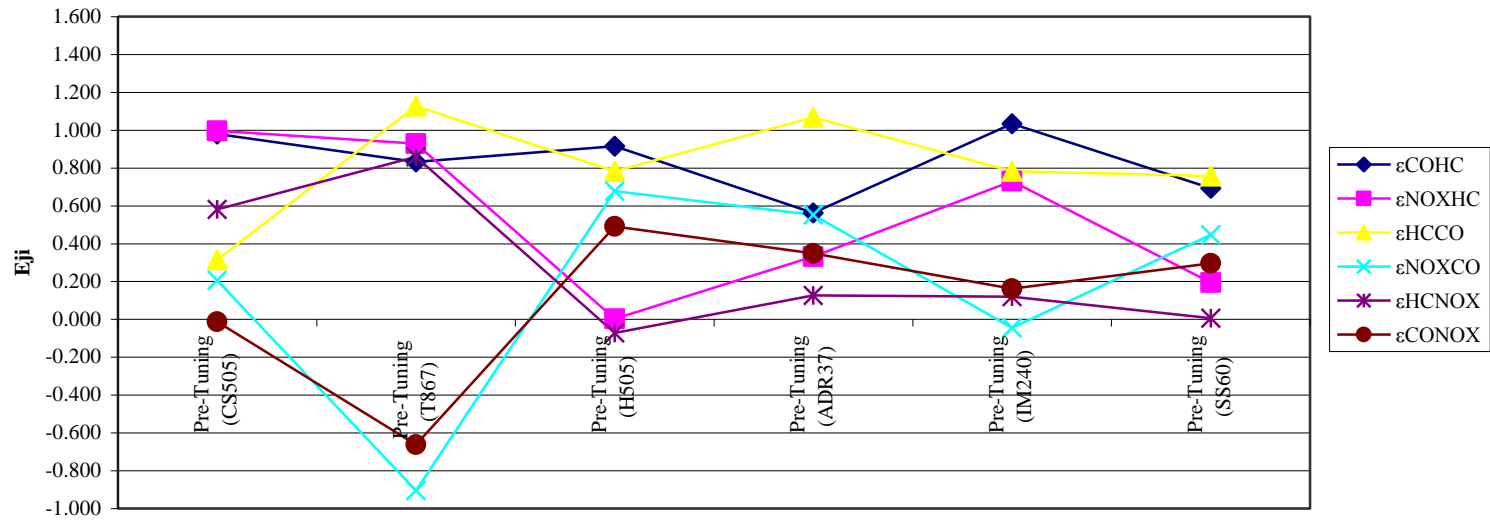


Figure 10-1 Measures of the Responses to Changes per Test Drive-Cycle: Pre-Tuning

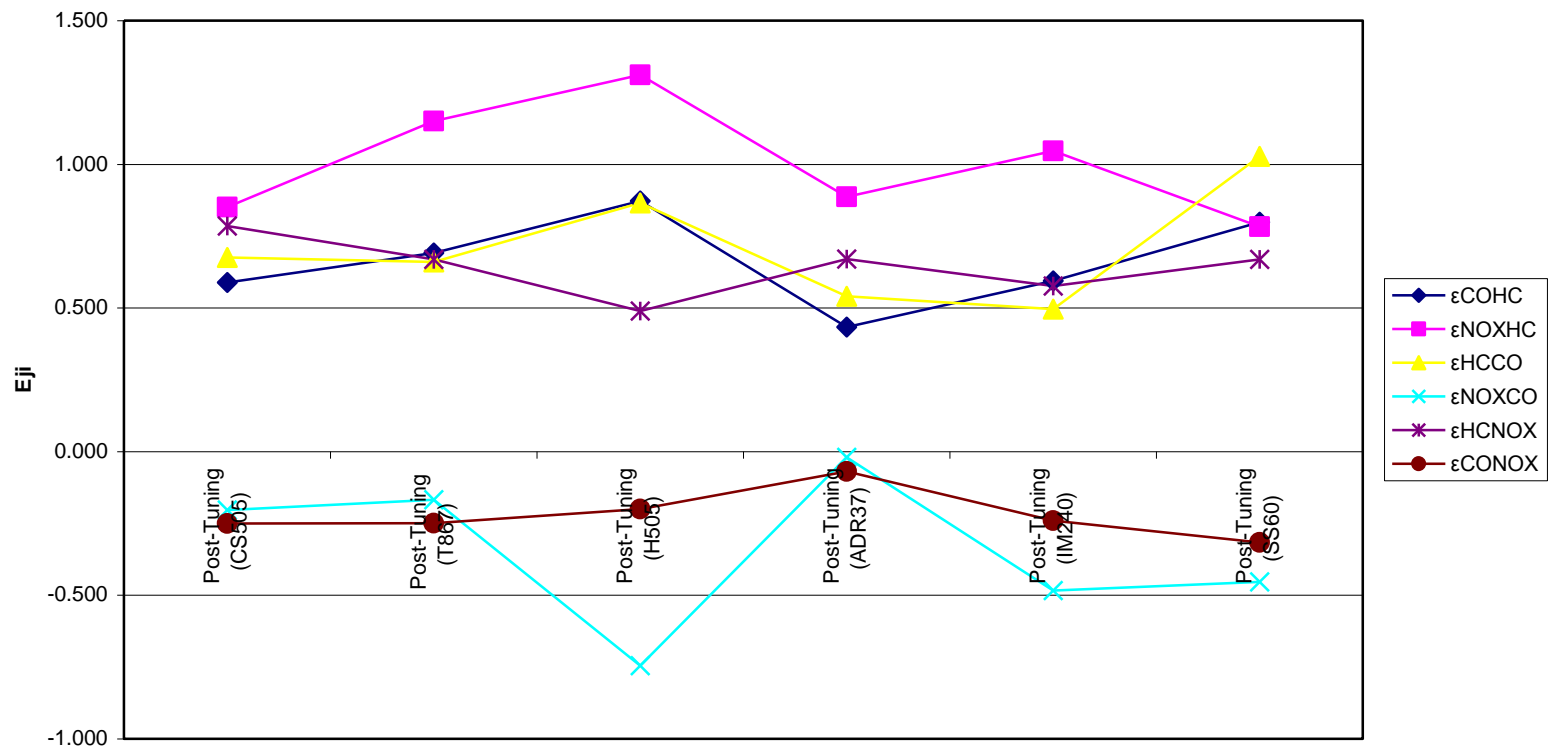


Figure 10-2 Measures of the Responses to Changes per Test Drive-Cycle: Post-Tuning

10.8 Interpretation of Modelling Vehicle Emissions Interdependencies

The modelling proposition of this thesis is that the formation of CO, HC, and NO_x emissions, within gasoline-fuelled engines for passenger vehicles, are combustion-chemistry related and are interdependent (Chapters 2 and 4). The main drivers that influence emissions, for each data set, are constrained, as follows: (i) the modal variables are limited to a specific test drive-cycle, because the models are separately formulated for each test drive-cycle; (ii) the observations are collected under standardised testing conditions; (iii) the testing responses of the engine, in terms of the air-fuel ratio and other engine parameters, are limited because of the vintage range of the engine technologies of the sample, i.e., between 1980 and 1991; and (iv) the air pollutant interdependencies are specified and discussed based on test drive-cycle averages.

In the context of this thesis, we find that HC, CO, NO_x emissions are endogenously dependent in a system of simultaneous-equations. We find sufficient evidence to reject that HC, CO, and NO_x emissions are not statistically significantly interdependent. We find for the thesis sample, that NO_x and CO are negatively correlated, whereas NO_x and HC are positively correlated. We also find that HC and CO are positively correlated. After inspecting the diagrams of HC, CO, and NO_x emissions versus air-fuel mixtures in Figure 4-11 of Chapter 4, the findings of this thesis line up with the fuel rich-side diagrams. Gasoline-fuelled engines operate within a fuel equivalence ratio (Φ) between 1.18 and 0.84 (see Section 4.5 in Chapter 4). Nevertheless, old vehicles are more likely to operate under fuel-rich operations (Kazopoula *et al.*, 2005). Moreover, vehicle kilometres travelled also strongly correlated with vehicle age (see Section 3.3.4.3 in Chapter 3).

We also investigate emission responses to a one percent increase in an emission with respect to the other emissions. We find the relations between CO and NO_x are of special interest. We find that a one percent increase in NO_x is associated with a 0.35 percent average decrease in CO and that a one percent increase in CO is associated with a 0.22 percent average decrease in NO_x for vehicles after they

were tuned. We find that emission responses to change with respect to the other emissions vary with various test drive-cycles (see Section 5.4.2 in Chapter 5). However, a band of upper and lower limits include these variations.

We find that

- A 1 percent increase in HC is associated a 0.5 to 0.8 percent increase in NO_x , and also is associated with a 0.5 to 1 percent increase in CO, for vehicles after they were tuned.
- A 1 percent increase in HC is associated with a 0.125 to 0.859 percent increase in NO_x , and with between a 0.315 to 1.127 percent increase in CO, for vehicles before they were tuned.
- A 1 percent increase in CO is associated with a 0.4 to 0.9 percent increase in HC, and with a 0.07 to 0.32 percent decrease in NO_x , for vehicles after they were tuned.
- A 1 percent increase in CO is associated with a 0.562 to 1.034 percent increase in HC, and with a 0.014 to 0.662 percent decrease in NO_x , for vehicles before they were tuned.
- A 1 percent increase in NO_x is associated with a 0.8 to 1.3 percent increase in HC, and with a 0.02 to 0.7 percent decrease in CO, for vehicles after they were tuned.
- A 1 percent increase in NO_x is associated with a 0.331 to 0.996 percent increase in HC, and with a 0.046 to 0.904 percent decrease in CO, for vehicles before they were tuned.

These measures of the responses are very important derivatives of the findings of the thesis. They estimate the impacts of traffic management schemes when reducing a targeted emission on the other non-target emissions.

We have so far developed models for testing the hypothesis of the thesis the interdependencies of HC, CO, and NO_x emissions. We have established that it is possible that an increase in one emission is associated with a decrease in another emission, *ceteris paribus*. We investigate the responses of a 1% increase in an emission on the other emissions (Table, 10-50). We demonstrate, for example, that

a 1% increase in NO_x is associated with a 0.02 to 0.7 percent decrease in CO (Table 10-50).

Table 10-50 Effects of Emission Responses to 1% Increase in the other emissions

	1% increase in HC	1% increase in CO	1% increase in NO _x	
HC	1%	1.0	1.0	M 1_Pre-Tuning
CO	0.3	1%	0.2	
NO _x	0.6	-0.01	1%	
Test cycle 1_CS505				
HC	1%	0.6	0.9	M 7_Post-Tuning
CO	0.7	1%	-0.2	
NO _x	0.8	-0.25	1%	
Test cycle 2_T867				
	HC	CO	NO _x	
HC	1%	0.8	0.9	M 2_Pre-Tuning
CO	1.1	1%	-0.9	
NO _x	0.9	-0.66	1%	
Test cycle 2_T867				
HC	1%	0.7	1.1	M 8_Post-Tuning
CO	0.7	1%	0.2	
NO _x	0.7	-0.25	1%	
Test cycle 3_H505				
	HC	CO	NO _x	
HC	1%	0.9	0.002	M 3_Pre-Tuning
CO	0.8	1%	0.7	
NO _x	-0.1	0.49	1%	
Test cycle 3_H505				
HC	1%	0.9	1.3	M 9_Post-Tuning
CO	0.9	1%	-0.7	
NO _x	0.5	-0.20	1%	
Test cycle 4_ADR37				
	HC	CO	NO _x	
HC	1%	0.6	0.3	M 4_Pre-Tuning
CO	1.1	1%	0.6	
NO _x	0.1	0.35	1%	
Test cycle 4_ADR37				
HC	1%	0.4	0.9	M 10_Post-Tuning
CO	0.5	1%	0.02	
NO _x	0.7	0.07	1%	
Test cycle 4_ADR37				
HC	1%	1.0	0.7	M5_Pre-Tuning
CO	0.8	1%	0.05	
NO _x	0.1	0.16	1%	

	1% increase in HC	1% increase in CO	1% increase in NO _x	
Test cycle 5_IM240				
HC	1%	0.6	1.0	M 11_Post-Tuning
CO	0.5	1%	-0.5	
NO _x	0.6	-0.24	1%	
Test cycle 6_SS60				
	HC	CO	NO _x	
HC	1%	0.7	0.19	M 6_Pre-Tuning
CO	0.8	1%	0.4	
NO _x	0.0	0.30	1%	
Test cycle 6_SS60				
HC	1%	0.8	0.8	M 12_Post-Tuning
CO	1.0	1%	-0.5	
NO _x	0.7	-0.32	1%	

The numbers with the diagonal shades are insignificantly correlated
 All numbers are in percentiles, e.g., 0.7 is 0.7%

10.9 The Chapter Summary

In this chapter, we estimate twelve models for vehicle emissions interdependencies under six test drive-cycles, for each of before and after vehicles were tuned using the 3SLS method. The models presented in the sets of Equations 10-1 through to 10-12, which shows linear additive of the other emissions, are designed to provide an improved understanding of the discussions of the results of Model 1 through to Model 12. These models, providing everything else is the same, are not as important as the evidence of testing the comprehensive hypothesis of the thesis, i.e., that HC, and CO, and NO_x emissions are jointly dependent (see also Section 10.5). In fact, the theory of the thesis demonstrates complex nature of relationships among HC, CO, and NO_x emissions (see Figures 4-11, 4-18, and 4-19 of Chapter 4, and also Appendix III). However, the nature of these behaviours across the on-road vehicles population and driving patterns is not obvious. Three-stage least-squares (3SLS) regression is employed to test the hypothesis of the thesis that vehicle emissions are interdependent. 3SLS regression is also employed to gain insights into the simultaneous effects of vehicle variables and other vehicle emissions on each emission. We use linear estimation of the system of three least squares equations, although Chapter 4 shows complex behaviour of HC, CO, and NO_x emissions (see Section 10.5). We estimate the formulated models and the maximum likelihood that the vehicle variables and other emissions will influence

simultaneously each of HC, CO, and NO_x emissions. We calculate direct elasticity to measure the responses of an emission to changes with respect to changes in the other two emissions. We then, investigate the effects of a 1 percent increase in an emission on the other two emissions. The results of the findings show clear variations, but also show general trends. They vary with various test drive-cycles; however, a band of upper and lower limits contain these variations

Based on the results of the estimations of the twelve models formulated, we find for the thesis sample, that NO_x and CO are negatively correlated, whereas HC and CO are positively correlated and HC and NO_x are positively correlated. We then investigate emission responses to a one percent increase in an emission with respect to the other emissions. The relations between CO and NO_x were of special interest, we find that a one percent increase in NO_x is associated with a 0.35 percent average decrease in CO and that a one percent increase in CO is associated with a 0.22 percent average decrease in NO_x, for vehicles after they were tuned.

The final results of the models, which indicate that HC, CO, and NO_x are inter-correlated, are not too surprising. The formation of CO, HC, NO_x emissions are combustion-chemistry related, and are interdependent (see Chapters 2 and 4). Nevertheless, previous modelling studies have not recognised the interaction effects of vehicle emissions, and have assumed independent formation of the emissions. Consequently, they have used ordinary least squares (OLS) regression to estimate HC, CO, NO_x emissions separately and independently of each other.

Within each data set, the main factors that affect emissions are constrained, as follows:

- The models, formulated in this chapter, are developed separately for each cycle, which constrains the modal variables to a specific test drive-cycle pattern.
- Observations are collected under standardised test drive-cycles. These standardised test drive-cycles control the testing conditions of each cycle, i.e., fuel properties, temperature, and humidity, and in turn constrain emissions.

