1 Introduction

The term ‘Air pollution’ is used to denote the presence of chemicals that are not present in the natural air composition or they are but in lowest quantities and that may be harmful for human beings, animals or vegetation or more in general may cause a short-term or long-term adverse effect.

The present-day atmosphere is indeed different from the natural atmosphere that existed before the Industrial Revolution (1760) in terms of chemical composition.

Gas	**Symbol**	**Ppm (Natural atm.)**	**Ppm (Current atm.)**
Carbon dioxide	CO_2	280	397
Methane	CH_4	0.750	1.79
Nitrous oxide	N_2O	0.270	0.322

In other words, it may be said that air pollution is the chemical composition that has followed the human activities began with the fuels burning.

Since the 1950s, we have known that vehicle exhaust fumes play a major role in the deterioration of air quality especially in urban areas. The first country to recognise the fact was the United States that gives the EPA (Environmental

Protection Agency) the responsibility and legal authority to control air pollution by setting limits on pollution from stationary area and mobile sources of emissions through the CAA (Clean Air Act) in 1970. Federal standards were emitted (known as National Ambient Air Quality Standards) to be set at levels that protect human health. Automobile emissions were arbitrarily set at a 90% reduction from the 1970 (for CO and hydrocarbons) or 1971 (for NOx) model year emissions to be achieved by 1975 (or 1976 for NOx). Since there was no proven way to achieve these goals when the law was enacted, the industry was in effect forced to develop new technologies to meet the standards by a certain deadline ("technology-forcing legislation"). Emission standards were to be written by the EPA for certain new industrial plants. This led to less polluting vehicles but the increase of population and gross domestic product reduce the innovations' effects.

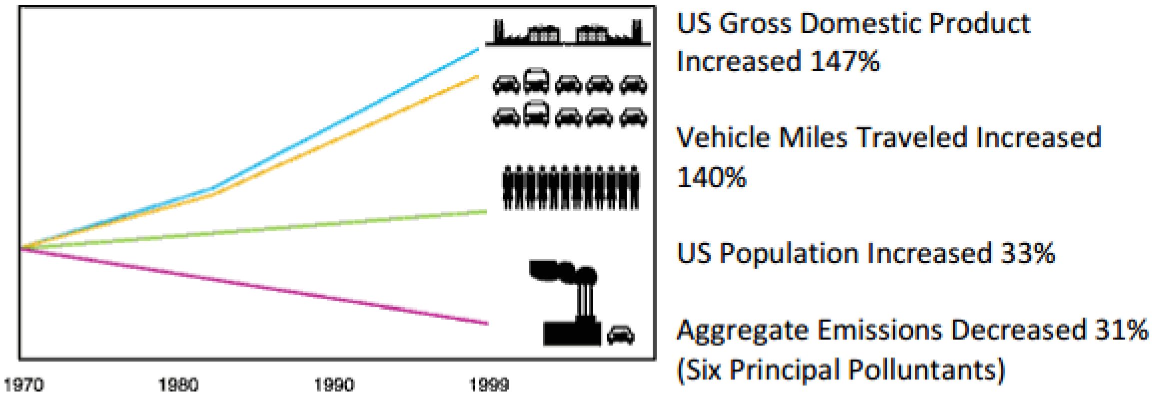

Figure 1 – EPA projections

The result is that the air is much cleaner and the pollutants concentrations (Figure 2) have decreased respect to the quantities of the 1970 but despite this further progress is not only required but necessary.

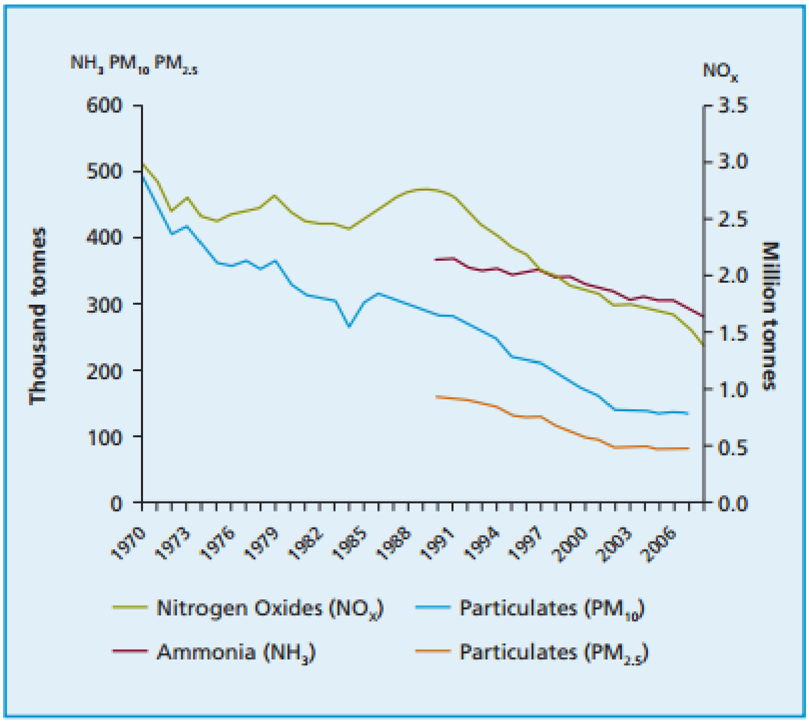

Figure 2

In the European Community the developing of a legislation has started in 1968 with the drafting of the regulation known as ECE 15. In ECE-15 regulation the procedure for the detection of vehicle emissions has been established. From 1974 onward a series of pronouncements has been emitted to regulate the approval of motor vehicles.

The Italian legislation about pollutants' emissions produced by motor vehicles is substantially made of a series of acts that transpose the provisions of the European community.

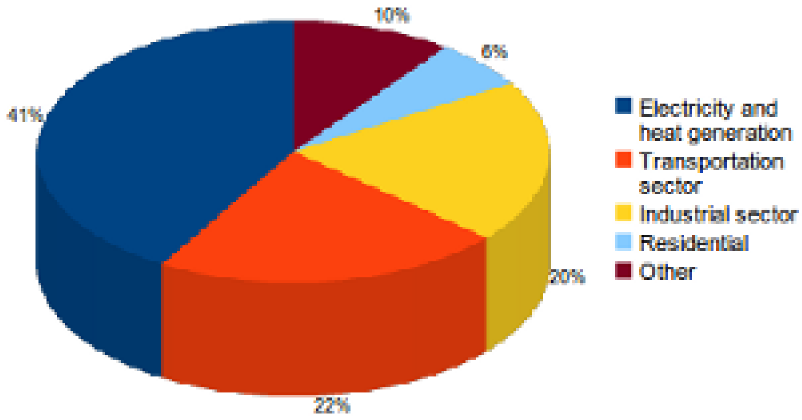

Figure 3 - Le Quéré, C. et al. (2013). The global carbon budget 1959-2011

Pollutants that come out from the motor vehicles are responsible of 22% of the total carbon dioxide emissions. This made national policy focusing their attention on better vehicles engine to respect Kyoto Protocol impositions.

The Kyoto Protocol is an international treaty which extends the 1992 United Nations Framework Convention on Climate Change that commits State Parties to reduce greenhouse gases emissions, based on the premise that: global warming exists and man-made CO_2 emissions have caused it. The Kyoto Protocol provides for reduce emissions of the greenhouse gases in a measure not lower than 5.2% respect to the emissions registered in 1990.

To understand in which measure the transportation sector is important in greenhouses reduction policies, it may be considered the Italian Government's program that with a view to reducing of the 7% the CO_2 emissions by the 2010 (110 Mt equivalent CO_2) planned to operate principally on transportation sector (with a contribute of 24 Mt equivalent CO_2) with the following measures:

- Urban traffic control

- Incentives for high efficiency vehicles
- Modernisation of railways and sea roads
- Displacement of freight transport from road to railway

1.1 Pollutant classification

Pollutants can be classified as *primary* or *secondary pollutants* (Zanetti, 2007). Primary pollutants are all the substances that are directly emitted into air from sources. The main primary pollutants known to cause harm in high enough concentrations are the following:

- Carbon compounds (CO, CO_2, CH_4, VOCs)
- Nitrogen compounds (NO, N_2O, NH_3)
- Sulphur compounds (H_2S and SO_2)
- Halogen compounds, such as chlorides, fluorides, and bromides
- Particulate matter (PM), either in solid or liquid form, which is categorized into the groups (base on the diameter of the particles):
    1. Particles less than 100 microns (called “inhalable”)
    2. Particles less than 10 microns (PM_{10})
    3. Particles less than 4 microns (often called “respirable”)
    4. Particles less than 2.5 micron ($PM_{2.5}$)
    5. Particles less than 0.1 microns ($PM_{0.1}$)

Secondary pollutant not directly emitted but forms when other pollutants (primary pollutants) react in the atmosphere.

Secondary pollutants are not directly emitted from sources, but instead form in the atmosphere from primary pollutants (also called “precursors”). The main secondary pollutants known to cause harm in high enough concentrations are the following:

- NO_2 and HNO_3 formed from NO
- Ozone (O_3) formed from photochemical reactions of nitrogen oxides and VOCs
- Sulfuric acid droplets formed from SO_2 and nitric acid droplets formed from NO_2
- Sulphates and nitrates aerosols (e.g., ammonium (bi)sulphate and ammonium nitrate) formed from reactions of sulfuric acid droplets and nitric acid droplets with NH_3, respectively
- Organic aerosols formed from VOCs in gas-to-particle reactions

This kind of pollution was first recognized in 1940 in the city of Los Angeles. In fact, after a long research, was found that nitrogen oxides and VOC were involved together (thanks to the sunlight) causing the production of ozone and other secondary chemicals (this is the reason why this phenomenon is also called *photochemical smog*).

1.2 An introduction to the main pollutants

1.2.1 Carbon monoxide

Carbon monoxide (CO) is a colourless, odourless, and tasteless gas that is slightly less dense than air. After carbon monoxide is breathed in, it enters your bloodstream and mixes with haemoglobin (the part of red blood cells that carry oxygen around your body), to form carboxyhaemoglobin. When this happens, the blood is no longer able to carry oxygen, and this lack of oxygen causes the body's cells and tissue to fail.

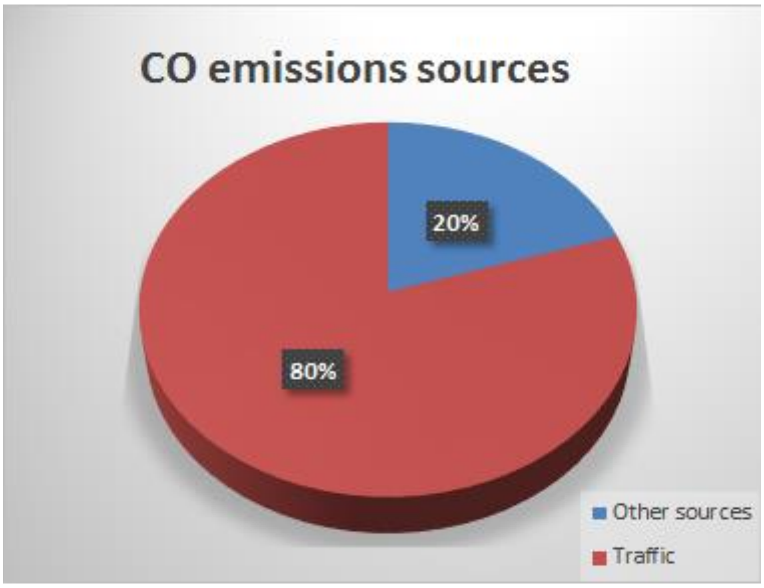

Figure 4 – Source Pennsylvania State University

Carbon monoxide is produced when fuels such as gas, oil, coal and wood don't burn fully. In a general way fuel combustion in residential housing, businesses, industry and utilities accounts for 10 to 20 percent of the total CO emissions, while mobile sources (cars, trucks, buses and off-road equipment such as marine engines and construction equipment) account for 80 to 90 percent.

So the vehicles are the main source of local air CO pollution. The presence of carbon monoxide is strictly linked to the traffic flows as it has been showed in the picture below representing the CO concentrations in the 24 hours of a day.

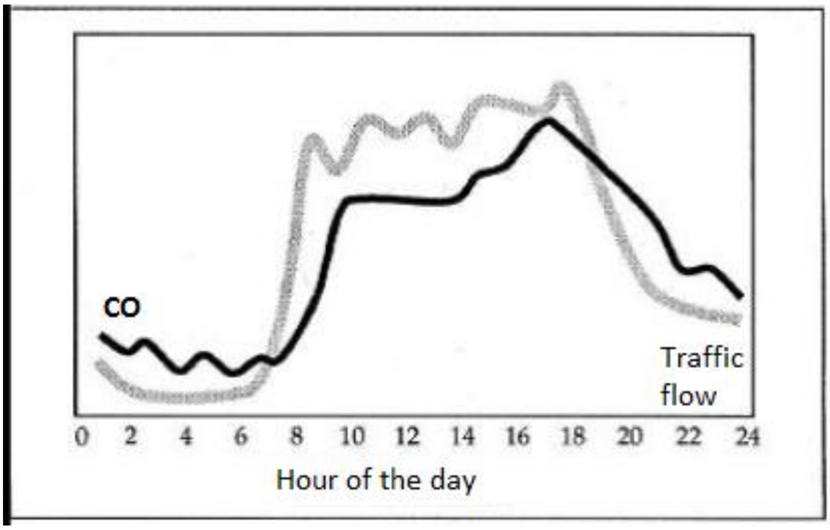

Figure 5

1.2.2 Carbon dioxide

Carbon dioxide (chemical formula CO_2) is a colourless and odourless gas vital to life on Earth. This naturally occurring chemical compound is composed of a carbon atom covalently double bonded to two oxygen atoms. Carbon dioxide exists in Earth's atmosphere as a trace gas at a concentration of about 0.04 percent (400 ppm) by volume.

Carbon dioxide is a significant greenhouse gas. Since the Industrial Revolution, anthropogenic emissions - including the burning of carbon-based fossil fuels and land use changes (primarily deforestation) - have rapidly increased its concentration in the atmosphere, leading to global warming. It is also a major cause of ocean acidification because it dissolves in water to form carbonic acid. Roughly a third of America's carbon dioxide (CO_2) emissions come from moving people or goods, and 80 percent of these emissions are from cars and trucks. In order to reduce CO_2 emissions from the transportation sector, policy makers are primarily pushing for more efficient vehicles and the use of alternative fuels. In terms of vehicle improvements, it is thought that:

- vehicles can be made lighter and smaller (while maintaining safety);
- further improvements can be made in terms of powertrain efficiency;
- alternative technologies can be developed, such as hybrid and fuel-cell vehicles.