- The technological groups of the sample, i.e., the model year range between 1980 and 1991, constrain the engine technologies, emission control systems, and electronic control module. Engine technologies govern the response of the engine to testing, in terms of air-fuel ratio and other parameters of the engine.

Because the primary drivers of emissions are constrained, within each data set, the responses of emissions to the cycles would likely be highly correlated, even if CO, HC, and NO_x formation were absolutely independent. Notwithstanding that, we acknowledge that the models are actually not as important as the general findings and conclusions of this thesis that vehicle emissions are interdependent. These findings provide useful insights within transport policy context (See Section 11.3 in Chapter 11).

Chapter Eleven

Conclusions

This chapter summarises the contributions and the main findings of the thesis. The chapter also identifies areas for further research.

11.1 The Thesis Contributions

The modelling proposition of this thesis is that the formation of CO, HC, and NO_x emissions within gasoline-fuelled engines of passenger vehicles are combustion-chemistry-related and interdependent (Chapter 2, Chapter 4, and Appendix III). Previous modelling studies, with rare exception, have not recognised that vehicle emissions are endogenously or jointly dependent and therefore, have assumed independent formation of CO, HC, and NO_x emissions. Consequently, they have used ordinary least-squares (OLS) regression to estimate HC, CO, and NO_x emissions independently of each other. These studies have considered that the interaction effects at the combustion-chemistry level and within the catalytic converter were insignificant, relative to the vehicle operating conditions, fuel characteristics, and the other environmental factors that influence air: fuel ratio, peak combustion temperature, and emissions control system efficiency. The major contribution of the thesis is to investigate the inter-correlations between vehicle emissions within a controlled dataset, and to test the hypothesis of vehicle emissions interdependencies.

The thesis employs three-stage least-squares (3SLS) regression to estimate twelve models formulated to test interdependencies among HC, CO, and NO_x emissions. We find for each model that HC, CO, and NO_x emissions are endogenously or jointly dependent in a system of three simultaneous-equations. The investigation in Chapter 10 of the hypothesis of vehicle emissions interdependencies shows strong evidence to reject the null hypothesis (H_0) - HC, CO, and NO_x emissions are not statistically significantly interdependent, in favour of the alternative hypothesis (H_1) - HC, CO, and NO_x emissions are statistically significantly interdependent.

We find, for the sample, that NO_x and CO emissions are negatively correlated, HC and CO emissions are positively correlated, and NO_x and HC emissions are positively correlated.

The thesis also identifies the emission responses to changes in the other emissions. The measures of responses to change are important derivatives of the investigations of the hypothesis of vehicle emissions interdependences. They estimate the impacts of reducing one targeted emission on the other non-targeted emissions, *ceteris paribus*. We derive emission responses to a one percent increase in an emission with respect to the other emissions. We find that emission responses to changes vary with various test drive-cycles (see Section 5.4.2 in Chapter 5). The results presented in Section 10.8 in Chapter 10 show clear variations, but they also show general trends. We find that the variations are contained within a band of upper and lower limits. For vehicles after they were tuned, a one percent increase in HC is associated with an increase in NO_x between 0.5 and 0.8 percent, and with an increase in CO between 0.5 percent and one percent. Also, for vehicles after they were tuned, a one percent increase in CO is associated with an increase in HC between 0.4 percent and 0.9 percent, and with a decrease in NO_x between 0.07 percent and 0.32 percent. Furthermore, a one percent increase in NO_x is associated with an increase in HC between 0.8 and 1.3 percent, and with a decrease in CO between 0.02 percent and 0.7 percent. We conclude that it is possible to establish estimates of emission responses to changes in other emissions. Most interestingly, we find that the relationship between CO and NO_x is of special interest. For vehicles after they were tuned, we find that those vehicles that exhibit a one percent increase in NO_x exhibit simultaneously a 0.35 percent average decrease in CO. Similarly, we find that those vehicles that exhibit a one percent increase in CO exhibit simultaneously a 0.22 percent average decrease in NO_x .

We investigated the inter-correlations between HC, CO, and NO_x emissions within a well-controlled dataset, also we provide discussions on associated related effects and policy implications. The findings of the thesis, after investigating vehicle emissions interdependencies, yield insights that advance our knowledge regarding vehicle emissions, and also bridge an important gap in the current vehicle

emissions state of art. The thesis provides decision-makers with valuable knowledge on how changes in the operation of the transport system might affect urban air-quality, and hence they can identify effective traffic management schemes that counteract the most adverse impacts of traffic pollution on the urban air-quality. A better understanding of the relationship between vehicle emissions can help decision-makers to reach reasoned decisions with regards to mitigating the worse impacts of vehicle emissions. The thesis informs policymakers of the complex nature of the formation of vehicle emissions, and also that a set of vehicle drivers function together and are collectively accountable for producing emissions. The thesis alerts transport policymakers to the fact that an emission control strategy that is implemented to mitigate one vehicle emission may actually elevate other vehicle emissions (Chapter 3). Therefore, strategically speaking, actions undertaken within a transport policy and urban air-quality context should target reducing the most adverse impacts of traffic pollution (see Chapter 3 and Appendix IV). Furthermore, the findings shed more light on the way that vehicle emissions influence enhanced greenhouse gases, and thereby degrade air-quality (Chapter 1 and Dabbas, 2004). A study by Yedla *et al.* (2005) found that urban transport strategies that target mitigating local pollution, such as HC and total suspended particulate matter (TSP), also show potential to reduce a non-target pollutant, such as CO₂, an enhanced greenhouse gas.

The findings that HC, CO, and NO_x emissions are statistically significantly interdependent, bridge an important gap in the current vehicle emissions state of art, and has important implications in developing predictive models of vehicle emissions. The thesis highlights the need to use more accurate tools in estimating predictive models for vehicle emissions that support a modelling approach in which HC, CO, and NO_x emissions are estimated simultaneously. The interaction effects of vehicle emissions, in-engine and in-catalyst especially, may be important enough to represent in new forecasting models. However, larger and better designed datasets that represent traffic composition mix and drive operating conditions of on-road vehicles fleet are needed, in order to make the case.

11.2 Further Considerations

Although this thesis bridges a gap in our current knowledge on the estimations of vehicle emissions, additional, more detailed research with larger data sets that cut across more on-road driving conditions and represent the modern vehicle fleet is needed to address further issues. The empirical research predates the recent survey of passenger vehicle emissions performance (NISE-2), which was undertaken between December 2007 and December 2008 by the Commonwealth Department of Environment, Water, Heritage, and the Arts. The findings herein however, reinforce the need for NISE-2 to take into account, in analysis using more recent data, the interdependencies between emissions. Moreover, we recommend that NISE-2 study collect more detailed data, especially employing test drive-cycles that represent better the actual on-road drive operating conditions, such as enrichment vehicle events.

Avenues for further research considerations are listed below. We recommend:

- (1) investigating several databases on vehicle emissions, for example NISE-2, in order to establish common measures of the responses of emissions to changes with respect to changes in the other emissions.
- (2) that the ongoing NISE-2 study collect more detailed information, particularly which shows the air: fuel ratio reading with time and speed readings for each test cycle and sub-cycle. This would allow further research to predict using vehicle characteristics when vehicles become high emitters.
- (3) the undertaking of comparative studies of vehicle emission prediction models that accounts for the endogenous relations between HC, CO, and NO_x emissions and other prediction models that do not take these endogenous relations into consideration
- (4) extending the research to investigate the interdependencies

- a. of other vehicle emissions, such as CO₂ and PM.
 - b. of vehicle emissions for other vehicles, such as freight vehicles, and
 - c. of vehicle emissions for other types of fossil fuels, such as diesel.
- (5) investigating present vehicle engine technologies and the impacts of their use and the use of other alternative design options on minimising a target emission on the other vehicle emissions.

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Appendix I
Initial Coding of the Raw Data

Table 1 Raw Data Codings

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
LABORATORY	LAB	alpha		1 = FORD 2 = NSW 3 = VIC		0.0%
AGB Mc Nair #	ID_No	numeric (categorical)			Each vehicle sourced by AGB McNair was allocated an AGB ID	0.0%
Vehicle Make	MAKE	alpha		1 = Ford 2 = Holden 3 = Mitsubishi 4 = Nissan 5 =Toyota		0.0%
Vehicle Model	MODEL	alpha		10= Ford Cortina 11 = Ford Fairlane 12 = Ford Falcon 13 = Ford Laser 14 = Ford Telstar 15 = Ford Fairmont 16 = Ford escort 17 = Ford LTD	Falcon / Fairmont / / Fairlane Telstar Laser / Meteor Cortina	
				18 = Ford Corsair	Escort	

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
				19 = Ford Meteror 20 = Holden Calais 21 = Holden Camira 22 = Holden Commodor 23 = Holden Gemini 24 = Holden Statesman 25 = Holden Sunbird 26 = Holden Astra 27 = Holden Apollo 28 = Holden Nova	Commodore/Berlina/ /Calais/Vacationer Statesman Camira Apollo Astra Nova Torana/Sunbird	0.0%
				30 = Mits Colt 31 = Mits Magna 32 = Mits Sigma 33 = Mits Lancer	Magna Sigma Colt	
				40 = Nissan Bluebird	Pintara	
				41 = Nissan Pulsar 42 = Nissan Stanza 43 = Nissan Pintara 44 = Nissan Skyline 45 = Nissan Pinjarra 46 = Nissan 200B	Bluebird Pulsar Datsun 120Y Datsun 200B	
				50 = Toyota Corolla 51 = Toyota Corona	Lexcen Camry	

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
				52 = Toyota Camry 53 = Toytoa Corolla Tercel 4WD 54 = Toyota Lexcen	Corona Corolla	
Body Type	BODY	alpha		1=Sedan 2=Wagon 3=Van 4= H/ Top 5= Hatch		0.0%
Compliance Date	COMP_DAT	date		1980		0.0%
Emission Standard	ADR	numeric (categorical)		27 37		0.0%
Vehicle Mass	MASS	numeric (continuous)	Kg			0.0%
Odo Reading	ODOMETER	numeric (continuous)	Km		Cell (159xI) contains 117297 Odo not working	0.185%
Engine Management System	ENG_SYS	alpha		1 = Y 2 = N		0.0%
Type of Air Injection System	A_IJ_SYS	alpha		4 = NF 15 = PA 16 = AP		0.0%
Engine Displacement	ENG_DIS	numeric	Liters			

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
		(continuous)				0.0%
No. of Cylinders	N_CYLIND	numeric (categorical)		4, 6, 8		0.0%
Engine Configuration	ENG_CONF	alpha		18=I 19=V		0.0%
Transmission on I Gears	GEAR_TYP	alpha		15=A3 16=A4 17=M3 18=M4 19=M5	Could be a Typing Error One cell contains the letter "A " Cell (287x S), must be A4 Similar to the above & below row	0.0%
Fuel System	FUEL_SYS	alpha		17 = C 18 = I		0.0%
Choke	CHOKE	alpha		3=NA 4=NF 15=A 16=M		0.0%
Catalyst Present	CATALYST	alpha		1=Y 2=N 3=NA		0.0%

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
Air Conditioning	AIR_COND	alpha		1=Y 2=N		0.0%
Inertia Category	INERTIA	numeric (continuous)	(Kg)			0.185%
Exhaust Comp Secure?	EXHASUT	alpha		1=Y 2=N		0.0%
Engine Oil OK?	ENG_OIL	alpha		1=Y 2=N		0.0%
Trans. Fluid Level OK?	FLUID_LV	alpha		1=Y 2=N		0.0%
Trans Fluid level Action	FLD_LV_A	alpha		2 = N 20=AD		54.6%
Radiator Coolant level Ok?	RD_CL_LV	alpha		1=Y 2=N		0.0%
Battery Water level OK?	BAT_W_LV	alpha		1=Y 2=N 6=P		0.0%
Fuel Filter Ok?	FUEL_FLT	alpha		1=Y		

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
				2=N 3=NA		0.0%
Air Filter OK?	AIR_FLT	alpha		1=Y 2=N 6=P		0.0%
Distributor Functional?	DIST_FUN	alpha		1=Y 2=N		0.00%
Test for Catalyst Converter Rattle	CATYST_TS	alpha		3=NA 1=Y 2=N 3=NA		0.00%
EGR Operational?	EGR_OPER	alpha		1=Y 2=N 3=NA		0.00%
EGR Action Taken	EGR_ACT	alpha		2=N 10=clean 11=RE 12=RECONNECT 15=REPLACE 14=REPAIR 15=FIX		0.185%
Evap Canister Fitted &	EVP_CANS	alpha		1=Y		

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
Operational				2=N 3=NA		0.00%
Canister Action Taken	CANS_ACT	alpha		2=N 11=RE 12=RECONNECTED	Could be a Typing Error in cell (471x AH) contains RECO must be RECONNECTED	4.43%
Vacuum Hose Condition Ok?	V_HOS_CT	alpha		1=Y 2=N		19.37%
Vacuum Hose Action Taken	V_HS_ACT	alpha		2 = N 11=RE		19.37%
O ₂ Sensor Fitted & Operational	O2_SENS	alpha		1=Y 2=N 3=NA		0.00%
Air Preheat Fitted & Operational	AR_BH_F	alpha		1=Y 2=N 3=NA	Could be a Typing Error in cell (143x AK) & (533x Ak) contain " Y" must be instead "Y"	52.03%
Air Preheat Action Taken	AR_BH_AC	alpha				

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
				2=N 11=RE 12=RECONNECTED 13=REPLACE		3.69%
EEMS Operational?	EEMS_OPR	alpha		1=Y 2=N 3=NA		0.00%
High Tension Leads OK?	H_T_LEAD	alpha		1=Y 2=N		0.00%
Timing (Air On) Pre test	TM_ARO_B	numeric & alpha		various words	2ATDC,AM,5ATDC,no. B, OK,SPEC,NOTCH,NA,T DC	3.69%
Timing Spec	TM_SPEC	numeric & alpha		various words	SPEC,NOTCH,5ATDC,v alue+value value+-value, value+/- value	0.74%
Timing (Air On) Post Tune	TM_ARO_P	numeric & alpha		various words	2ATDC,AM, 5ATDC,no.B, OK,SPEC,NOTCH,NA,T DC	1.48%
Spark Plug Condition/Gap	SPARK_GAP	alpha		6=P 7=OK		0.00%

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
Plug Gap Pre test	PLG_GAPB	numeric & alpha		3=NA 5=NR	value-value	3.69%
Plug Gap Spec	PLG_GAPS	numeric & alpha		8=NS	value+-value, value+/- value value+/- value-value, value+/- 0+BJ470.o5	0.18%
Plug Gap Post Tune	PLG_GAPP	numeric & alpha		5=NR		0.55%
Points Condition	PTS_CONT	alpha		3 = NA 6 = P 7 = OK		0.00%
Dwell Angle Pre Test	DW_ANG_B	numeric & alpha		3=NA 5=NR		25.28%
Points/DweII Spec	DW_SPEC	numeric & alpha		3=NA 8=NS	value+-value, value+/- value value- value,cell(173xAY)49to5 0	11.62%
Points/DweII Post Tune	DW_ANG_P	numeric & alpha		3=NA		27.31%
Idle CO% Pre Test Air On	ICO_B_AO	numeric & alpha	%	3=NA 5=NR	>value	10.33%
Idle CO% Pre Test Air off	ICO_B_AF	numeric & alpha	%	3=NA 5=NR	>value	1.85%
Idle CO% Spec	ICO_SPEC	numeric & alpha	%	8=NS	value+-value, value+/- value	