For those that are technology-ready and have started to enter the market, it will still probably take several years for a majority of the existing fleet to be turned over before a significant impact on CO_2 can be seen. With all that being said, it can be pointed out that comparatively less attention has been given to CO_2 emissions associated with traffic congestion and possible short-term CO_2 reductions as a result of improved traffic operations. Traffic congestion can be considered as a supply management problem. The transportation infrastructure (i.e., roadways) can be considered as supply for use by drivers (demand). If these supplies are limited in terms of capacity and demand is high, congestion is likely to occur.

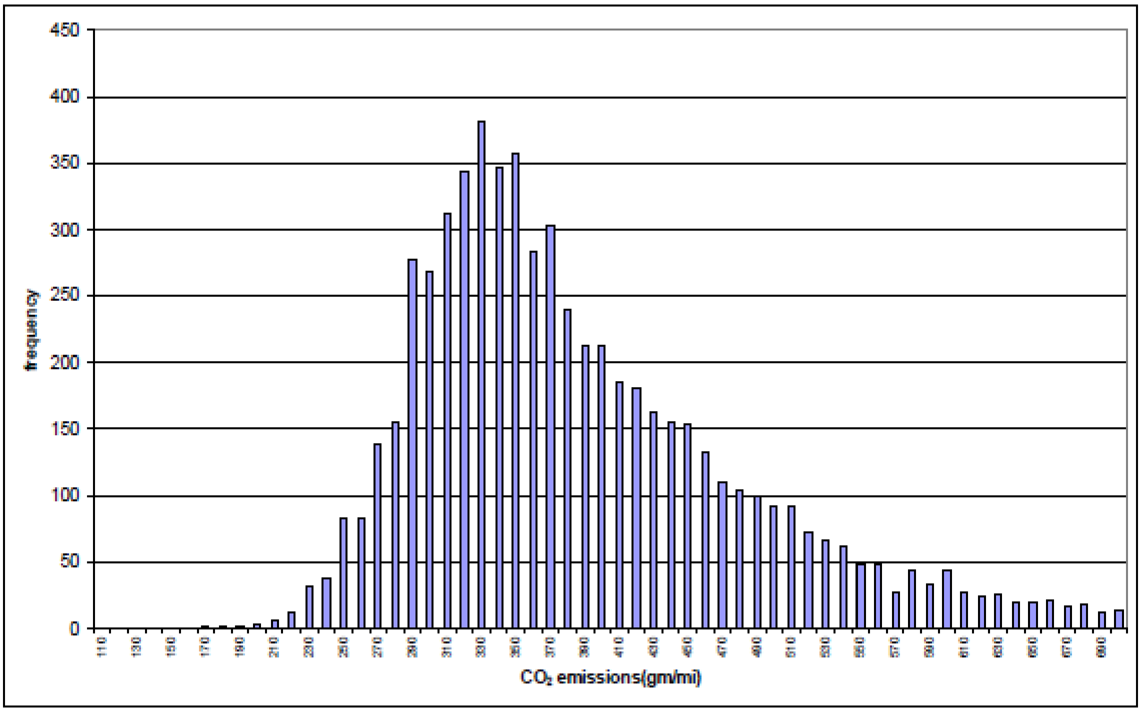

Figure 6 - CO_2 emissions histogram for a representative database of trip in Southern California

1.2.3 Hydrocarbons

Hydrocarbons are the simplest organic compounds. Containing only carbon and hydrogen, they can be straight-chain, branched chain, or cyclic molecules. Carbon tends to form four bonds in a tetrahedral geometry. Hydrocarbon derivatives are formed when there is a substitution of a functional group at one or more of these positions.

Hydrocarbon, any of a class of organic chemical compounds composed only of the elements carbon (C) and hydrogen (H). The carbon atoms join together to form the framework of the compound; the hydrogen atoms attach to them in many different configurations. Hydrocarbons are the principal constituents of petroleum and natural gas. They serve as fuels and lubricants as well as raw materials to produce plastics, fibres, rubbers, solvents, explosives, and industrial chemicals.

Hydrocarbons are released through the exhaust when fuel is unburned or incompletely burned. Considerable amounts also reach the atmosphere due to fuel evaporation. Hydrocarbons evaporate from the fuel tank and other fuel feed elements, such as the fuel line, carburettor, filter, reserve canister, etc.. Hydrocarbons also vaporize when fuel station storage depots and motors vehicles tanks are filled.

A study conducted by the American Chemical Society on the aerosols related to vehicle emissions in the Mexico City in 2002 metropolitan area reported that Median total particulate PAH concentrations along Mexico City's roadways range from 60 to 910 ng m-3, averaged over a minimum of 1 hour. This is unfortunately the situation of many of the cities among the PVS countries.

The exposure to vehicle-related PAH emission is in a particular way dangerous: such levels may present an important public health risk.

1.2.4 Nitrogen oxides

NOx is a generic term for the mono-nitrogen oxides NO and NO_2 (nitric oxide and nitrogen dioxide). They are produced from the reaction among nitrogen, oxygen and even hydrocarbons (during combustion), especially at high temperatures. In areas of high motor vehicle traffic, such as in large cities, the amount of nitrogen oxides emitted into the atmosphere as air pollution can be significant. NOx gases are formed whenever combustion occurs in the presence of nitrogen – as in an air-breathing engine; they also are produced naturally by lightning. In atmospheric chemistry, the term means the total concentration of NO and NO_2. NOx gases react to form smog and acid rain as well as being central to the formation of tropospheric ozone.

The three primary sources of NOx in combustion processes:

- *thermal NOx*: Thermal NOx - The concentration of “thermal NOx” is controlled by the nitrogen and oxygen molar concentrations and the temperature of combustion. Combustion at temperatures well below 1,300C (2,370F) forms much smaller concentrations of thermal NOx.
- *fuel NOx*: It is estimated that transportation fuels cause 54% of the anthropogenic (i.e. human-caused) NOx. The major source of NOx production from nitrogen-bearing fuels such as certain coals and oil, is the conversion of fuel bound nitrogen to NOx during combustion. [13] During combustion, the nitrogen bound in the fuel is released as a free radical and ultimately forms free N_2, or NO. Fuel NOx can contribute as much as 50% of total emissions when combusting oil and as much as 80% when combusting coal.
- *prompt NOx*: This third source is attributed to the reaction of atmospheric nitrogen, N_2, with radicals such as C, CH, and CH2 fragments derived from fuel.

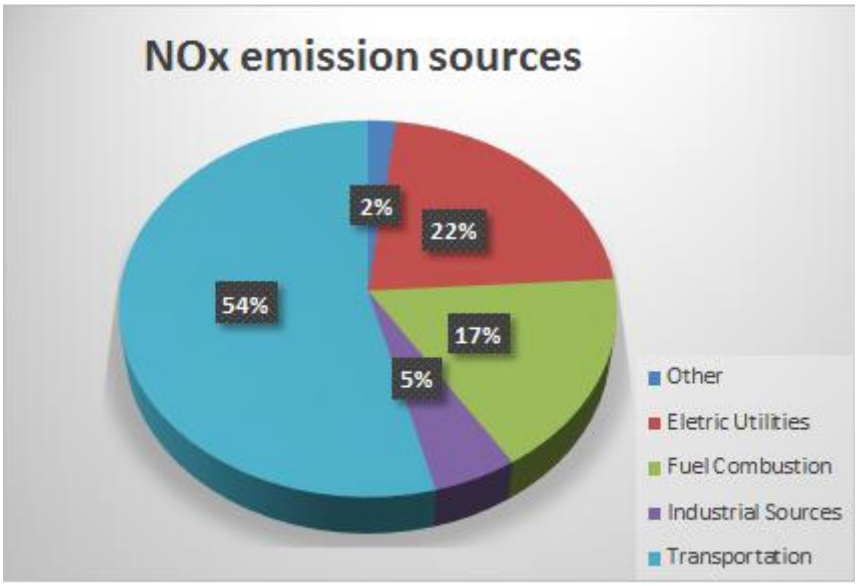

Figure 7 – Source Sylvatek studies

1.2.5 Particulate matter

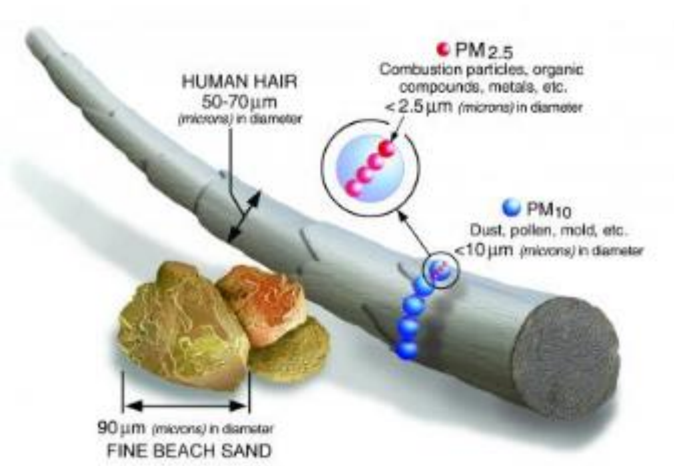

Figure 8 - Size comparison for PM particle

Atmospheric particulate matter – also known as particulate matter (PM) or particulates – is microscopic solid or liquid matter suspended in the Earth's atmosphere. The term aerosol commonly refers to the particulate/air mixture, as opposed to the particulate matter alone. Sources of particulate matter can be man-made or natural: some are emitted directly from a source, such as construction sites, unpaved roads, fields, smokestacks or fires and others form in the atmosphere because of complex reactions of chemicals such as sulphur dioxide and nitrogen oxides, which are pollutants emitted from power plants, industries and automobiles.

Recent studies show that no exhaust particulate matter emissions from road traffic are also an important source of this air pollutant (Thorpe, 2008). Non-exhaust particulate emissions involve abrasive processes such as tire wear, brake wear and road surface wear, these processes can lead to the deposition of particles on the road surface. The other process is the resuspension of road dust which is due to traffic induced turbulence, tire friction or the action of the wind. A study conducted in three European cities investigated the sources of road dust particles. It concluded that road dust resuspension is the dominant source of PM_{10} in Spain (60%), while in Zürich it only represents 30% of road dust loadings (Amato, 2011). Another study conducted in Beijing investigated the characteristics of resuspended road dust and its impact on the urban air, this research concluded that resuspended road dust from traffic is one of the major sources of aerosols in Beijing. The contribution of non-exhaust road traffic emissions to the total PM_{10} emissions can be as high as 90% in northern European countries (Beltran).

Below it is shown the graphical correlation among Weekday PM2.5 patterns tracked local ITS traffic volume and vehicle-hours well in the morning Weekday hours in the city of Baltimore (Maryland).

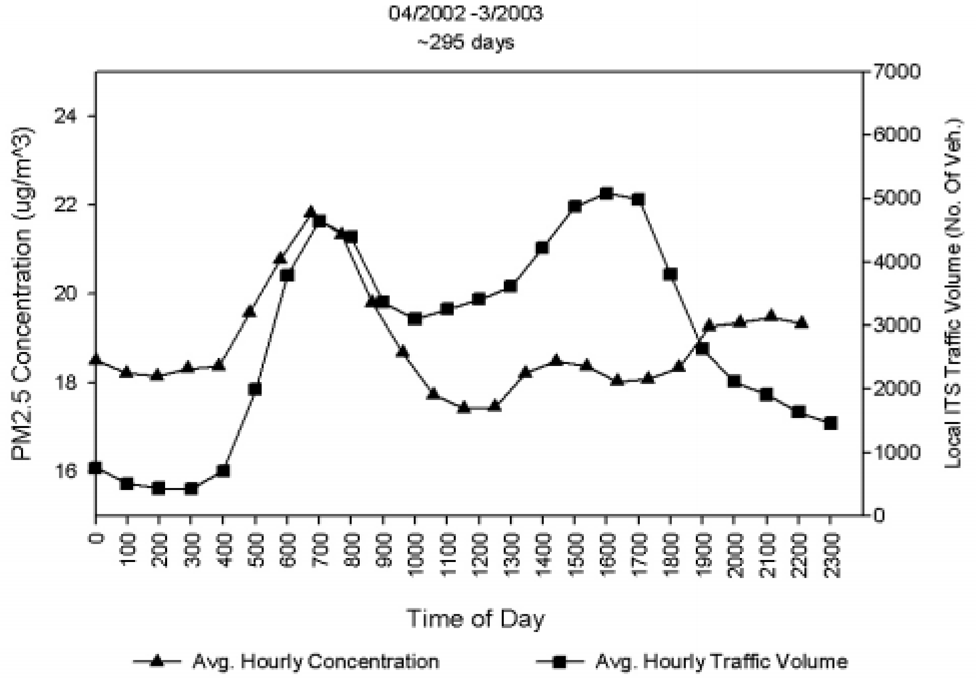

Figure 9 - PM2.5 Concentrations versus Traffic for Baltimore Maryland

1.3 Effects of the air pollution

When the researchers talk about the effects of air pollution, they always precise that many of them are not measurable. In a general way, the ones that are measurable may be divided into the categories that follow.

1.3.1 Effects on health and human welfare (Boubel, 1994)

The effects of pollutants on human beings have been the major reason for efforts to understand and control their sources. The presence of air pollutants in the surrounding ambient air is only one aspect of determining the impact on human beings.

Most persons do not have the luxury of choosing the air they breathe. Air pollution principally affects the respiratory, circulatory and olfactory systems. The respiratory system is the principal route of entry air pollutants some of which may alter the function of the lungs.