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
		alpha			value-value,0.5+BR482 0.05+BR537, SEALED, <value value MAX	18.63%
Idle CO% Post Tune Air On	ICO_P_AO	numeric & alpha	%	5=NR		8.30%
Idle CO% Post Tune Air Off	ICO_P_AF	numeric & alpha	%	3=NA 5=NR		2.21%
Idle HC ppm Pre Test Air On	IHC_B_AO	numeric & alpha	(ppm)	5=NR		1.11%
Idle HC ppm Pre Test Air Off	IHC_B_AF	numeric & alpha	(ppm)	3=NA 5=NR 8=NS		0.00%
Idle HC ppm Spec	IHC_SPEC	alpha	(ppm)	3=NA 8=NS		31.18%
Idle HC ppm Post Tune Air On	IHC_P_AO	numeric & alpha	(ppm)	5=NR		2.40%
Idle HC ppm Post Tune Air Off	IHC_P_AF	numeric & alpha	(ppm)	3=NA 5=NR 8=NS		0.00%
Idle O2% Pre Test Air On	IO2_B_AO	numeric & alpha	%	5=NR	(542xBK)=0.4 general form (520xBK)=0.2 general form	6.46%
Idle O2% Pre Test Air Off	IO2_B_AF	numeric &	%	3=NA		

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
		alpha		5=NR 8=NS		1.85%
Idle O2% Spec	IO2_SPEC	numeric & alpha	%	8=NS		31.18%
Idle O2% Post Tune Air On	IO2_P_AO	numeric & alpha	%	3=NA 5=NR		5.35%
Idle O2% Post Tune Air Off	IO2_P_AF	numeric & alpha	%	3=NA 5=NR 8=NS		2.58%
Idle Speed rpm Pre Test Air On	IS_B_AO	numeric & alpha	rpm	5=NR	One cell (141xBP)contains value+/-value	0.55%
Idle Speed rpm Pre Test Air Off	IS_B_AF	numeric & alpha	rpm	3=NA 5=NR 8=NS		0.00%
Idle Speed rpm Spec	IS_SPEC	numeric & alpha	rpm	3=NA 8=NS	value+-value,value+/- value value-value,	0.37%
Idle Speed rpm Post Tune Air On	IS_P_AO	numeric & alpha	rpm	5=NR		1.66%
Idle Speed rpm Post Tune Air Off	IS_P_AF	numeric & alpha	rpm	3=NA 5=NR 8=NS		1.11%
Modifications to vehicle	MODIFY	alpha		1=Y		

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
affecting Emissions ?				2=N		0.00%
Type of Modifications	MODF_TYP	alpha		various parts in words		
Comments on Modifications	COM_MODF	alpha		various parts in words		
Is vehicle Fitted with proprietary parts ?	PROP_PRT	alpha		1=Y 2=N		0.00%
Oil Replaced in Tune-up?	OIL_CH_T	alpha		1=Y		0.00%
Oil Filter Replaced in Tune-up?	OLF_CH_T	alpha		1=Y		0.00%
Air Filter Replaced in Tune-up?	ARF_CH_T	alpha		1=Y		0.00%
POINTS Replaced in Tune-up?	PTS_CH_T	alpha		1=Y 2=N 3=NA		0.00%
SPARK PLUGS Replaced in Tune-up?	PLG_CH_T	alpha		1=Y 2=N		0.00%
FUEL FILTER	FUF_CH_T	alpha		1=Y		

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
Replaced in Tune-up?				2=N 3=NA		0.74%
DISTIBUT OR CAP Replaced in Tune-up?	DCAP_C_T	alpha		1=Y 2=N 3=NA		2.03%
ROTOR BUTTON Replaced in Tune-up?	RBUT_C_T	alpha		1=Y 2=N 3=NA		2.21%
HT LEADS Replaced in Tune-up?	HT_LDS_T	alpha		1=Y 2=N 3= NA		0.74%
FUEL CAP Replaced in Tune-up?	FCAP_C_T	alpha		1=Y 2=N	Could be a Typing Error in cells (470x CH) & (495xCH) contain n,must be N	2.21%
O2 SENSOR Replaced in Tune-up?	O2SN_C_T	alpha		1=Y 2=N 3=NA	Could be a Typing Error in cells (470x CH) & (495xCH) contain n,must be N	2.40%
CATALYST Replaced in Tune-up?	CTALS_C_T	alpha		1=Y 2=N 3=NA		2.40%
OTHER Item Replaced in Tune-up ?	ITM_CH_T	alpha		1=Y 2=N		10.52%

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
				words		
OTHER Item Replaced in Tune-up ?	ITM_C_T1	alpha		1=Y 2=N words		14.39%
OTHER Item Replaced in Tune-up ?	ITM_C_T2	alpha		1=Y 2=N words		14.76%
OTHER Item Replaced in Tune-up ?	ITM_C_T3	alpha		1=Y 2=N words		46.49%
TOTAL PARTS COST:	TP_COST	Currency			\$ Sign	0.00%
AJUSTED TOTAL PARTS COST	ATP_COST	Currency			\$ Sign	0.00%
HC Pre-CS505	HCbCS505	numeric	grams			0.0%
HC Post-CS505	HCpCS505	numeric	grams			0.0%
CO Pre-CS505	CObCS505	numeric	grams			0.0%
CO Post-CS505	COpCS505	numeric	grams			0.0%
NOx Pre-CS505	NOxbCS55	numeric	grams			

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
						0.0%
NOx Post-CS505	NOXpCS55	numeric	grams			0.0%
HC Pre-T867	HCb_T867	numeric	grams			0.0%
HC Post-T867	HCp_T867	numeric	grams			0.0%
CO Pre-T867	COb_T867	numeric	grams			0.0%
CO Post-T867	COp_T867	numeric	grams			0.0%
NOx Pre T867	NOXb T867	numeric	grams			0.0%
NOx Post-T867	NOXp T867	numeric	grams			0.185%
HC Pre-H 505	HCb_H505	numeric	grams			0.0%
HC Post-H 505	HCp_H505	numeric	grams			0.0%
CO Pre-H505	COb_H505	numeric	grams			0.0%
CO Post-H505	COp_H505	numeric	grams			0.0%
NOx Pre H505	NOXbH505	numeric	grams			

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
						0.0%
NOx Post-H505	NOXpH505	numeric	grams			0.0%
HC Pre-ADR27	HCbADR27	numeric	(g/km)			66.61%
HC Post-ADR27	HCpADR27	numeric	(g/km)			66.61%
CO Pre-ADR27	CObADR27	numeric	(g/km)			66.61%
CO Post-ADR27	COpADR27	numeric	(g/km)			66.61%
NOx Pre-ADR27	NOxbADR2	numeric	(g/km)			66.61%
NOx Post-ADR27	NOxpADR2	numeric	(g/km)			66.61%
Fuel Cons Pre-ADR27	FCb_ADR27	numeric	L/100km			66.61%
Fuel Cons Post-ADR27	FCp_ADR27	numeric	L/100km			66.61%
HC Pre-ADR37	HCbADR37	numeric	(g/km)			0.0%
HC Post-ADR37	HCpADR37	numeric	(g/km)			

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
						0.0%
CO Pre- ADR37	CObADR37	numeric	(g/km)			0.0%
CO Post-ADR37	COpADR37	numeric	(g/km)			0.0%
NOX Pre- ADR37	NOX bADR3	numeric	(g/km)			0.0%
NOX Post-ADR37	NOX pADR3	numeric	(g/km)			0.0%
Fuel Cons Pre-ADR37	FCb_ADR37	numeric	L/100km			0.0%
Fuel Cons Post-ADR37	FCp_ADR37	numeric	L/100km			0.00%
HC Pre-Shed	HCb_SHED	numeric & alpha	(g/test)	3=NA 5=NR		21.40%
HC Post-Shed	HCp_SHED	numeric & alpha	(g/test)	3=NA 5=NR		21.40%
HC Pre-SS60	HCb_SS60	numeric	(g/min)			0.37%
HC Post-SS60	HCp_SS60	numeric	(g/min)			1.11%
CO Pre-SS60	COb_SS60	numeric	(g/min)			0.18%

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
CO Post-SS60	COp_SS60	numeric	(g/min)			0.18%
NOx Pre-SS60	NOXbSS60	numeric	(g/min)			0.37%
NOx Post-SS60	NOXpSS60	numeric	(g/min)			0.37%
HC Pre-IM240	HCbIM240	numeric	(g/km)			0.55%
HC Post-IM240	HCpIM240	numeric	(g/km)			0.0%
CO Pre-IM240	CObIM240	numeric	(g/km)			0.18%
CO Post-IM240	COpIM240	numeric	(g/km)			0.0%
NOX Pre IM240	NOXbIM24	numeric	(g/km)			0.37%
NOX Post-IM240	NOXpIM24	numeric	(g/km)			?
HC Pre-ASM	HCb_ASM	numeric	(ppm)			8.67%
HC Post-ASM	HCp_ASM	numeric	(ppm)			9.04%
CO Pre-ASM	COb_ASM	numeric	(% vol)			12.92%

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
CO Post-ASM	COp_ASM	numeric	(% vol)			14.39%
NO Pre-ASM	NOb_ASM	numeric & alpha	(ppm)	5=NR	> Value	2.21%
NO Post-ASM	NOp_ASM	numeric & alpha	(ppm)	5=NR	> Value	2.58%
NOx Pre-ASM	NOxb_ASM	numeric & alpha	(ppm)	3=NA 5=NR	Value ++	19.74%
NOx Post-ASM	NOxp_ASM	numeric & alpha	(ppm)	3=NA 5=NR		20.11%
HC Pre-Idle	HCb_IDLE	numeric	(ppm)			5.72%
HC Post-Idle	HCp_IDLE	numeric	(ppm)			5.17%
CO Pre-Idle	COb_IDLE	numeric & alpha	(% Vol)		One cell (151xEW) contains >10.5	11.62%
CO Post-Idle	COp_IDLE	numeric	(% Vol)			12.55%
HC Pre- High Idle	HCb_HIDL	numeric	(ppm)			13.84%
HC Post- High Idle	HCp_HIDL	numeric	(ppm)			10.70%

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
CO Pre- High Idle	COb_HIDL	numeric	(% vol)			11.25%
CO Post High Idle	COp_HIDL	numeric	(% vol)			11.62%
NO Pre-ASM Chem	NOb_ASMC	numeric & alpha	(ppm)	5=NR	>Value Value+	19.6%
NO Post- ASM Chem	NOp_ASMC	numeric & alpha	(ppm)	5=NR	>Value, One cell(18xFD) contains Typing error 1141..7	19.7%
NOX Pre-ASM chem	NOxbASMC	numeric & alpha	(ppm)	5=NR	>Value Value+	19.7%
NOX Post-ASM chem	NOxpASMC	numeric & alpha	(ppm)	5=NR	>Value Value> Value+	19.6%
IM240 purge Pre	FLObIM24	numeric & alpha	L	3=NA 5=NR	>Value Value>	23.1%
IM240 purge Post	FLOpIM24	numeric & alpha	L	3=NA 5=NR	>Value Value>	22.9%
Inlet to catalyst shrouded?	CAT_I_TYP	alpha		1=Y 2=N 3=NA		0.0%
Catalyst Temp Inlet-Pre	CTA_T_Ib	numeric& alpha	°C	3=NA 5=NR		12.7%
Catalyst Temp Inlet-Post	CTA_T_Ip	numeric&	°C	3=NA		

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
		alpha		5=NR 8=NS		12.7%
Outlet from Catalyst shrouded?	CAT_O_TYP	alpha		1=Y 2=N 3=NA 5=NR		0.0%
Catalyst Temp Outlet -Pre	CTA_T_Ob	numeric& alpha	°C	3=NA 5=NR		12.73%
Catalyst Temp Outlet -Post	CTA_T_Op	numeric& alpha	°C	3=NA 5=NR		14.76%
Catalyst Temp difference-Pre	CTA_T_db	numeric& alpha	°C	3=NA		16.24%
Catalyst Temp difference-Post	CTA_T_dp	numeric& alpha	°C	3=NA		15.68%
Fuel Filler Cap Emissions Pre	CAPe_HCb	numeric& alpha	(HC in ppm)	3=NA 5=NR		22.5%
Fuel Filler Cap Emissions Post	CAP e_HCp	numeric& alpha	(HC in ppm)	3=NA 5=NR		23.4%
Raw HC Pre-SS60	rHCbSS60	numeric	(g/min)			58.1%
Raw HC Post-SS60	rHCpSS60	numeric	(g/min)			

Description Variables	Acronym 8-character	Type of Data	Unit of Measurements	Levels	Comments	% missing data
						58.5%
Raw CO Pre- SS60	rCObSS60	numeric	(g/min)		Typing Error in cell (492xFU) ..01	60.7%
Raw CO Pre- SS60	rCOpSS60	numeric	(g/min)			61.6%
Raw NO Pre- SS60	rNObSS60	numeric & alpha	(g/min)	5=NR	one cell no(491xFW) contains NR	57.0%
Raw NO Pre- SS60	rNOpSS60	numeric	(g/min)			57.0%
Canister HC-Pre	CANS_HCb	numeric& alpha		5=NR	value> >value	48.0%
Canister HC-Post	CANS_HCp	numeric& alpha		5=NR	value> >value	47.8%

Appendix II

The Detailed Results of the Estimations of Twelve 3SLS Models for Testing the Hypothesis of the Thesis

Model No. 1 Pre-Tuning (CS505)

(1) The Estimates for the equation on HCBCS505

Diagnostic Log-L = -1264.156
 Restricted (b=0) Log-L = -1419.614

HCBCS505 Mean = 8.638
 S.D. = 4.810

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			-7.138	-5.527	
COBCS505	CO Pre-Tuning (CS505)	grams	0.069	10.721	122.528
NOXBCS55	NO _x Pre-Tuning (CS505)	grams	0.784	10.934	10.973
MAKE1 MAKE	Ford Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	1.956	4.221	0.324
MAKE2 MAKE	Toyota Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	2.719	6.676	0.253
MAKE3 MAKE	Nissan Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	1.338	2.820	0.097
MAKE4 MAKE	Holden Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	3.085	5.965	0.208
ENG_DIS	Engine Displacement Engine capacity	Liters	-0.989	-3.587	2.460
ENG_CONF	Engine Configuration V-shape, Inline	0,1	-3.128	-3.840	0.909
TRANMISN	Transmission Automatic, Manual	0,1	2.608	6.732	0.343
FUEL_SYS	Fuel System Carburetor, Injection (MPI, TBI)	0,1	4.268	8.486	0.465
AIR_COND	Air Conditioning No, Yes	0,1	-1.325	-3.305	0.733

Model No. 1 Pre-Tuning (CS505)

(2) The Estimates for the equation on COBCS505

Diagnostic Log-L = -2492.039 COBCS505 Mean = 122.528
 Restricted (b=0) Log-L = -2685.322 S.D. = 69.091

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			108.628	10.707	
HCBCS505	HC Pre-Tuning (CS505)	grams	4.464	4.092	8.638
NOXBCS55	NO _x Pre-Tuning (CS505)	grams	2.296	2.141	10.973
MAKE2 MAKE	Toyota Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	-39.583	-7.781	0.253
MAKE3 MAKE	Nissan Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	-18.033	-2.646	0.097
MAKE4 MAKE	Holden Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	-15.329	-2.471	0.208
FUEL_SYS	Fuel System Carburetor, Injection (MPI, TBI)	0,1	-63.123	-11.125	0.465
TRANMISN	Transmission Automatic, Manual	0,1	-15.928	-2.943	0.343