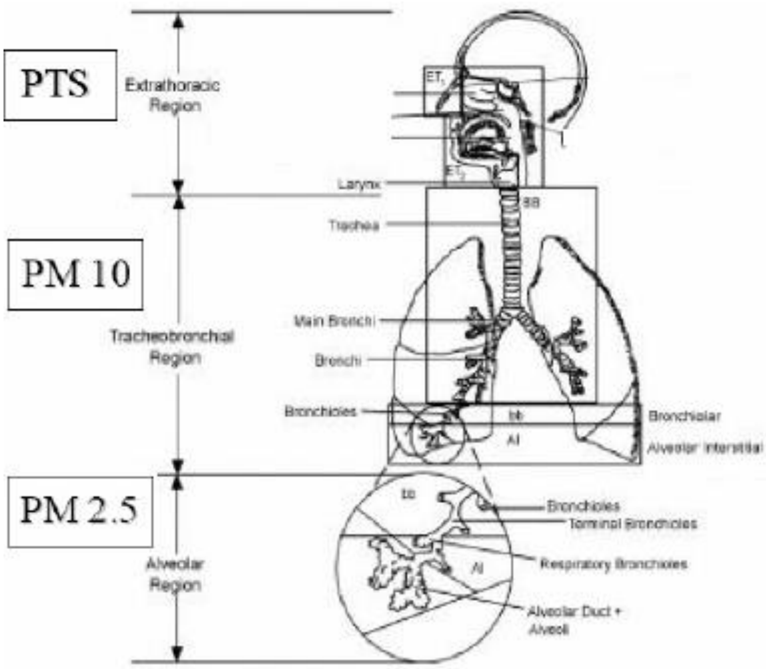

Figure 10 – PM path into respiratory ways

The behavior of particles and gases in the respiratory system is greatly influenced by the region of the lung in which they are located. In *Figure 10 – PM path into respiratory ways* it should be seen how different pollutants (PTS, PM10 and PM5) are able to affect different part of the respiratory system. Larger particles are deposited in the nasal region by impaction on the hairs of the nose or at the bends of the nasal passages. Smaller particles pass through the nasal region and are deposited in the tracheobronchial and pulmonary regions.

The effects attributed to air pollutants range from mild eye irritation to mortality. In most cases, the effect is to aggravate preexisting diseases or to degrade the health status, making persons more susceptible to infection or development of a chronic respiratory disease. Some of the effects associated with specific pollutants are listed below.

Pollutant	Effects
CO	Reduction in the ability of the circulatory system to transport O_2 Impairment of performance on tasks requiring vigilance Aggravation of cardiovascular disease.
NO_2	Increased susceptibility to respiratory pathogens
O_3	Decrement in pulmonary function Coughing, chest discomfort Increased asthma attacks
Lead	Neurocognitive and neuromotor impairment Heme synthesis and hematologic alterations
Peroxyacyl nitrates, aldehydes	Eye irritation
SO_2/particulate matter	Increased prevalence of chronic respiratory disease Increased risk of acute respiratory disease

Figure 11 – Effects of some pollutants according to EPA

1.3.2 Effects on vegetation and animals

When we talk about effects on vegetation we should differentiate air pollution damage from air pollution injury. Injury is considered to be any observable alteration in the plant when exposed to air pollution. Damage is defined as an economic or aesthetic loss due to interference with the intended use of a plant.

The effects of air pollution on plants range from subtle to catastrophic. These effects can be classified as visible symptoms (e.g. the leaf is severely discoloured, early senescence, leaf drop) and non-visual or subtle effects (i.e. reduced plant growth, alteration of physiological and biochemical processes).

The cost of air pollution damage is difficult to estimate. However, estimates indicate crop losses of $1-$5 billion for the United States (source EPA). Figure 12 lists some of the types of plants injured by exposure to these pollutants showing how important it is the exposure of a plant to a pollutant.

				Injury threshold		
Pollutant	Symptoms	Maturity of leaf affected	Part of leaf affected	ppm (vol)	$\mu g\ m^{-3}$	Sustained exposure
Sulfur dioxide	Bleached spots, bleached areas between veins, chlorosis; insect injury, winter and drought conditions may cause similar markings	Middle-aged leaves most sensitive; oldest least sensitive	Mesophyll cells	0.3	785	8 h
Ozone	Flecking, stippling, bleached spotting, pigmentation; conifer needle tips become brown and necrotic	Oldest leaves most sensitive; youngest least sensitive	Palisade or spongy parenchyma in leaves with no palisade	0.03	59	4 h
Peroxyacetyl nitrate (PAN)	Glazing, silvering, or bronzing on lower surface of leaves	Youngest leaves most sensitive	Spongy cells	0.01	50	6 h
Nitrogen dioxide	Irregular, white or brown collapsed lesions on intercostal tissue and near leaf margin	Middle-aged leaves most sensitive	Mesophyll cells	2.5	4700	4 h

Figure 12

Effects of pollutant from road traffic also affect forest ecosystems states. The greatest impact of air pollution on forest is caused by the phenomena known as *Acid Deposition.* Acid deposition refers to the transport of acid constituents from the atmosphere to the earth's surface. This process includes dry deposition of SO_2, NO_2, HNO_3 to surfaces. This process is widespread and alters distribution of plant and aquatic species, soil composition, pH of water, and nutrient content, depending on the circumstances. Numerous studies have shown that large European and North American areas are being altered by acid deposition.

Forest damage is a complex problem involving the interaction of acid deposition, other air pollutants, forestry practices, and naturally occurring soil conditions. As in all ecosystems, forest must always be understood as complex, integrated systems with myriad interrelation

1.4 Effects on materials and structures

1.4.1 Effects on metals

The principal effects of air pollutants on metals are corrosion of the surface, with eventual loss of material from the surface, an alteration in the electrical properties of metals. It’s not very easy do understand the effects of pollutants on materials because the rate of corrosion of metals is influenced by three factors: moisture, type of pollutant and temperature, and because of that every situation could be completely different from the other.

1.4.2 Effects on limestone

The primary concern regarding air pollution is the soiling and deterioration of limestone, which is widely used as a building material and for marble statuary. The following figure shows the long-term effects of urban air pollution on the appearance of stone masonry. Many buildings in older cities have been exposed to SO_2 and CO_2 for decades. The surfaces have become soiled and are subjected to chemical attack by acid gases.

Figure 13 – Pock marks in marble column

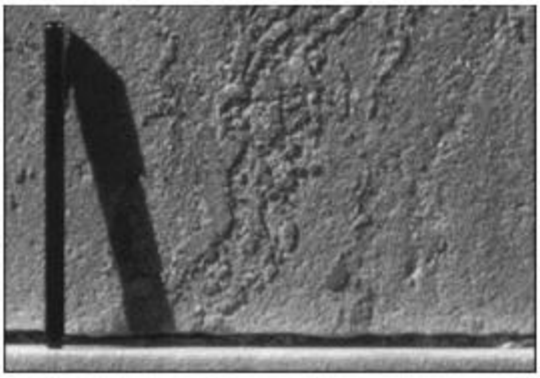

Figure 14 – Marble block shows erosion

1.5 Effects on the atmosphere

Warming on the global scale is expected to occur as a result of the increase of carbon dioxide (CO_2) and other greenhouse gases (those that absorb and reradiate portions of the infrared radiation from the earth).

The average temperature of the earth is difficult to measure, but most measurements show a very small overall change that would not be detectable to humans due to short-term and regional variations. Overall, however, a majority scientific evidence appears to indicate that the temperature of the earth is increasing. About the matter, Charles Keeling, measure CO_2 concentrations in the atmosphere using an infrared gas analyser obtaining the Keeling curve.