Model No. 1 Pre-Tuning (CS505)

(3) The Estimates for the equation on NOXBCS55

Diagnostic Log-L = -1384.066 NOXBCS55 Mean = 10.973
 Restricted (b=0) Log-L = -1427.493 S.D. = 4.891

Variable	Variable definition	Units	Coefficient	t-value	Variable Mean
Constant			-0.295	-0.215	
HCBCS505	HC Pre-Tuning (CS505)	grams	0.738	9.237	8.638
COBCS505	CO Pre-Tuning (CS505)	grams	-0.001	-0.199	122.528
TRANMISN	Transmission Automatic, Manual	0,1	-1.626	-3.124	0.343
MAKE1	Ford Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	-2.033	-4.219	0.324
MAKE4	Holden Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	-2.119	-3.558	0.208
ENG_DIS	Engine Displacement Engine capacity	Liters	1.059	3.650	2.460
ENG_CONF	Engine Configuration V-shape, Inline	0,1	3.350	3.845	0.909
AIR_COND	Air Conditioning No, Yes	0,1	1.406	3.226	0.733

Model No. 2 Pre-Tuning (T867)

(1) The Estimates for the equation on HCBT867

Diagnostic Log-L = -1135.557 HCBT867 Mean = 4.983
 Restricted (b=0) Log-L = -1434.889 S.D. = 4.754

Acronym	Variable definition	Units	Coefficient	t-value	Mean of X
Constant			-3.076	-4.964	
COBT867	CO Pre-Tuning (T867)	grams	0.060	22.725	69.288
NOXBT867	NO _x Pre-Tuning (T867)	grams	0.704	10.393	6.568
ENG_CONF	Engine Configuration V-shape, Inline	0,1	-1.880	-4.469	0.909
TRANMISN	Transmission Automatic , Manual	0,1	1.393	5.366	0.332
AIR_COND	Air Conditioning No, YES	0,1	-1.194	-4.099	0.737
EEMS	Engine Electronic Management System No, Yes	0,1	3.176	9.542	0.446

(2)The Estimates for the equation on COBT867

Diagnostic Log-L = -2461.762 COBT867 Mean = 69.288
 Restricted (b=0) Log-L = -2753.516 S.D. = 73.317

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			45.400	4.441	
HCBT867	HC Pre-Tuning (T867)	grams	15.677	23.007	4.983
NOXBT867	NO _x Pre-Tuning (T867)	grams	-9.541	-6.643	6.568
EEMS1 EEMS_OPR	NO Engine Electronic Management System Operational No, Yes ,Not Applicable	1,0	-48.105	-6.310	0.068
EEMS2 EEMS_OPR	YES Engine Electronic Management System Operational No, Yes ,Not Applicable	1,0	-51.046	-9.519	0.373
TRANMISN	Transmission Automatic , Manual	0,1	-21.577	-5.145	0.332
AIR_COND	Air Conditioning No, YES	0,1	18.464	4.091	0.737
ENG_CONF	Engine Configuration V-shape, Inline	0,1	26.890	3.953	0.909

Model No. 2 Pre-Tuning (T867)

(3)The Estimates for the equation on NOXBT867

Diagnostic Log-L = -1232.212

NOXBT867 Mean = 6.568

Restricted (b=0) Log-L = -1315.301

S.D. = 3.710

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			-0.105	-0.166	
HCBT867	HC Pre-Tuning (T867)	grams	1.132	12.013	4.983
COBT867	CO Pre-Tuning (T867)	grams	-0.063	-7.582	69.288
EGR1 EGR_OPER	No Exhaust Gas Re- circulation Operational? not working / working	1,0	0.634	2.495	0.199
TRANMISN	Transmission Automatic , Manual	0,1	-1.565	-4.830	0.332
ENG_CONF	Engine Configuration V-shape, Inline	0,1	2.669	5.370	0.909
CHOKE1 CHOKE	Automatic Choke Automatic ,Manual, NA	1,0	3.982	8.211	0.548
CHOKE2 CHOKE	Manual Choke Automatic ,Manual, NA	1,0	3.834	4.472	0.056
AIR_COND	Air Conditioning No, YES	0,1	1.295	3.657	0.737

Model No. 3 Pre-Tuning (H505)

(1)The Estimates for the equation on HCBH505

Diagnostic Log-L = -1133.716
 Restricted (b=0) Log-L = -1327.563

HCBH505 Mean = 4.519
 S.D. = 3.805

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			1.895	2.648	
COBH505	CO Pre-Tuning (H505)	grams	0.079	14.001	52.445
NOXBH505	NO _x Pre-Tuning (H505)	grams	0.001	0.015	10.354
TRANMISN	Transmission Automatic, Manual	0,1	1.506	6.815	0.340
AIR2 A_IJ_SYS	PA Type of Air Injection System AP, PA, NF	1,0	-4.807	-9.277	0.276
O2_SENS	O ₂ Sensor Fitted & Operational (Not working / working)	0,1	-1.714	-4.086	0.415

(2)The Estimates for the equation on COBH505

Diagnostic Log-L = -2415.285
 Restricted (b=0) Log-L = -2517.308

COBH505 Mean = 52.445
 S.D. = 44.913

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-46.321	-5.420	
HCBH505	HC Pre-Tuning (H505)	grams	9.087	13.859	4.519
NOXBH505	NO _x Pre-Tuning (H505)	grams	3.430	6.595	10.354
O2_SENS	O ₂ Sensor Fitted & Operational (not working / working)	0,1	23.617	4.060	0.415
AIR2 A_IJ_SYS	PA Type of Air Injection System AP, PA, NF	1,0	61.082	8.757	0.276
TRANMISN	Transmission Automatic, Manual	0,1	-12.833	-6.013	0.340

Model No. 3 Pre-Tuning (H505)

(3)The Estimates for the equation on NOXBH55

Diagnostic Log-L = -1496.373

Restricted (b=0) Log-L = -1482.913

NOXBH55 Mean = 10.354

S.D. = 5.252

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			8.689	7.411	
HCBH505	HC Pre-Tuning (H505)	grams	-0.166	-0.958	4.519
COBH505	CO Pre-Tuning (H505)	grams	0.097	6.832	52.445
O2_SENS	O ₂ Sensor Fitted & Operational (not working / working)	0,1	-2.559	-2.623	0.415
AIR2 A_IJ_SYS	PA Type of Air Injection System AP, PA, NF	1,0	-5.834	-4.715	0.276

Model No. 4 Pre-Tuning (ADR37)

(1)The Estimates for the equation on HCBADR37

Diagnostic Log-L = -135.908

HCBADR Mean = 0.961

Restricted (b=0) Log-L = -541.317

S.D. = 0.741

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			0.137	1.146	
COBADR37	CO Pre-Tuning (ADR37)	g/km	0.041	12.432	13.144
NOXBADR3	NO _x Pre-Tuning (ADR37)	g/km	0.222	3.216	1.430
ENG_DIS	Engine Displacement Engine capacity	Liters	0.066	3.340	2.455
CATALYST	Catalyst Present No, Yes	0,1	-0.464	-8.035	0.719
MAKE2 MAKE	Toyota Vehicle Make Ford, Toyota , Nissan, Holden, Mitsubishi	1,0	0.104	2.530	0.248
MAKE4 MAKE	Holden Vehicle Make Ford, Toyota , Nissan, Holden, Mitsubishi	1,0	0.198	4.940	0.211
TRANMISN	Transmission Automatic, Manual	1,0	0.211	5.843	0.333

Model No. 4 Pre-Tuning (ADR37)

(2) The Estimates for the equation on COBADR37

Diagnostic Log-L = -1660.737 COBADR37 Mean = 13.144
 Restricted (b=0) Log-L = -1826.502 S.D. = 10.547

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-9.04	-4.37	
HCBADR37	HC Pre-Tuning (ADR37)	g/km	14.58	17.04	0.96
NOXBADR3	NO _x Pre-Tuning (ADR37)	g/km	5.08	4.34	1.43
ENG_DIS	Engine Displacement Engine capacity	Liters	-1.09	-3.24	2.45
MAKE1 MAKE	Ford Vehicle Make Ford, Toyota , Nissan, Holden, Mitsubishi	1,0	1.38	2.31	0.30
MAKE2 MAKE	Toyota Vehicle Make Ford, Toyota , Nissan, Holden, Mitsubishi	1,0	-1.71	-2.47	0.25
MAKE4 MAKE	Holden Vehicle Make Ford, Toyota , Nissan, Holden, Mitsubishi	1,0	-3.15	-4.50	0.21
TRANMISN	Transmission Automatic, Manual	0,1	-3.40	-5.41	0.33
CATALYST	Catalyst Present No, Yes	0,1	7.47	7.25	0.72

(3) The Estimates for the equation on NOXBADR3

Diagnostic Log-L = -481.046 NOXBADR3 Mean = 1.430
 Restricted (b=0) Log-L = -508.801 S.D. = 0.693

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			0.799	14.378	
HCBADR37	HC Pre-Tuning (ADR37)	g/km	0.186	2.123	0.961
COBADR37	CO Pre-Tuning (ADR37)	g/km	0.038	5.848	13.144
MAKE1 MAKE	Ford Vehicle Make Ford, Toyota , Nissan, Holden, Mitsubishi	1,0	-0.151	-2.316	0.304

Model No. 5 Pre-Tuning (IM240)

(1) The Estimates for the equation on HCBIM240

Diagnostic Log-L = -181.484
 Restricted (b=0) Log-L = -429.259

HCBIM240 Mean = 0.672
 S.D. = 0.588

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-0.668	-9.415	
COBIM240	CO Pre-Tuning (IM240)	g/km	0.078	16.924	8.884
NOXBIM24	NO _x Pre-Tuning (IM240)	g/km	0.275	7.683	1.786
MAKE1 MAKE	Ford Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	-0.234	-6.485	0.312
POINT2 PTS_CONT	OK Points Condition Poor, Ok, NA	1,0	0.259	4.068	0.076
TRANMISN	Transmission Automatic, Manual	0,1	0.157	4.332	0.341
EEMS1 EEMS	No Engine Electronic Management System Operational No, Yes, Not Applicable	1,0	0.362	5.062	0.070
EEMS2 EEMS	Yes Engine Electronic Management System Operational No, Yes, Not Applicable	1,0	0.343	7.059	0.372

Model No. 5 Pre-Tuning (IM240)

(2) The Estimates for the equation on COBIM240

Diagnostic Log-L = -1421.245 COBIM240 Mean = 8.884
 Restricted (b=0) Log-L = -1650.412 S.D. = 7.330

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			2.913	2.689	
HCBIM240	HC Pre-Tuning (IM240)	g/km	10.348	13.780	0.672
NOXBIM24	NO_x Pre-Tuning (IM240)	g/km	-0.227	-0.513	1.786
CATALYST	Catalyst Present No, Yes	0,1	1.634	2.993	0.715
MAKE1 MAKE	Ford Vehicle Make FORD, Toyota , Nissan, Holden, Mitsubishi	1,0	2.694	6.555	0.312
POINT2 PTS_CONT	OK Points Condition Poor, Ok, NA	1,0	-2.902	-3.939	0.076
TRANMISN	Transmission Automatic, Manual	0,1	-1.763	-4.193	0.341
EEMS1 EEMS	No Engine Electronic Management System Operational No, Yes, Not Applicable	1,0	-4.155	-5.135	0.070
EEMS2 EEMS	Yes Engine Electronic Management System Operational No, Yes, Not Applicable	1,0	-3.976	-7.701	0.372

Model No. 5 Pre-Tuning (IM240)

(3)The Estimates for the equation on NOXBIM24

Diagnostic Log-L = -577.434

Restricted (b=0) Log-L = -663.666

NOXBIM24 Mean = 1.786

S.D. = 0.954

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			1.669	7.772	
HCBIM240	HC Pre-Tuning (IM240)	g/km	0.318	1.532	0.672
COBIM240	CO Pre-Tuning (IM240)	g/km	0.032	2.496	8.884
CATALYST	Catalyst Present No, Yes	0,1	-0.566	-3.435	0.715
EGR1 EGR_OPER	No Exhaust Gas Re- Circulation Operational? Working/ Not Working No, Yes, Not Applicable	1,0	0.112	2.039	0.202

Model No. 6 Pre-Tuning (SSL60)

(1) The Estimates for the equation on HCBSS60

Diagnostic Log-L = 95.173 HCBSS60 Mean = 0.350
 Restricted (b=0) Log-L = -203.046 S.D. = 0.369

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			0.065	0.939	
COBSS60	CO Pre-Tuning (SS60)	g/min	0.046	10.721	5.282
NOXBSS60	NO _x Pre-Tuning (SS60)	g/min	0.091	1.883	0.743
ENG_DIS	Engine Displacement Engine Capacity	Liter	0.040	4.638	2.471
CATALYST	Catalyst present No, Yes	0,1	-0.224	-6.856	0.709
FUEL_SYS	Fuel System Carburetor, Injection (MPI, TBI)	0,1	0.081	2.589	0.443

(2) The Estimates for the equation on COBSS60

Diagnostic Log-L = -1403.134 COBSS60 Mean = 5.282
 Restricted (b=0) Log-L = -1580.338 S.D. = 6.473

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-2.051	-3.783	
HCBSS60	HC Pre-Tuning (SS60)	g/min	11.440	12.069	0.350
NOXBSS60	NO _x Pre-Tuning (SS60)	g/min	3.178	3.607	0.743
AIR2 A_IJ_SYS	PA Type of Air Injection System AP, PA, NF	1,0	3.562	7.442	0.274

(3) The Estimates for the equation on NOXBSS60

Diagnostic Log-L = -344.462 NOXBSS60 Mean = 0.743
 Restricted (b=0) Log-L = -363.118 S.D. = 0.515

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			0.779	6.441	
HCBSS60	HC Pre-Tuning (SS60)	g/min	0.009	0.044	0.350
COBSS60	CO Pre-Tuning (SS60)	g/min	0.029	3.042	5.282
CATALYST	Catalyst present No, Yes	0,1	-0.270	-2.852	0.709

Model No. 7 Post-Tuning (CS505)

(1) The Estimates for the equation on HCPCS505

Diagnostic Log-L = -1184.674 HCPCS505 Mean = 7.617
 Restricted (b=0) Log-L = -1299.991 S.D. = 3.761

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-2.646	-4.353	
COPCS505	CO POST (CS505)	grams	0.042	10.135	106.626
NOXPCS55	NOX POST (CS505)	grams	0.634	13.314	10.223
ENG_CONF	Engine Configuration V-Shape, Inline	0,1	-1.628	-3.796	0.909
TRANMISN	Transmission Automatic, Manual	0,1	2.075	7.262	0.335
MAKE4 MAKE	Holden Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	0.384	2.055	0.209

(2) The Estimates for the equation on COPCS505

Diagnostic Log-L = -2430.713 COPCS505 Mean = 106.626
 Restricted (b=0) Log-L = -2586.441 S.D. = 56.755

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			75.012	7.535	
HCPCS505	HC POST (CS505)	grams	9.454	9.107	7.617
NOXPCS55	NO _x POST (CS505)	grams	-2.126	-2.012	10.223
EEMS	Electronic Engine Management System N, Y	0,1	-31.897	-7.248	0.456
TRANMISN	Transmission Automatic, Manual	0,1	-12.310	-2.486	0.335

Model No. 8 Post-Tuning (T867)

(1) The Estimates for the equation on HCPT867

Diagnostic Log-L = -1135.934 HCPT867 Mean = 4.293
 Restricted (b=0) Log-L = -1370.818 S.D. = 4.138

Acronym	Variable	Units	Coefficient	t-value	Mean of X
	Meanings				
Constant			-5.900	-15.101	
COPT867	CO Post-Tuning (T867)	grams	0.061	13.514	48.744
NOXPT867	NO _x Post-Tuning (T867)	grams	0.843	18.150	5.854
EEMS	Engine Electronic				
	Management System	0,1	0.957	6.131	0.445
	No, Yes				
TRANMISN	Transmission	0,1	1.067	4.124	0.315
	Automatic, Manual				
N_CYLIND	No. of cylinders				
	4 , > 4 (= 6 or 8)	0,1	1.622	5.909	0.337
P_ATCOST	Adjusted Total Parts				
	Cost Replaced in	\$	0.004	4.037	201.863
	Tune-up				
MAKE3	Nissan	1,0	0.726	1.965	0.091
MAKE	Vehicle Make				
	Ford, Toyota, Nissan,				
	Holden, Mitsubishi				
MAKE4	Holden	1,0	0.870	3.056	0.213
MAKE	Vehicle Make				
	Ford, Toyota, Nissan,				
	Holden, Mitsubishi				

Model No. 8 Post-Tuning (T867)

(2) The Estimates for the equation on COPT867

Diagnostic Log-L = -2302.559 COPT867 Mean = 48.744
 Restricted (b=0) Log-L = -2538.394 S.D. = 46.413

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			36.234	5.643	
HCPT867	HC Post-Tuning (T867)	grams	7.492	11.111	4.293
NOXPT867	NO _x Post-Tuning (T867)	grams	-1.397	-1.219	5.854
EEMS	Engine Electronic Management System No, Yes	0,1	-25.758	-6.529	0.445

(3) The Estimates for the equation on NOXPT867

Diagnostic Log-L = -1184.811 NOXPT867 Mean = 5.854
 Restricted (b=0) Log-L = -1283.857 S.D. = 3.456

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			5.753	15.090	
HCPT867	HC Post-Tuning (T867)	grams	0.912	22.751	4.293
COPT867	HC Post-Tuning (T867)	grams	-0.030	-4.996	48.744
TRANMISN	Transmission Automatic, Manual	0,1	-1.349	-4.161	0.315
N_CYLIND	No. of cylinders 4, > 4 (= 6 or 8)	0,1	-2.049	-5.983	0.337
P_ATCOST	Cost Replaced in Adjusted Total Parts Tune-up	\$	-0.005	-4.053	201.863
MAKE3	Nissan Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	-0.917	-1.971	0.091
MAKE4	Holden Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	-1.098	-3.051	0.213

Model No. 9 Post-Tuning (H505)

(1) The Estimates for the equation on HCPH505

Diagnostic Log-L = -1145.653
 Restricted (b=0) Log-L = -1290.223

HCPH505 Mean = 4.039
 S.D. = 3.445

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-5.666	-14.871	
COPH505	CO Post (CS505)	grams	0.085	16.744	41.223
NOXPH505	NO _x Post (CS505)	grams	0.564	13.678	9.399
TRANMISN	Transmission Automatic, Manual	0,1	0.404	2.906	0.331
MAKE2 MAKE	Toyota Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	0.908	4.796	0.241
MAKE3 MAKE	Nissan Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	0.610	2.286	0.099
MAKE4 MAKE	Holden Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	2.260	8.234	0.210

Model No. 9 Post-Tuning (H505)

(2) The Estimates for the equation on COPH505

Diagnostic Log-L = -2219.566 COPH505 Mean = 41.223
 Restricted (b=0) Log-L = -2385.496 S.D. = 32.803

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			44.843	9.067	
HCPH505	HC Post (CS505)	grams	8.832	18.980	4.039
NOXPH505	NO _x Post (CS505)	grams	-3.267	-5.591	9.399
MAKE2 MAKE	Toyota Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	-12.949	-4.986	0.241
MAKE3 MAKE	Nissan Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	-8.702	-2.358	0.099
MAKE4 MAKE	Holden Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	-21.977	-7.540	0.210

(3) The Estimates for the equation on NOXPH505

Diagnostic Log-L = -1346.678 NOXPH505 Mean = 9.399
 Restricted (b=0) Log-L = -1448.231 S.D. = 4.768

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			7.532	16.892	
HCPH505	HC Post (CS505)	grams	1.137	11.884	4.039
COPH505	CO Post (CS505)	grams	-0.046	-3.061	41.223
MAKE4 MAKE	Holden Vehicle Make Ford, Toyota, Nissan, Holden, Mitsubishi	1,0	-2.146	-4.537	0.210
TRANMISN	Transmission Automatic, Manual	0,1	-1.210	-3.055	0.331

Model No. 10 Post-Tuning (ADR37)

(1) The Estimates for the equation on HCPADR37

Diagnostic Log-L = -265.115 HCPADR37 Mean = 0.870
 Restricted (b=0) Log-L = -506.798 S.D. = 0.656

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-0.010	-0.052	
COPADR37	CO Post-Tuning (ADR37)	g/km	0.037	6.011	10.229
NOXPADR3	NO _x Post-Tuning (ADR37)	g/km	0.548	12.129	1.407
ODOMETER	Odo Readings	Km	.128590D-05	4.194	115365.155
ENG_CONF	Engine Configuration V-shape, Inline	0,1	-0.165	-2.448	0.919
ENG_DIS	Engine Displacement Engine Capacity	Liters	0.078	4.359	2.493
POINTST	Points condition after points replaced in Tune-up NA, OK	0,1	-0.288	-3.079	1.851
TRANMISN	Transmission Automatic, Manual	0,1	0.231	5.645	0.316

(2) The Estimates for the equation on COPADR37

Diagnostic Log-L = -1480.162 COPADR37 Mean = 10.229
 Restricted (b=0) Log-L = -1711.579 S.D. = 6.991

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			5.993	7.155	
HCPADR37	HC Post-Tuning ADR37	g/km	6.355	9.634	0.870
NOXPADR3	NO _x Post-Tuning ADR37	g/km	-0.149	-0.218	1.407
EEMS1 EEMS_OPR	N Electronic Engine Management System Operational? N, Y, NA	1,0	-3.988	-5.423	0.067
EEMS2 EEMS_OPR	Y Electronic Engine Management System Operational? N, Y, NA	1,0	-4.387	-7.458	0.363
AIR_COND	Air Conditioning No, Yes	0,1	1.041	2.274	0.749

Model No. 10 Post-Tuning (ADR37)

(3) The Estimates for the equation on NOXPADR37

Diagnostic Log-L = -515.150
 Restricted (b=0) Log-L = -580.701

NOXPADR3 Mean = 1.407
 S.D. = 0.758

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			0.482	4.286	
HCPADR37	HC Post-Tuning ADR37	g/km	1.084	10.466	0.870
COPADR37	CO Post-Tuning ADR37	g/km	-0.010	-0.806	10.229
ODOMETER	Odo Meter	Km	-.172662D-05	-3.089	115365.155
TRANMISN	Transmission Automatic, Manual	0,1	-0.333	-5.104	0.316
ENG_CONF	Engine Configuration V-shape, Inline	0,1	0.418	3.737	0.919

Model No. 11 Post-Tuning (IM240)

(1) The Estimates for the equation on HCPIM240

Diagnostic Log-L = -170.637 HCPIM240 Mean = 0.584
 Restricted (b=0) Log-L = -376.596 S.D. = 0.535

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-0.584	-7.069	
COPI240	CO Post-Tuning (IM240)	g/km	0.048	8.365	7.261
NOXPIM24	NO _x Post-Tuning (IM240)	g/km	0.393	7.770	1.556
ENG_DIS	Engine Displacement Engine Capacity	Liters	0.062	3.315	2.493
ODOMETER	Odo Readings	Km	.101592D-05	3.906	112777.419
POINTST	Points condition after points replaced in Tune-up NA, OK	0,1	0.271	2.470	0.139
TRANMISN	Transmission Automatic, Manual	0,1	0.117	3.362	0.328
ENG_CONF	Engine Configuration V-shape , Inline	0,1	-0.148	-2.431	0.914

(2)The Estimates for the equation on COPIM240

Diagnostic Log-L = -1345.218 COPIM240 Mean = 7.261
 Restricted (b=0) Log-L = -1510.77 S.D. = 5.828

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			8.918	8.352	
HCPIM240	HC Post-Tuning (IM240)	g/km	6.173	7.464	0.584
NOXPIM24	NO _x Post-Tuning (IM240)	g/km	-2.257	-3.234	1.556
O2_SENST	O ₂ Sensor fitted & Operational after replaced in Tune-Up NA, Y/Action	0,1	-4.112	-7.587	0.425

Model No. 11 Post-Tuning (IM240)

(3) The Estimates for the equation on NOXPIM24

Diagnostic Log-L = -529.816 NOXPIM24 Mean = 1.556
 Restricted (b=0) Log-L = -610.307 S.D. = 0.875

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			0.819	6.467	
HCPIM240	CO Post-Tuning (IM240)	g/km	1.537	10.211	0.584
COPIM240	CO Post-Tuning (IM240)	g/km	-0.052	-3.201	7.261
ODOMETER	Odo Readings	Km	-.176962D-05	-2.704	112777.419
TRANMISN	Transmission Automatic, Manual	0,1	-0.198	-2.539	0.328
ENG_CONF	Engine Configuration V-shape , Inline	0,1	0.525	4.150	0.914

Model No. 12 Post-Tuning (SS60)

(1) The Estimates for the equation on HCPSS60

Diagnostic Log-L = -17.120 HCPSS60 Mean = 0.317
 Restricted (b=0) Log-L = -169.661 S.D. = 0.343

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			-0.432	-9.838	
COPSS60	CO Post-Tuning (SS60)	g/min	0.065	17.560	3.903
NOXPSS60	NO _x Post-Tuning (SS60)	g/min	0.348	9.005	0.713
ENG_DIS	Engine Displacement	Liters	0.101	8.262	2.499
POINTST	Points condition after replaced in Tune-up NA, OK	0,1	0.142	2.172	0.142
TRANMISN	Transmission Automatic, Manual	0,1	-0.074	-3.360	0.320

(2) The Estimates for the equation on COPSS60

Diagnostic Log-L = -1278.741 COPSS60 Mean = 3.903
 Restricted (b=0) Log-L = -1450.856 S.D. = 4.765

Acronym	Variable Meanings	Units	Coefficient	t-value	Mean of X
Constant			4.594	6.364	
HCPSS60	HC Post-Tuning (SS60)	g/min	12.635	16.990	0.317
NOXPSS60	NO _x Post-Tuning (SS60)	g/min	-2.480	-3.521	0.713
ENG_DIS	Engine Displacement	Liters	-1.209	-5.975	2.499
TRANMISN	Transmission Automatic, Manual	0,1	1.412	3.757	0.320
POINTST	Points condition after replaced in Tune-up NA, OK	0,1	-2.561	-2.194	0.142

(3) The Estimates for the equation on NOXPSS60

Diagnostic Log-L = -356.697 NOXPSS60 Mean = 0.713
 Restricted (b=0) Log-L = -408.58 S.D. = 0.560

Acronym	Variable Description	Units	Coefficient	t-value	Mean of X
Constant			0.877	10.496	
HCPSS60	HC Post-Tuning (SS60)	g/min	1.504	10.284	0.317
COPSS60	CO Post-Tuning (SS60)	g/min	-0.058	-4.137	3.903
ENG_DIS	Engine Displacement	Liters	-0.166	-6.212	2.499

Appendix III

The Theoretical and Physical Principles for Exhaust Emissions from Gasoline-Fuelled Engines: A Background

1. Introduction

Many researchers have investigated the effects of engine design and vehicle operating variables on vehicle emissions. Existing literature provides a considerable body of evidence that suggest these variables are inter-related and affect vehicle emissions simultaneously. The literature also demonstrates that it is difficult to study the effects of one variable in isolation of the other variables. A change that reduces one emission often increases one or more other emissions.

Appendix III reviews briefly the theoretical and physical principles that underlie automotive emissions. In the beginning, we describe the combustion process in the engine, and we review critically the physical features and operating characteristics of the engine. We then describe briefly several exhaust after-treatment systems. In the end, we outline the overall efficiency of the engine in terms of combustion, thermal, mechanical, and volumetric efficiencies.

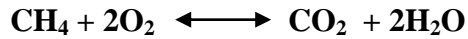
2. The Engine Combustion Process

The combustion process in gasoline-fuelled internal combustion engines produces power, heat, and emissions. Combustion is divided into three main regions (Pulkrabek, 1997):

- **flame ignition:** spark plugs initiate a flame and ignite the air-fuel mixture.
- **flame propagation:** the flame propagates after burning between 5 percent and 10 percent of the air-fuel mixture. The propagation of the flame elevates both the temperature and pressure in the cylinder, and forces the piston downwards.
- **flame termination:** the flame is terminated after between 90 percent and 95 percent of the air-mixture is burnt. The flame is terminated by heat transfer and viscous drag with the walls at the extreme edges of the chamber

2.1 Reactions of Combustion

Combustion is burning fuel with air. Fuel, e.g., gasoline, is hydrocarbons, i.e., hydrogen (H_2) and carbon (C). Air consists, in molar terms, of 21 percent oxygen (O_2) and 79 percent atmospheric nitrogen (N_2^*), of which 78 percent nitrogen (N_2), and 1 percent argon and other traces. Nitrogen and argon are inactive in combustion, but affect the temperature and pressure of combustion. The main elements involved in combustion are oxygen (O_2) and nitrogen (N_2) from the ambient air, and carbon (C) and hydrogen (H_2) from the fuel in the tank (Figure 1) (Houghton, 1995). A complete oxidation of the fuel releases theoretically carbon dioxide (CO_2) and water (H_2O).



However, it is not possible to burn all fuel. The combustion efficiency, i.e., fraction of the burnt fuel, is between 0.95 and 0.98 typically (Pulkrabek, 1997). The exhaust includes emissions of complete, incomplete, and by-products of combustion. The main products of combustion are carbon dioxides (CO_2), water (H_2O), nitrogen (N_2), HC, CO, NO_x , and other compounds, such as Aldehydes (H-C-O compounds), lead compounds for leaded fuels, sulphur dioxides (SO_2) for fuels with sulphur (Schäfer and Basshuysen, 1995).