The Keeling curve shows that there has been more than 15% increase in CO_2 concentration which is a substantial rise given the short time in which the measurements have been taken. It is likely that our present CO_2 levels are double what they were in pre-industrial revolution times, providing ample evidence that global warming is indeed occurring.

Another hypothesis for this rise in temperature is that the presence of certain gases in the atmosphere is not allowing the earth to reflect enough of the heat energy from the sun back into space. The absorptive potential of several important gases is shown in Figure 15 along with the spectra for the incoming light (short wavelength) radiation and the outgoing heat (long wavelength) radiation.

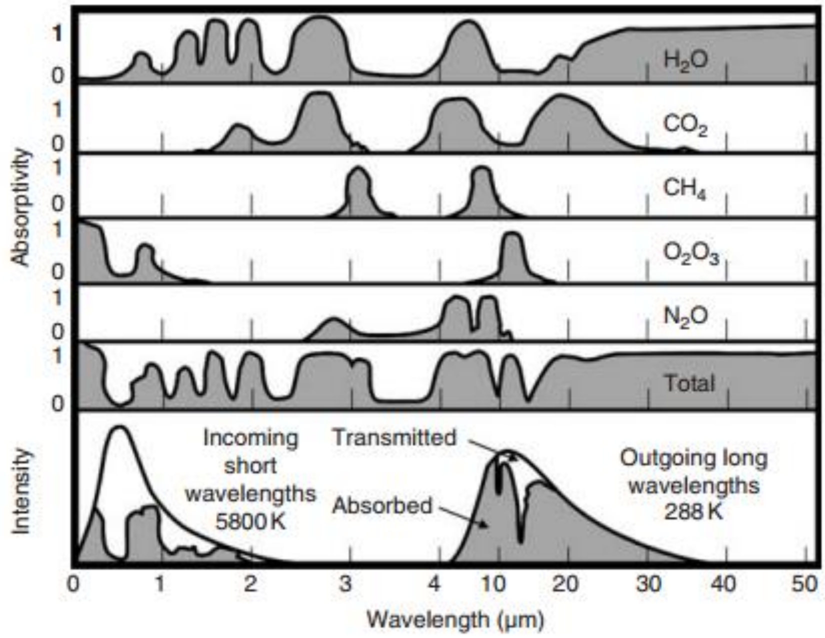

Figure 15

The effectiveness of a particular gas to promote global warming is known as *forcing*. Many processes are now contributing to forcing the Earth's climate away from a natural state. To get a sense of the net effect, you can add all the components of forcing that are positive and negative and you end up with a view of the total forcing in the climate system of Earth. The gases of most importance in forcing are shown in Figure 16. Climate change results from natural internal processes and from external forcings. These types of forcings are often referred to as radiative forcing and can be quantified in units of the extra energy in watts per meter squared (W m-2) entering the Earth near the top of the atmosphere (TOA).

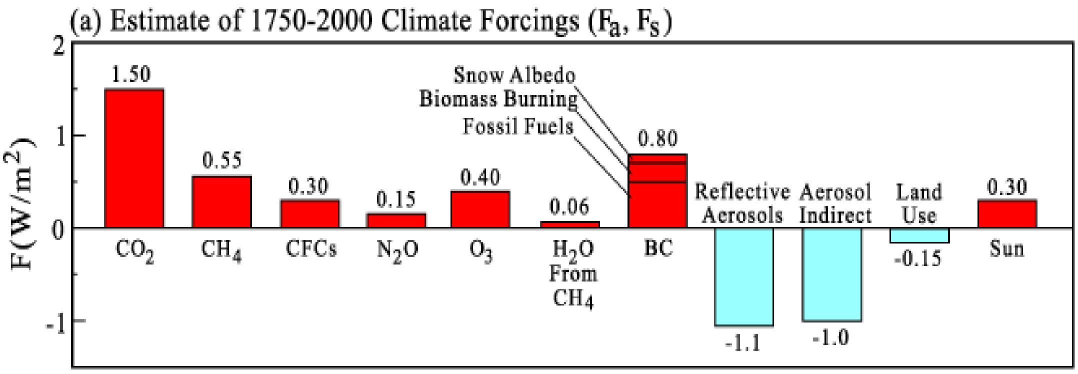

Figure 16

The greenhouse gases, consisting of carbon dioxide (CO2), methane (CH4), nitrous oxide (N20) and chlorofluorocarbons (CFCs), are obviously responsible for global warming (and the natural forcing is not able to cancel their negative effect).

The Intergovernmental Panel on Climate Change (IPCC) established in 1988 by the WMO (World Meteorological Organization) predicted that if no significant actions are taken to curtail consumption of fossil fuel worldwide, the global mean temperature will increase at a rate of 0.2-0.5°K per decade over the next century.

Most recently, in “Climate Change 2007: The Physical Science Basis—Summary for Policymakers”, the IPCC has stated that “warming of the climate system is unequivocal, as is now evident from observations of increases in global average air and ocean temperatures, widespread melting of snow and ice, and rising global average sea level.” They also assert:

- Average Arctic temperatures increased at almost twice the global average rate in the past 100 years. Satellite data since 1978 show that annual average Arctic sea ice extent has shrunk by 2.7% (2.1–3.3%) per decade, with larger decreases in summer of 7.4% (5.0–9.8%) per decade.
- Temperatures at the top of the permafrost layer have generally increased since the 1980s in the Arctic (by up to 3°C). The maximum area covered by seasonally frozen ground has decreased by about 7% in the Northern Hemisphere since 1900, with a decrease in spring of up to 15%.
- Long-term trends from 1900 to 2005 have been observed in precipitation amount over many large regions. Significantly increased precipitation has been observed in eastern parts of North and South America, northern Europe and northern and central Asia. Drying has been observed in the Sahel, the Mediterranean, southern Africa, and parts of southern Asia. Precipitation is highly variable spatially and temporally, and data are limited in some regions. Long-term trends have not been observed for the other large regions assessed

Another pollutants' effect is that linked to the decrease in ozone in the stratosphere (commonly known as "ozone holes"). Stratospheric ozone is in a dynamic equilibrium with a balance between the chemical processes of formation and destruction. The primary components in this balance are ultraviolet (UV) solar radiation, oxygen molecules (O_2), and oxygen atoms (O) and may be represented by the following reactions:

$$O_2 + hv \rightarrow O + O$$

$$O + O_2 + M \rightarrow O_3 + M$$

$$O_3 + hv \rightarrow O_2 + O$$

Where hv represents a photon with energy dependent on the frequency of light, *v*, and M is a molecule of oxygen or nitrogen. The cycle starts with the photodissociation of O_2 to form atomic oxygen O. O atoms react with O_2 in the presence of a third molecule (O_2 or N_2) to form O_3. Ozone absorbs UV radiation and can undergo photodissociation to complete the cycle of formation and destruction.

At a given altitude and latitude, a dynamic equilibrium exists with a corresponding steady-state ozone concentration. This interaction of UV radiation with oxygen and ozone prevents the penetration of shortwave UV to the earth's surface. Stratospheric ozone thus provides a UV shield for human life and biological processes on the earth's surface.

2 Literature review of traffic Emission Models

Emission models represent the mathematical relationship among the pollutants emitted by vehicles and the physical characteristics of the motion that strictly influence those pollutants.