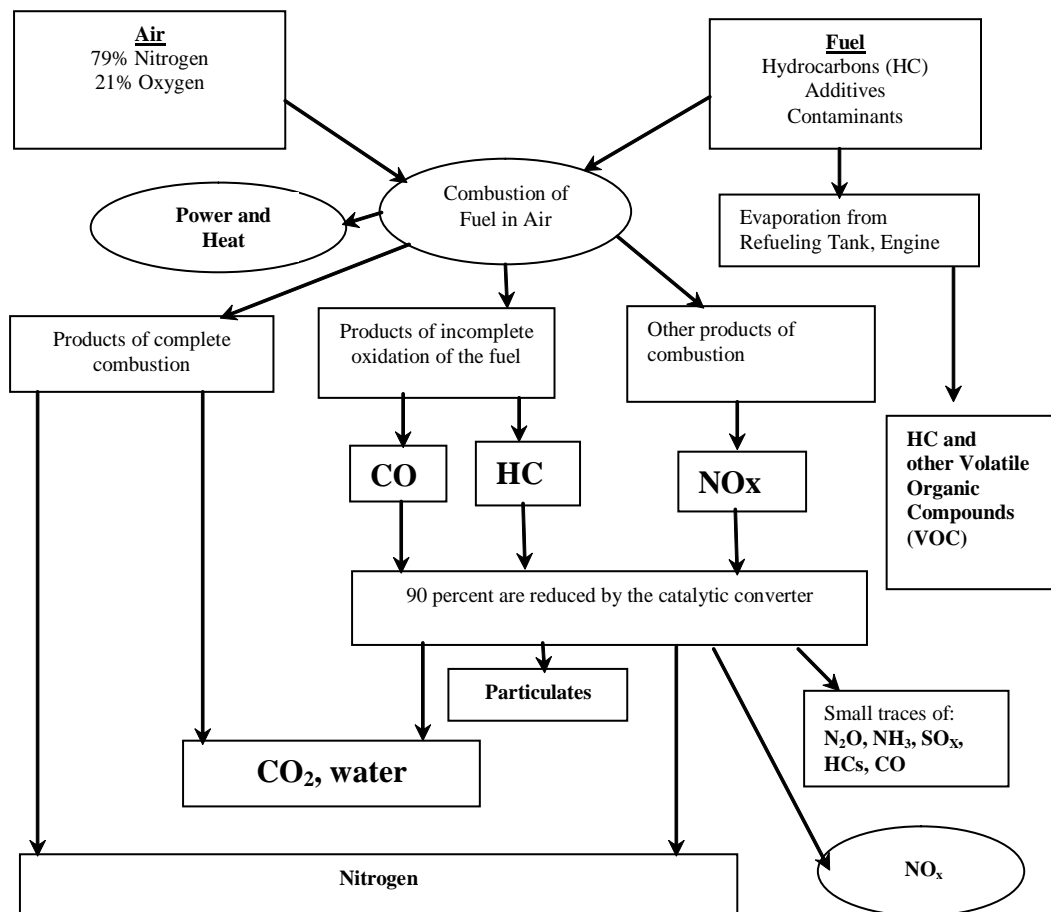


Figure 1 Combustion in Gasoline-Fueled Automobiles

Source: Houghton (1995)

2.2 Air / Fuel mixtures

Air fuel mixtures are important to ensure efficient operations of the engine. Air-fuel mixtures must be chemically correct, in order to produce a complete combustion, a reliable ignition, and proper flame propagation. The fuel delivery system, such as fuel injector or carburettor, supplies the fuel necessary for any airflow to form air-fuel mixtures (Schäfer and Basshuysen, 1995). Air-fuel mixtures are described by air/fuel and fuel/air ratios. The air/fuel ratio is the ratio of air mass to fuel mass, and the fuel /air ratio is the ratio of fuel mass to air mass, as follows:

$$\text{Air / Fuel ratio} = \frac{m_a}{m_f}$$

$$\text{Fuel / Air ratio} = \frac{m_f}{m_a}$$

where: m_a = air mass (kg) m_b = fuel mass (kg)

Air-fuel mixtures are stoichiometric, i.e., chemically correct, for both gasoline-fuelled and diesel-fuelled vehicles, when the ratio of air mass to fuel mass is 14.6 kg of air to 1.0 kg of fuel (Schäfer and Basshuysen, 1995). Ideally, combustion occurs with air/fuel equals 14.6, and is possible for air/fuel between 6 and 19. When air/fuel is less than 6 the mixture is too rich to sustain combustion and when it is greater than 19 the mixture is too lean and combustion becomes unstable (Pulkrabek, 1997). Gasoline-fuelled engines operate with air-fuel ratio between 12 and 18, but it varies with various operating conditions (Pulkrabek, 1997).

The strength of the mixture is a significant determinant of vehicle emissions (Figure 2). It affects the mixture susceptibility to ignite without a spark, i.e., spontaneously. The strength of the air-fuel mixture is known by fuel equivalence ratio (Φ). For example, Fuel equivalence ratio (Φ) with 25 percent excess air is defined, as follows (Stone, 1992):

$$\Phi = \frac{\text{Actual (Fuel / Air) ratio}}{\text{Stoichiometric (Fuel / Air) ratio}} = \frac{\text{Stoichiometric (Air / Fuel) ratio}}{\text{Actual (Air / Fuel) ratio}} = \frac{1}{1.25} = 0.8$$

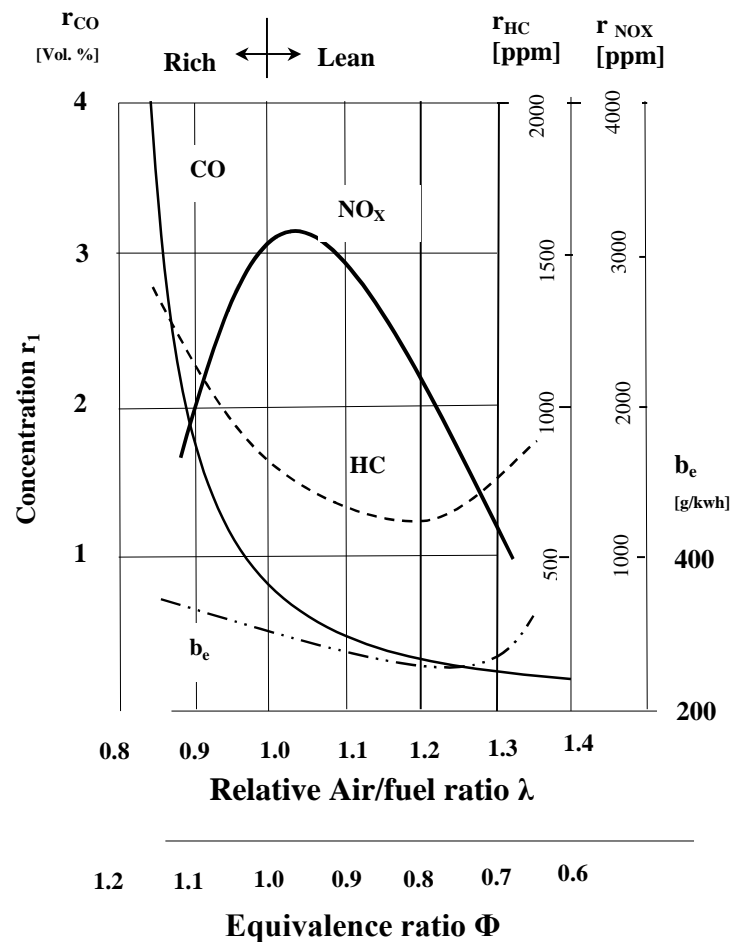


Figure 1 Vehicle Emissions function of the Air-Fuel Ratio

Source: Stone (1992), Schäfer and Basshuysen (1995)

When $\Phi = 1$, the mixture is stoichiometric and maximum energy is released. For $\Phi > 1$ the engine runs rich and increases CO and HC emissions. For $\Phi < 1$ the engine runs lean and produces oxygen (O_2). A fuel-lean mixture burns slowly, and has lower temperature and pressure. Lower temperatures and pressures reduce the tendency to self-ignition and produce undesirable knock. The knock affects the vehicle driveability, because it generates pulses of pressure that induces surge and unsteady forward progressions (Schäfer and Basshuysen, 1995).

2.3 Pollutants of the Engine

Fuel composition has profound effects on exhaust gas composition (Schäfer and Basshuysen, 1995). A typical exhaust under the ECE test drive-cycle is shown in Figure 3. For non-catalyst equipped vehicles, the total mass of the flow in the

exhaust consists of 1.10 percent pollutants, 18.10 percent CO₂, 8.20 percent H₂O, 1.20 percent argon, and 1.10 percent O₂.

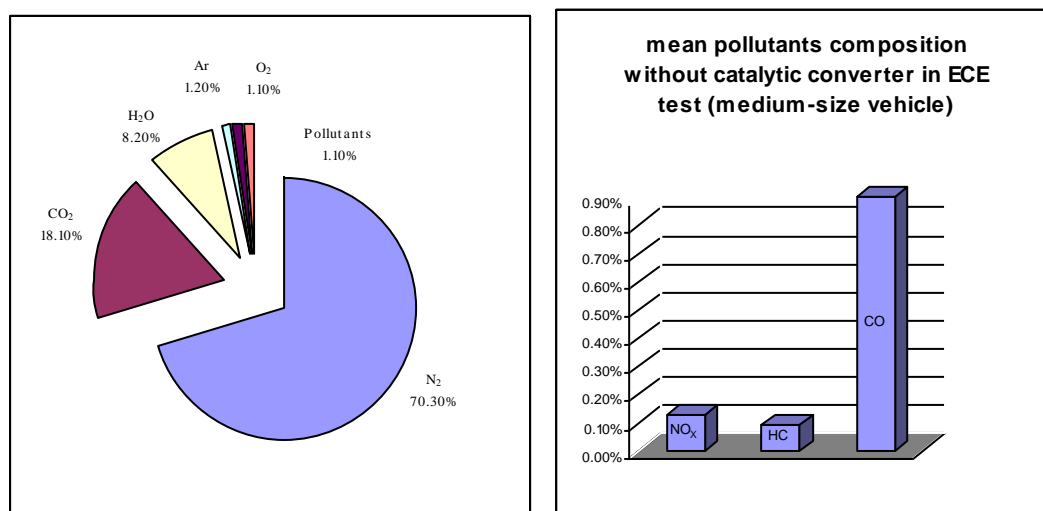


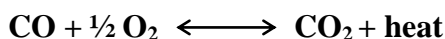
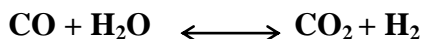
Figure 2 Average Exhaust for non-Catalyst Vehicles under the ECE Test Drive-Cycle

Source: Schäfer and Basshuysen (1995)

Carbon monoxide (CO)

CO is a product of inhomogeneous air-fuel mixtures. It is the product of poor mixing of fuel with air in the engine. It is also, the product of the incomplete combustion that is caused by the termination of the flame (Schäfer and Basshuysen, 1995). CO depends primarily on the air/fuel ratio. Fuel-rich mixtures, such as under starting, accelerating, and high loads, produce higher CO emissions, while fuel-lean mixtures produce lower CO emissions (Pulkrabek, 1997; Figure 2).

CO is elevated with fuel-rich mixtures, because oxygen is not sufficient to transform all carbons (C) into CO₂ (Schäfer and Basshuysen, 1995). CO is not only an emission, but also represents thermal energy that was not used (Pulkrabek, 1997).



CO depends strongly on the pressure in the cylinder, especially during the expansion phase. Therefore, parameters that do not affect the pressure in the cylinder, such as ignition timing, compression ratio, injection timing, and engine speed, do not have significant impacts on CO (Schäfer and Basshuysen, 1995).

Hydrocarbons (HC)

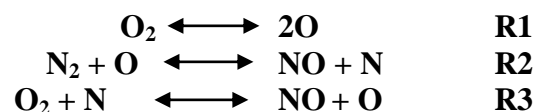
Hydrocarbons (HC), such as aromatic substances (benzene, toluene, and ethyl benzene), olefins (propene and ethylene), and paraffins (CH₄), depend on the chemical composition of the fuel. The variables that contribute to incomplete

combustion, e.g., shape of the chamber, increase HC. Schäfer and Basshuysen (1995) listed the main factors that contribute to elevating hydrocarbons (HC) emissions, as follows:

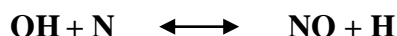
- (1) **Non-stoichiometric air /fuel ratio:** HC depends strongly on the air/fuel ratio. Air/fuel ratios approaching misfire limits produce higher HC, one misfire out of 1000 cycles gives one gram of emissions for every one kg fuel. Also, fuel-rich mixtures, such as under starting, rapid accelerations, and high engine loads, elevate HC emissions.
- (2) **Incomplete combustion:** Pulkrabek (1997) listed several factors that contribute to incomplete combustion:
 - Inhomogeneous mixing of fuel with air, which result in some fuel not finding enough oxygen to react with.
 - flame quenching, particularly around gaps in the chamber, in the grooves of the piston ring, and around spark plugs, which is caused by:
 - inability of the flame to propagate to the cylinder walls, because the walls that are relatively cold will extinguish the flame.
 - expansion that lowers the temperature and pressure in the cylinder, and therefore slows combustion and quenches the flame.
 - high residual under low engine loads and idling conditions that quenches the flame.
 - weak and mistimed spark (Schäfer and Basshuysen,1995).
- (3) **Expulsion of the oil film:** The expulsion of oil film that serves as a lubricant between the piston and the walls of the cylinder contributes to elevating hydrocarbons (HC) emissions.

Nitrogen Oxides (NO_x)

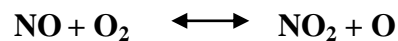
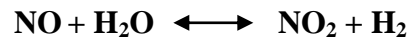
Nitrogen oxides (NO_x) are formed by Zeldovich's mechanism in a chain of complex reactions (Stone, 1992), as follows:



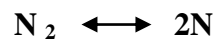
An additional reaction becomes important in Zeldovic's mechanism, especially for mixtures with equivalence ratio (Φ) >1.2, (Schäfer and Basshuysen, 1995), as follows:



Both NO and NO₂ are known as NO_x. NO accounts for between 90 percent and 98 percent approximately of all NO_x. NO reacts further to produce NO₂ by various reactions, as follows (Pulkrabek, 1997):



Nitrogen oxides (NO_x) are directly related to the thermal energy of the combustion process, in addition to the quantity of the airflow into the chamber. Higher temperatures shift the equilibria of reactions R1, R2, and R3 to the right, and enhance the formation of NO (Jacob, 1999). Higher temperatures also enhance the splitting of N_2 and O_2 into two reactive molecules. The excess air ensures oxygen is available to complete the reactions of NO_x (Pulkrabek, 1997):



The reactions of nitrogen oxides are relatively slow (Schäfer and Basshuysen, 1995). The kinetics of the reactions increases as the temperature of the flame increases. The latter enhances strongly the formation of NO and other nitrogen oxides. NO_x also depends on the speed of the flame (Stone, 1992), particularly for mixtures that are slightly fuel-rich mixtures. The higher are the speeds of the flame, the higher is NO_x . While, fuel-lean mixtures take longer time to form NO_x . Also, NO_x depends on the location where it is being formed. NO_x is higher around areas that have high temperatures, such as around spark plugs.

NO_x is maximum for slightly lean mixtures with excess air, i.e. for Φ between 0.9 and 0.95 (Figure 2), although the maximum temperature of the flame occurs at $\Phi = 1$. Almost all variables that affect the temperature and the rate of combustion do affect NO_x , such as ignition angle, ignition timing, and compression ratio. Ignition timing in particular affects NO_x significantly. Advanced ignition increases the temperature in the cylinder and produces higher NO_x .

NO_x requires several non-instantaneous chemical reactions with complex kinetics. NO_x is higher than predicted by thermodynamics. The rate of forward reaction is different from the rate of backward reaction. Also, there is insufficient time to reach equilibrium (Mattavi and Amann, cited by Stone, 1992). Research is being undertaken to predict accurately NO_x emissions because of the complexity of its chemical reactions (Stone, 1992; 1999).

2.4 Minimising CO, HC, and NO_x emissions

CO emissions can be reduced with fuel-lean operations, but lean operations have negative effects on the power of the engine. Similar to CO, HC is reduced with fuel-lean operations until flammability of the mixture is reduced, thereafter lean operations increase HC emissions. Also, HC can be reduced if a second spark plug is added to the chamber; starting the flame at two points will reduce both the path of flame proceeding and the reaction time, and thereby will reduce flame quenching (Pulkrabek, 1997).

Unlike HC and CO, NO_x is reduced by several ways. NO_x is reduced with reducing either the duration or the temperature of combustion. Also, NO_x is

reduced with retarding ignition, because it reduces the peak temperature and pressure of combustion. However, retarding ignition has negative effects on both the power and fuel economy. Additionally, re-circulating a fraction of the exhaust gas reduces NO_x . Exhaust gas re-circulation (EGR) increases residuals in the cylinder by reducing both the temperature of combustion and the flame speed, and thereby reduces NO_x . An EGR between 5 percent and 10 percent is likely to halve NO_x , but also is likely to lower the engine overall efficiency by reducing its limits for operating lean.

3. Engine Design Parameters and Operating Characteristics

3.1 The Engine

The engine affects both emissions and fuel consumption. Internal combustion engines are classified according to several criteria, as follows (Pulkrabek, 1997):

Types of Ignition: Internal combustion engine are two main types (Stone, 1992):

- (a) **Spark ignition engine** – for gasoline engines – a spark plug ignites the mixture just before the piston will reach its upper position. A gasoline engine is started on very fuel-rich mixtures, and continues to operate with rich mixtures until reaching the optimal temperature under steady-state conditions.
- (b) **Compression ignition engine** –for diesel engines– fuel is ignited spontaneously by increasing both the pressure and temperature under compression.

Types of the Cycle: designs of conventional gasoline-fuelled engines are similar to reciprocating engines, where pistons reciprocate back and forth or move repeatedly up and down in the cylinders. Conventional gasoline-fuelled engines are either four-stroke or two-stroke cycles (Stone, 1992):

- (a) **Four-Stroke Cycle:** is completed every two revolutions of the crankshaft. The movement of the piston is transferred through connecting rods to the crankshaft and ultimately to the wheels, as shown in Figure 4.
- (b) **Two-Stroke Cycle:** the piston moves twice each cycle.

Types of the Cylinder

- **In-line Engine:** consists of several cylinders, and one is behind another on a straight line along the crankshaft. In-line engines with four cylinders are common for automobiles.

- **V-Engine:** consists of two banks of cylinders at an angle along the crankshaft. The angle between the two banks is between 15° and 120°, and is commonly between 60° and 90°. Engines have even numbers of cylinders, and V6s and V8s are common in automobiles.
- **Others:** such as the opposed cylinder engine, W-engine, the opposed piston engine, the radial engine, etc.

Position of the Intake and Exhaust Valves

Air Intake

- **Naturally Aspirated:** where the pressure in the intake of air is not boosted.
- **Supercharged:** where the pressure in the intake of air is increased and the compressor is being driven off the crankshaft.
- **Turbocharged:** where the pressure in the intake of air is increased and the turbine-compressor is driven by the flow in the exhaust.
- **Crankcase compressed**

Fuel Delivery Systems

- Carburetted
- Multiple Port Fuel Injections: one or more injectors at each the intake cylinder
- Throttle Body Fuel Injection: injectors are upstream in the intake manifold

Types of Cooling

- Air cooled
- Liquid cooled, water cooled

3.2 The Mechanism of Four-stroke Cycle in Internal Combustion Engines

The engine is a key element that influences both fuel consumption and emissions largely. The overall engine efficiency, in terms of combustion, thermal, mechanical, and volumetric efficiencies, depends on many factors, such as the type of the engine, the valve timing, injection/ignition timing, number of valves per cylinders, and the presence of turbo or intercooler (Stone, 1992). More importantly, it depends largely on the mechanism of the cycle. We describe the mechanism of four-stroke cycle in internal combustion engines, as follows (Stone, 1999;Figure 4):

- (1) **Intake stroke or induction:** when the inlet valve opens, the piston moves downward, and the air-fuel mixture flows into the cylinder.
- (2) **Compression stroke:** at the end of the intake stroke, the intake valve shuts down, and the piston starts to move upward and compress the mixture. As the piston approaches the top, the spark plug gives a spark, and combustion starts.
- (3) **Expansion or power stroke:** the spark ignites the compressed mixture, and elevates the pressure and temperature in the cylinder. Therefore, the burnt gases expand, and thereby force the piston downwards.

- (4) **Exhaust stroke:** at the end of the power stroke, the exhaust valve opens. As the piston starts moving upward, products of the combustion flow through the exhaust valve.

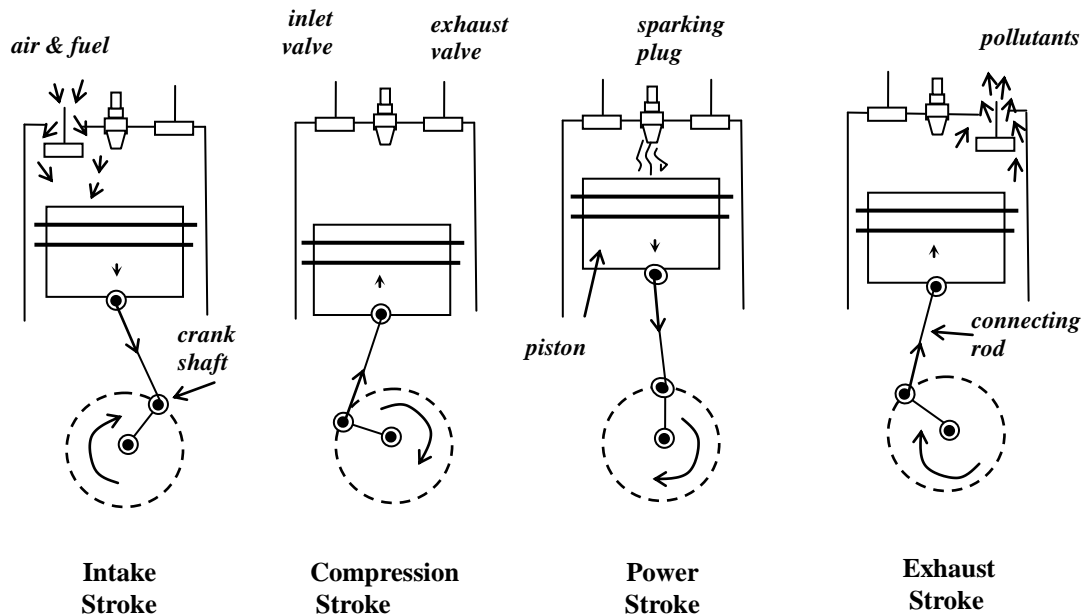


Figure 4 3 Four-Stroke Cycle in Internal Combustion Engine

Source: Stone (1999)

3.3 Engine Design and Operational Variables

Both emissions and fuel consumption are influenced by several variables, such as the air/fuel ratio, power of the engine, speed of the engine, ignition timing, pressure in the exhaust, overlaps of the intake and exhaust valves, the design of the chamber, compression ratio, and engine size. Therefore, it is difficult to correlate one engine to another (Schäfer and Basshuysen, 1995). We review critically the effects of several parameters on vehicle pollutants, as follows:

3.3.1 Engine Displacement

The displacement and the piston bore/stroke ratio affect both emissions and fuel consumption. For a given power, increasing the engine capacity will increase the potential of the engine to consume and burn fuel (Van den Brink and Van Wee, 2001). Small engines, at full power consume more fuel than larger engines with lower engine speed (rpm), because the higher is the engine speed, the higher are the friction losses, and more fuel is injected than is theoretically possible to burn. Thereby, power increases and temperatures in the exhaust are reduced. These affect adversely the catalytic converter, which produce higher HC and NO_x.

Reducing the number of cylinders and increasing the displacement of the cylinder reduce HC. Larger displacements emit higher NO_x but lower HC. The longer is the stroke relative to the engine bore, the lower are both HC and fuel consumption. However, there are almost always constraints on the designs of the engine capacity and the bore to stroke ratio, where other criteria, such as mass, chamber design, available installation space, and production equipments, allow only small variations in the designs.

3.3.2 Combustion Chamber

The shape of the chamber influences directly the compression ratio. Higher compression ratio creates lean-burn conditions that save fuel considerably. A compact combustion chamber that provides a small surface – volume ratios emit lower HC and higher NO_x emissions. A small ratio of the chamber-surface to the chamber-volume will reduce flame quenching, and thereby will reduce HC emissions. Also, a compact combustion chamber with a central spark plug will reduce the combustion time to minimum, and hence will reduce HC.

3.3.3 Deposits on the walls of the Combustion Chamber

Engines with larger compression ratios accumulate higher deposits on the walls of the engine. The absorption capacity of the walls for the deposits relates directly to the pressure in the chamber. The higher the pressure in the chamber, the higher is the absorption capacity of the walls for the deposits. Similarly, the lower the pressure, the lower is the absorption capacity of the walls for the deposits. The pressure is maximal during the compression stroke, and is minimal during the exhaust stroke when the exhaust valve is opened. Therefore, particles desorbed back into the cylinder during the exhaust stroke. Older engines have larger deposits, and hence emit higher HC. HC from deposits on the cylinder walls have increased with eliminating lead as a gasoline additive, because lead treats the metal walls of the engine (Pullarek, 1997).

3.3.4 Spark Plugs

The shape and location of the spark plug affect significantly vehicle emissions. For a given air-fuel ratio, the larger is the volume between the spark plug and the piston crown, or the larger is the distance between the electrode of the spark plug and crown of the piston, the better is combustion. Central spark plugs in engines with four and five valves have shorter flame paths, and therefore reduce both HC and fuel consumption.

3.3.5 Ignition timing

Ignition timing affects significantly vehicle emissions. Ignition timing is either electronic or mechanical. Ignition timing must be accurate. If ignition is too late, it is more likely that combustion will be incomplete and the exhaust valves are overheated. On the other hand, early ignition with peak pressure and temperature induce a knock.

Ignition timing is adjusted to give maximum power. However, ignition timing that gives the best power and driveability does not always give the lowest emissions. For full throttle and low speeds of the engine, retarding ignition will reduce the power efficiency of the engine. The more the timing is retarded, the lower emissions are. Retarding ignition increases temperature of the exhaust; therefore, enhances combustion. Also, it lowers the peak temperature of combustion hence reduces NO_x .

Advancing ignition increases NO_x and HC for a wide range of air-fuel mixtures, particularly for the stoichiometric mixture. Advancing ignition decreases the peak temperatures in the exhaust, worsen post-reactions, and increases HC. Although retarded ignitions are very effective in reducing vehicle emissions, particularly under warming-up and early light-offs of the catalytic converter, but they increase fuel consumption and CO_2 .

3.3.6 The Crevices in the Combustion Chamber

Approximately 80 percent of all HC are from the engine crevices. The spark plug forms the largest proportion of the crevices. Therefore, location of the spark plug relative to the top ring is an important determinate of HC emissions. The larger is the distance between the spark plug and the top ring, the more fuel is forced into the gaps prior to combustion. Thus, the larger are HC emissions. The crevices that are around the piston rings are largest when the engine is cold, because of the different coefficients of thermal expansion for various materials (Pulkrabek, 1997).

3.3.7 Compression Ratio

Compression ratio is the ratio of the cylinder volume with the piston being at the lowest position, to the cylinder volume with the piston being at the upper position (Van den Brink and Van Wee, 2001). Compression ratio should be as high as possible to secure high thermal efficiency and to reduce fuel consumption. Higher compression ratios increase the combustion temperatures and reduce NO_x . The improvement of thermal efficiency is important to reduce the temperature of the exhaust and to weaken post-oxidation reactions of HC and CO. Nonetheless, the reduction of the temperatures of the exhaust has negative impacts on the light-offs of the catalytic converter, especially under warming-up operations, and therefore produce more CO, HC, and NO_x emissions.

3.3.8 Valve Overlaps

When both the exhaust and intake valves are overlapping, a direct flow of the air-fuel mixture into the exhaust occurs. A well-designed engine minimises this flow. The flow is maximal under idle and low engine speed when the real time of overlapping is the longest (Pulkrabek, 1997).

3.3.9 Leak Past the Exhaust Valve

During the compression stroke, the pressure increases and some of the mixture is forced into the crevices. In particular, those are around the edges of the exhaust valve, and between the valve and valve seats. As a result, a small flow leaks beyond the valve into the exhaust manifold. When the exhaust valve is open, an

instant peak in HC occurs, especially at the beginning of the exhaust stroke (Pulkrabek, 1997).

3.3.10 Engine Management System

Engine management systems are two main types that are either used individually or in combination:

- the first uses an electronic memory to save the optimum discrete engine-operating conditions, such as ignition timing and mixture strength; and
- the second type uses an adaptive or a self-tuning control system to adjust continuously the engine-operating conditions for the optimal settings.

Engines that are controlled electronically are able to adjust many variables, such as ignition timing and strength of the mixture. Thus, they are able to reduce both emissions and fuel consumption. However they must meet several essential parameters, such as adaptation of the air-fuel mixture to a wide range of operating conditions, distributing the mixture equally into the cylinders, and adjusting timing of injecting fuel for various loads.

Engine management systems can adjust the pre-injection angle of the fuel for various loads. Therefore, they reduce HC emissions. Large pre-injection angles produce lower HC for partial loads. However, in case of full throttle, wide ranges of angles produce lower HC. Proper correlations of the injection timing relative to the opening of the inlet valve are required. Experiments with simultaneous and sequential injection, show that the proper correlations has positive effects on lean-burn operations, and therefore on HC and NO_x. Simultaneous injection requires that fuel be injected in all cylinders at the same moment. Hence, the time to prepare the air-fuel mixture in the intake rail differs from one cylinder to another. Simultaneous injection affects adversely emissions under transient operating conditions, such as under accelerating and warming-up.

3.3.11 Air-Fuel Mixture

Air-fuel mixtures affect largely both fuel consumption and emissions, especially under transient operating conditions. Air-fuel mixtures vary with various power levels, engine-operating conditions, engine speeds, and engine loads (Heywood, 1988). Air-fuel mixtures are formed by the fuel delivery system, which mixes the fuel in the tank with the ambient air. During induction, air-fuel mixtures are drawn into the cylinder. The optimum air-fuel mixture gives theoretically, the smoothest operations, but emission control systems require a different air-fuel mixture. Also, they require re-circulating a fraction of the exhaust gases (EGR) into the input system (Heywood, 1988).

Stringent emission standards require improving the mixture by several measures, such as adjusting the pre-injection angle, creating an air-envelope around the injection jet, and using multi-point injection. A mixture that has slightly excess air requires lower fuel consumption, and produces lower HC, CO, and maximum NO_x. The mixture is fuel-rich when fuel equivalence ratio (Φ) is less than one. As a

result, CO is increased significantly. The mixture reaches misfire limits when Φ is greater than 1.2 and HC increases sharply. Improvements in the air-fuel mixture improve the conversion efficiency of the catalytic together with the oxygen that have positive impacts on the mixture stability.

3.3.12 Engine Load

Increasing engine load and the exhaust temperatures would reduce HC. The engine loads have no effects on HC under constant engine speeds, constant air/fuel ratio, and a MBT spark. Similarly, engine loads do not affect CO under constant air/fuel ratio. Increasing engine load and the airflow will increase both HC and CO. Hence small, light, and fuel-efficient cars produce lower emissions.

3.3.13 Engine Speed

The optimum ratio of engine speed (N) – measured in a number of revolutions per unit of time – to vehicle velocity (V), i.e., (N/V), is tradeoffs between several criteria, such as performance, fuel economy, and emissions. The trend has been to lower N/V ratios to improve fuel economy and engine noise (Wong, 2001). High engine speeds improve combustion and therefore reduce emissions. The speed of the engine does not affect CO under normal temperatures of the exhaust, because oxidation of CO in the exhaust is kinetically limited. On the one hand, increasing the speed of the engine will increase HC. On the other hand, decreasing the speed of the engine will increase NO_x.