So, the problem of the emission models is to find the variables that are conditioning the fuel consumption of vehicles and then understand in which way each pollutant is linked to this value and formulate a mathematical equation that take into account its chemical characteristics.

The category of atmospheric pollutants emitted from road vehicles as a result of combustion is divided into three main categories:

- *Hot/Cold emissions*: those produced during the functioning of the engine at the exercise temperature (around 90 °C) and during the warming phases of the engine, respectively.
- *Evaporative emissions*: those dependent by the evaporation of the fuel (made only by the VOC’s, volatile organic compounds).
- *Particulate matter:* that comes from: tyre and brake wear, road surface wear, and re-suspension phenomena.

Exhaust emissions of carbon monoxide (CO), volatile organic compounds (VOCs), oxides of nitrogen (NOx) and particulate matter (PM) belong to the set of criteria air pollutants: all those which cause smog, acid rain and health hazards and for this reason are regulates by UE.

A set of unregulated gaseous pollutants are also emitted, including greenhouse gases carbon dioxide (CO_2), nitrous oxide (N_2O) and methane (CH_4). Except for CO_2, unregulated pollutants have been characterised in less detail than the regulated ones.

Source/process	Pollutant(s) emitted	
Hot and cold-start exhaust emissions	Regulated pollutants	CO VOCs NO_x PM
	Unregulated pollutants	
Evaporative emissions	VOCs (regulated)	
Tyre and brake wear Road surface wear Resuspension	PM (regulated)	

Figure 17 (Source: Transport Research Laboratory (TRL) of New Zealand)

As it has been said all emission models must consider the various factors affecting emissions, although the manner and detail in which they do so can differ substantially. They can be divided in the following categories:

- *Vehicle characteristics:* typical features of a certain vehicle category (as for example: engine, type of fuel, horsepower, aerodynamic efficiency etc…).
- *Mechanical state of the vehicle*: state of wear and maintenance.
- *Operational conditions of the vehicle in real traffic conditions:* all the characteristics that are related to the dynamic of the engine (e.g. engine rotation speed) and to the thermodynamic state of the fluid inside the cylinder of the engine (that determines the way in which the combustion happens).

Models for estimating emissions from road vehicles can be classified in several different ways, and they differ each other for the type of input data (and so the emission calculation approach) and for the type of function used (based on continuous or discrete emission functions).

Generic type	Example	Type of emission factor/function	Type of input data	Typical application
Aggregated emission factors	NAEI	Discrete, trip-based	Road type	Emission inventories, EIA[5], SEA[6]
Average speed	COPERT, DMRB	Continuous, trip- or link-based	Average trip speed	Emission inventories, dispersion modelling
Adjusted average speed	TEE	Continuous, link-based	Average speed, congestion level	Emission inventories, dispersion modelling
Traffic situation	HBEFA	Discrete, link-based	Road type, speed limit, level of congestion	Inventories, EIA, SEA, area-wide assessment of urban traffic management schemes, dispersion modelling
Multiple linear regression	VERSIT+	Discrete, link-based	Driving pattern	Emission inventories, dispersion modelling
'Simple' modal	UROPOL	Discrete, link-based	Distribution of driving modes	Local assessment of urban traffic management schemes
Instantaneous – speed based	MODEM, DGV	Discrete, trip-based	Driving pattern	Detailed temporal and spatial analysis of emissions, dispersion modelling
Instantaneous – power based	VeTESS, PHEM	Discrete, trip-based	Driving pattern, gradient, vehicle data	Detailed temporal and spatial analysis of emissions, dispersion modelling

Figure 18 (Source: Transport Research Laboratory (TRL) of New Zealand)

2.1 Aggregated emission factors models

Aggregated emission factor models are the simplest models among all and have mainly found their space on the largest spatial scales. There is only one emission factor used to represent a certain type of vehicle and a type of driving. The emission factors are calculated as mean values of measurements on a few vehicles over given driving cycles.

2.2 Average speed models

Average-speed emission models work on functions that make the emission factor for a certain pollutant and a given type/category of vehicles depends on the average speed during a trip. These models have been widely used in local air pollution prediction models, especially after the European Environment Agency has developed the COPERT software based on an exemplified average speed model. In Figure 19 (Source: Transport Research Laboratory (TRL) of New Zealand) it's shown a typical average speed emission function (red line) for NOx emission. In that case the curve is fitted to the emission factors measured for several vehicles over a range of driving cycles' measurements (blue points).

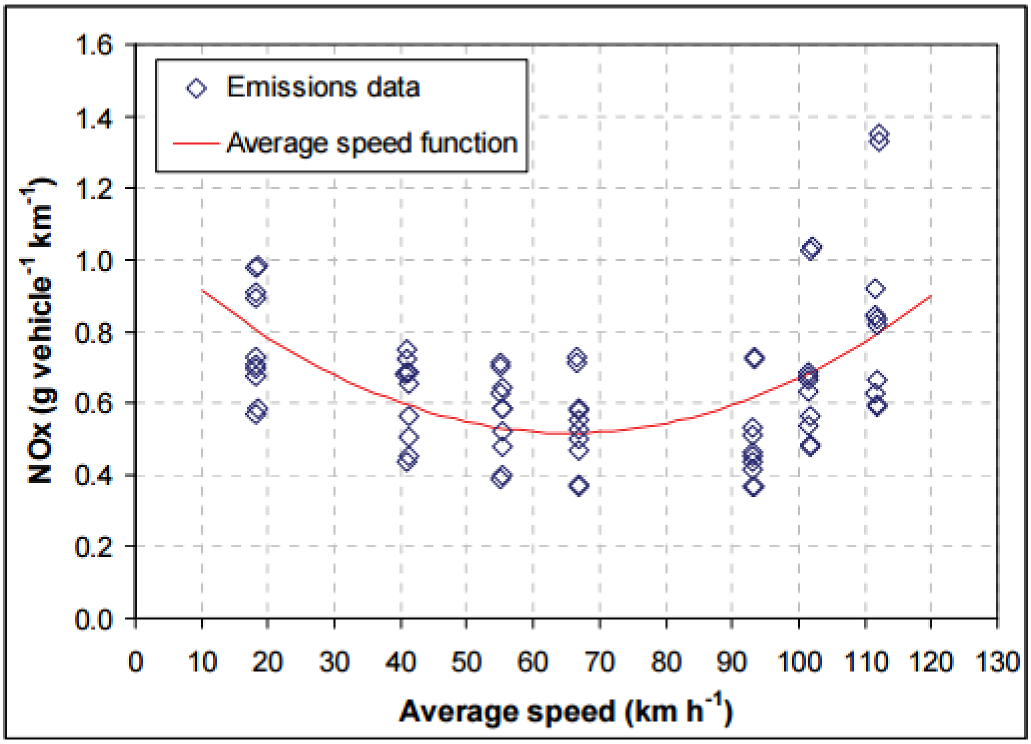

Figure 19 (Source: Transport Research Laboratory (TRL) of New Zealand)

However, such models do not capture the variation of the speed of the traffic flow. Hence, using average speed models means have less accuracy. The only way to reduce the estimation error is to use the average speed at every sampling time step (as many models already do).