3.3.14 The Fuel Delivery System

Either a carburettor or a fuel injector controls the flow of fuel into the intake manifold and distributes the fuel across the air stream. Carburettors are most commonly used and are still used widely, although current legislations have reduced the scope for using them (Heywood, 1988). Carburettors are of two main types, fixed jet and variable jet. Fuel injectors in spark ignition engines, are of two types, multi-point and single-point.

3.3.15 Exhaust Gas Re-circulation (EGR)

Exhaust gas re-circulation (EGR) re-circulates the flow in the exhaust into the air inlet. EGR are two main types:

- external EGR that externally feeds the exhaust flow into the intake system; and
- internal EGR that operates when the intake and exhaust valves are overlapping. The overlapping of valves weakens the cleaning and the removing of impurities from the cylinder. Hence, it increases residuals in the cylinder. Excessive residuals, especially under idle operations cause engine misfires and rough operations, and thereby increase HC.

Exhaust gas re-circulation (EGR) is increased for higher compression ratio, because misfire limits are shifted towards leaner operations. Therefore, NO_x is reduced and fuel economy is improved. Exhaust gas re-circulation reduces NO_x by:

- reducing the combustion temperatures;
- replacing some of the air in the chamber with the exhaust that has low oxygen; and
- reducing the rates of the combustion reactions to reduce further the temperature in the exhaust.

4. Exhaust After-Treatment Systems

Exhaust after treatment systems are of several types, such as, catalytic converters, secondary air injection, insulation of exhaust manifold, thermal reactors, filters (traps), and particulate retention systems. The type used depends on the type of the engine and fuel. Three-way catalytic converters are the most common types for gasoline-fuelled vehicles. They convert CO, HC, and NO_x into CO₂, H₂O, and N₂. Three-way catalytic converters are capable to minimise CO, HC, and NO_x simultaneously, provided that the air-fuel mixture is stoichiometric (Heywood, 1988).

4.1 Catalytic Converter Systems

Catalytic converters are four basic designs:

(1) Oxidation catalytic converters

Oxidation catalytic converters convert the exhaust into H₂O and CO₂, provided excess air is available. The excess air is available through either lean mixtures or secondary air injections. Oxidation catalytic converters do not require any complex control systems.

Oxidation catalytic converters were first used in 1975 on the U.S. vehicles. They are no longer used on passenger vehicles, but are used widely on diesel engines because they convert soluble particulate matter in addition to CO, HC, and NO_x.

(2) Dual-bed catalytic converters

Dual-bed catalytic converters consist of two catalyst systems arranged in a line. The first is a reduction catalyst for reducing NO_x, and the second is an oxidation catalyst for reducing HC and CO. Dual-bed converters require fuel-rich mixture, consume more fuel, and hence increase CO₂ and ammonia (NH₃) emissions. Unlike oxidation converters, they do not require any complex control systems. Dual-bed conversion efficiency for NO_x is less than three-way catalytic converters.

(3) Three-way catalytic converters

Three-way closed-loop catalytic converters are the most efficient catalyst used on internal-combustion engines. They reduce NO_x, HC, and CO with a very high efficiency, but unlike both the dual-bed and oxidation systems

require a complex control system. The uncontrolled three-way catalytic converters achieve between 40 percent and 50 percent conversion efficiency, whereas computer-controlled systems achieve more than 95 percent.

(4) Denox or lean-burn catalytic converters

Denox converters are being developed, but have already scored conversion efficiency greater than 50 percent. They convert CO, HC, and NO_x (Schäfer and Basshuysen, 1995).

Conversion efficiency is the percentage of emissions reduced. It depends on two factors:

- (i) **Light-off behaviour or the exhaust temperature:** is the temperature of the catalytic when converting 50 percent of the exhaust, and is normally between 260°C and 280°C but varies with different pollutants and catalytic converter systems. Ninety-percent of CO and NO_x are converted at 300 °C.
- (ii) **The air/fuel ratio or conversion behaviour:** is converting CO, HC, and NO_x for various air/fuel ratio. Higher conversion efficiencies are for mixtures that are chemically correct. Conversion efficiency decreases gradually with the operating life of the catalytic converter, due to:
 - **Thermal ageing:** is overheating of the catalytic, which starts at the inlet of the catalytic converter and is responsible for the loss of the active surface-area of the catalytic. To prevent thermal ageing in ceramic-made catalytic, temperatures of the catalytic should not exceed 900°C while the vehicle is in motion,
 - **Contamination:** are deposits from chemical reactions that alter the active-surface of the catalytic to partially inactive surface because of either:
 - o **chemical contamination:** reacting with foreign substances, such as fuel or oil additives, or
 - o **mechanical contamination:** blocking the pores of the coat by fuel additives, such as lead or oil sulphur, or by the metal compounds in the engine oil, such as Zinc (Zn), Magnesium (Mg), and Calcium (Ca).

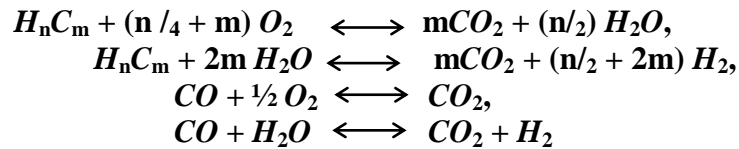
4.2 The Principles of Catalytic Converters

The activation energy of the catalytic converter is sufficiently reduced to increase the speeds and decrease the temperatures of post-combustion reactions in the exhaust, and therefore enhance further the oxidation and reduction in the exhaust. Post-combustion reactions reduce CO, HC, and NO_x, provided the right temperature and oxygen are available. Oxidation reactions reduce both HC and CO,

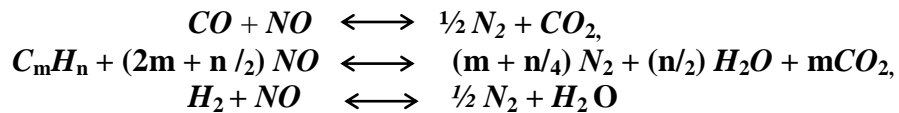
and reduction reactions reduce NO_x (Patterson and Henein, 1972). Reducing HC and CO requires excess oxygen, but reducing NO_x requires less oxygen.

Post-combustion reactions are increased by reducing the heat losses and by injecting air into the exhaust

- **Oxidation reactions** transform HC and CO into CO_2 and H_2O , but increase enhanced greenhouse emissions.



- **Reduction reactions** decompose NO and NO_x , as follows:



4.3 Oxygen Sensors

Oxygen sensors are placed ahead of three-way catalytic converters to improve the stability of the mixture. Oxygen sensors alter the air-fuel mixture to a chemically correct mixture for higher conversion efficiency. V-engines are sometimes fitted with two oxygen sensors.

Oxygen sensor is a galvanic cell, which has gas permeable solid electrolyte made of zirconium and yttrium oxide, which behaves similar to a pure oxygen conductor. Ceramic-made sensor becomes conductive for temperatures greater than 300 °C. Both sides of the solid electrolyte are bonded with porous electrodes that create an electrical voltage due to the difference in oxygen concentrations on both sides. This voltage is a measure of the concentrations of oxygen in the exhaust. In order to achieve high conversion efficiency, the mixture strength must remain approximately equal to one, i.e., between 0.995 and 1.005.

5. The Engine Overall Efficiency

The engine is a key element that influences both fuel consumption and emissions. The engine efficiency depends on many factors, such as fuel type and engine type, valve timing, injection/ignition timing, number of valves per cylinders and the presence of turbo or intercooler (Stone, 1992). The engine overall efficiency is defined in terms of combustion, thermal, mechanical, and volumetric efficiencies.

Combustion efficiency η_c

The efficiency of combustion is the percentage of the burnt fuel. The combustion efficiency (η_c) is typically between 0.95 and 0.98 (Pulkrabek, 1997).

Thermal efficiency η_t

Air and fuel, or the reactants, enter the engine at ambient temperature (T_0) and pressure (p_0). However, the products leave at a temperature greater than T_0 and a pressure equal to p_0 . Ideally, both reactants and products should enter and leave the engine at ambient temperature and pressure. The thermal efficiency and the heat added are related (Pulkrabek, 1997), as follows:

$$Q_{in} = m_f Q_{HV} \eta_c$$

$$\eta_t = \frac{W}{Q_{in}} = \frac{W^\circ}{Q_{in}^\circ} = \frac{W^\circ}{m_f^\circ Q_{HV} \eta_c} = \frac{\eta_f}{\eta_c}$$

where:

- η_t = engine thermal efficiency
- η_f = fuel conversion efficiency
- η_c = combustion efficiency = 0.95-0.98
- W = Work or Energy per a cycle (KJ)
- W° = power (KW)
- m_f° = fuel mass flow rate
- Q_{HV} = heating value of a fuel
- Q_{in} = the heat added per cycle per cylinder

The specific fuel consumption (sfc) is defined by the rate of fuel consumed per unit of power, such as kg/MJ or kg/kW.h. It is inversely related to the arbitrary overall efficiency η_0 and the fuel calorific value, as follows:

$$sfc \propto \frac{1}{-\Delta H_0 \eta_0}$$

where:

$$\eta_0 = \frac{W}{-\Delta H_0}$$

The rate of fuel consumed per a unit of power output is:

$$sfc = \frac{\dot{m}_f}{W} \text{ (kg/J)} \quad \text{specific fuel consumption kg / kW.h}$$

\dot{m}_f = fuel mass flow rate

W = power (J)

Mechanical efficiency η_m

The mechanical efficiency is the ratio between the indicated thermal efficiency and the brake thermal efficiency:

$$\eta_m = \frac{(\eta_t)_b}{(\eta_t)_i}$$

$(\eta_t)_b$ = thermal brake $\approx 30\%$

$(\eta_t)_i$ = indicated thermal $\approx 50\% - 60\%$

The indicated thermal efficiency is between 50 percent and 60 percent, and the brake thermal efficiency is approximately 30 percent. The mechanical efficiency is between 50 percent and 60 percent.

Volumetric efficiency η_v

The power of the engine depends on the quantity of the air that flows into the cylinder per a cycle. More air means more fuel is burnt, and thereby more of the energy produced is converted to power.

$$\tau = \frac{\eta_f \eta_v V_d Q}{2\pi n} \quad \text{[Torque N. m]}$$

$$P = \frac{\eta_f}{n} \quad \text{[Output power kW]}$$

Drawing in a relatively small volume of the liquid fuel into the cylinder is much easier than drawing in a large volume of the gaseous air. Ideally, the mass of air that flows in per cycle equals to the density of the ambient air times the cylinder displacement. However, in reality, less than the ideal air enters the cylinder due to

the short available time and flow constraints, such as air cleaner, carburettor, intake manifold and intake valves. The volumetric efficiency is:

$$\eta_v = \frac{\mathbf{m}_a}{\rho_a \mathbf{V}_d} = \frac{\mathbf{n} \mathbf{m}_a^\circ}{\rho_a \mathbf{V}_d \mathbf{N}}$$

where:

m_a = mass of the air into the engine (or cylinder) each cycle

m[°]_a = air steady-state flow into the engine

V_d = displacement volume

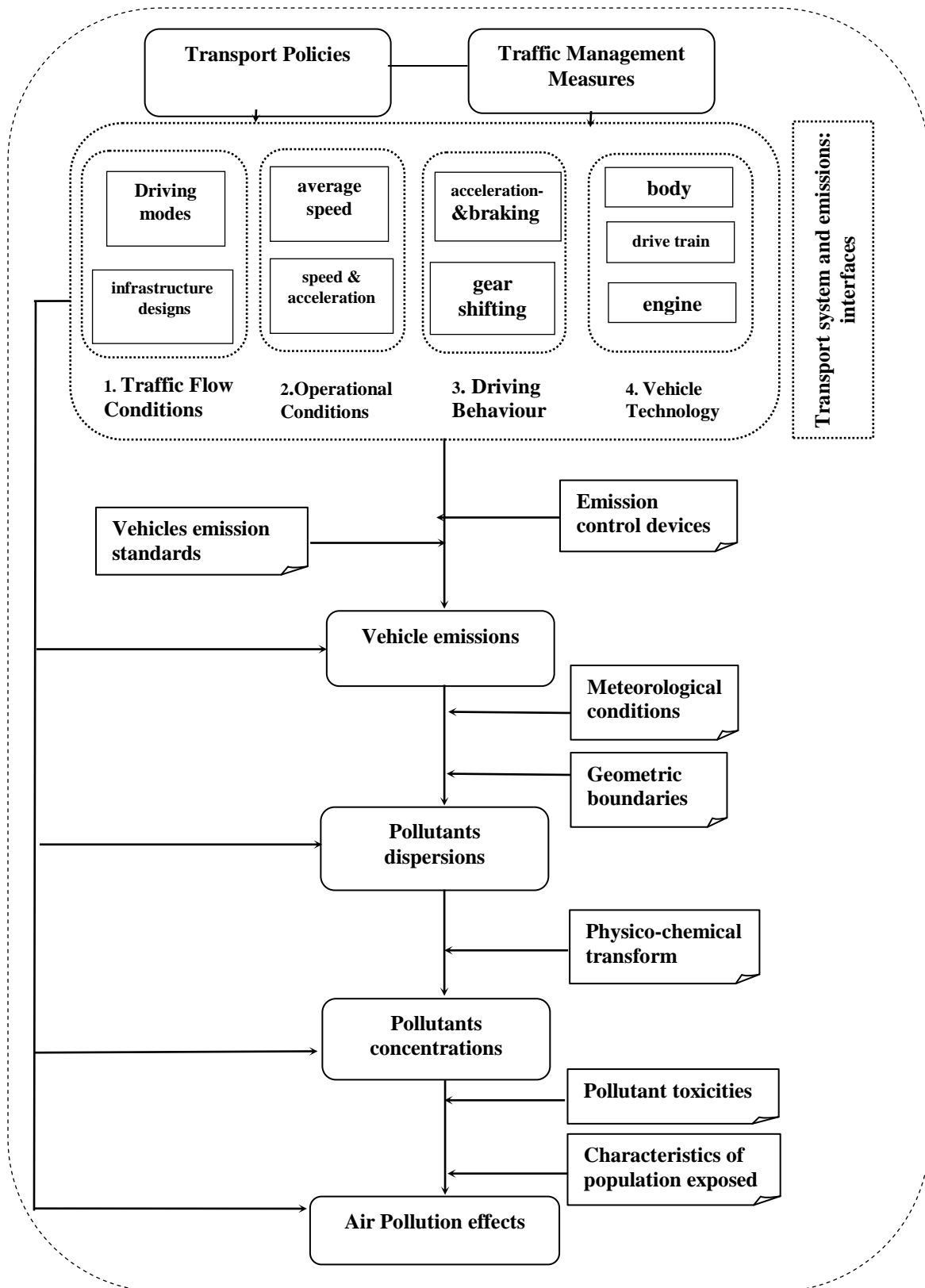
N = engine speed

n = number of revolutions per cycle.

The volumetric efficiency is between 75 percent and 90 percent for wide-open throttle (WOT) conditions. However, when the throttle is closed, it is much lower. Closing the throttle restricts the flow of air into the engine and limits the power produced.

Appendix IV

**Transport Planning and Air-Pollution of Vehicle Emissions:
A Framework**



Transport Planning and Air-Pollution Effects: A framework