A mathematical formulation of the Average Speed Models may be provided as follows:

$$E_i = \sum_c \sum_l VehKm * N_c * BER_l (s_l, c) \quad (1)$$

Where:

- c is the vehicle category;
- l is the index of a link (which average speed is s_l)
- *VehKm* are the vehicle-kilometres travelled in a given time interval on the link l
- N_c is the percentage of vehicles of category c
- $BER_i(s_l,c)$ is the base emission rate per kilometre for a species i. This factor is determined from standard driving cycles at a particular average speed s_l, for each vehicle category c. For that reason, base emission may be called also cycle emission.

It may be that the same average speed correspond to significantly different driving conditions and emission may result consequently misestimate. For such reason, it has been thought a variation of this type of models: the TEE (Traffic Energy and Emissions) model that adds a “corrected average-speed”: the effect of congestion on emissions at a certain average speed can be expressed by means of a “correction factor” derived from average speed, green time percentage, link length and traffic density. The emission factor for the average speed can be adjusted using the correction factor (Negrenti, 1998).

2.2.1 MOVES

MOVES (Motor Vehicle Emission Simulator) is a state-of-the-science emission modelling system that estimates emissions for mobile sources thought by United States Environmental Protection Agency (EPA).

Emissions in MOVES are calculated for all the significant vehicle emission processes: running emissions, start emissions, evaporative emissions, extended idle emissions, crankcase emissions, tirewear and brakewear.

In MOVES, default information is contained in a default input database. MOVES can work with inputs at the national level, with allocation to specific counties if desired, or MOVES can work at the county or project level, with inputs specific to that time and place (agency, 2011).

The MOVES model includes a “default” input database, which uses national data and allocation factors to approximate results for the 3222 counties in the USA and is capable of modelling emissions from the calendar years 1990 until

2050 (Kumar, 2015). The generated results are indeed influenced by the following input data:

- Study area Data Collection
- Meteorology data
- Source type population
- Volume count
- Age distribution
- Average Speed Distribution
- Vehicle Miles Travelled
- Fuel type and technologies
- Inspection and maintenance programs

MOVES' internal emission calculators consider the type of source as the specific combination of vehicle type and fuel type. Based on the input provided by the user, MOVES defines "source bins", with each bin having unique fuel consumption and emissions patterns associated with it. This ensures that several emission rates are used in calculations reflecting the variability of types of vehicles and types of fuels.

Additionally, MOVES also considers "operating modes" as another dimension to estimating total emissions. Total activity for some processes are further divided into different operating modes, which represent several combinations of "Vehicle Speed Power" (commonly indicated with VSP) and speed.

So, for running emissions, the key concept underlying the definition of operating modes is “vehicle-specific power (VSP, Pv). This parameter represents the tractive power exerted by a vehicle to move itself and its cargo or passengers. It is estimated in terms of a vehicle’s speed and mass, as shown in the equation below:

$$VSP = \frac{Av_t + Bv_t^2 + Cv_t^3 + m * v_t * a_t}{m}$$

In that form, VSP (Pv,t, KW/Mg) is estimated in terms of vehicles’:

- Speed at time t (vt)
- Acceleration at
- Mass *m* (Mg)
- A, B and C representing rolling resistance, rotational resistance and aerodynamic drag.

This equation does not include the terms accounting for others factors such as road grade and meteorological conditions because the data used in this analysis was measured on chassis dynamometers.

On the basis of VSP, speed and acceleration, a total of 23 operating modes are defined for the running-exhaus process. Aside from deceleration/braking, which is defined in terms of acceleration, and idle, which is defined in terms of speed alone, the remaining 21 modes are defined in terms of VSP within broad speed classes.

Operating Mode	**Operating Mode Description**	**Vehicle-Specific Power (VSP_t, kW/Mg)**	**Vehicle Speed (v_t, mi/hr)**	**Vehicle Acceleration (a_t, mi/hr-sec)**
0	Deceleration/Braking			$a_t \le -2.0$ OR ($a_t < -1.0$ AND $a_{t-1} < -1.0$ AND $a_{t-2} < -1.0$)
1	Idle		$-1.0 \le v_t < 1.0$	
11	Coast	$VSP_t < 0$	$1 \le v_t < 25$	
12	Cruise/Acceleration	$0 \le VSP_t < 3$	$1 \le v_t < 25$	
13	Cruise/Acceleration	$3 \le VSP_t < 6$	$1 \le v_t < 25$	
14	Cruise/Acceleration	$6 \le VSP_t < 9$	$1 \le v_t < 25$	
15	Cruise/Acceleration	$9 \le VSP_t < 12$	$1 \le v_t < 25$	
16	Cruise/Acceleration	$12 \le VSP_t$	$1 \le v_t < 25$	
21	Coast	$VSP_t < 0$	$25 \le v_t < 50$	
22	Cruise/Acceleration	$0 \le VSP_t < 3$	$25 \le v_t < 50$	
23	Cruise/Acceleration	$3 \le VSP_t < 6$	$25 \le v_t < 50$	
24	Cruise/Acceleration	$6 \le VSP_t < 9$	$25 \le v_t < 50$	
25	Cruise/Acceleration	$9 \le VSP_t < 12$	$25 \le v_t < 50$	
27	Cruise/Acceleration	$12 \le VSP < 18$	$25 \le v_t < 50$	
28	Cruise/Acceleration	$18 \le VSP < 24$	$25 \le v_t < 50$	
29	Cruise/Acceleration	$24 \le VSP < 30$	$25 \le v_t < 50$	
30	Cruise/Acceleration	$30 \le VSP$	$25 \le v_t < 50$	
33	Cruise/Acceleration	$VSP_t < 6$	$50 \le v_t$	
35	Cruise/Acceleration	$6 \le VSP_t < 12$	$50 \le v_t$	
37	Cruise/Acceleration	$12 \le VSP < 18$	$50 \le v_t$	
38	Cruise/Acceleration	$18 \le VSP < 24$	$50 \le v_t$	
39	Cruise/Acceleration	$24 \le VSP < 30$	$50 \le v_t$	
40	Cruise/Acceleration	$30 \le VSP$	$50 \le v_t$	

Figure 20 – MOVES operating modes

According to the found emission rates, the fuel consumption (FC) can be determined. For example, is reported the sulphur dioxide (SO2) emission algorithm.

$$SO2(g) = FC(g) * [S](ppm) * \frac{MW_{SO_2}}{MW_S} * fSO_2 * (\frac{10^{-6}}{ppm})$$

Where:

- FC(g)=fuel consumption (g), and
- [S](ppm)=relative fuel-sulfur concentration (ppm)

- $(MW\_SO_2)/(MW\_S)$ is the ratio of the molecular weight of sulfur dioxide.

2.2.2 COPERT

The Computer programme to calculate emissions from road transport (COPERT) was financed by the European Environment Agency for the compilation of CORINAIR emission inventories. The motor vehicles classification provided in the CORINAIR emission inventory guidebook it has been judged not sufficient to reproduce emitted pollutant rates, so it has been provided a more accurate classification that take into account the year of vehicle production, the engine and after-treatment technology which is implemented for achieving the emission standards (as an example a part of the classification table has been reported in Figure 21).

Vehicle Type	Class	Legislation
Passenger Cars	Gasoline <1,4l	PRE ECE
		ECE 15/00-01
		ECE 15/02
		ECE 15/03
		ECE 15/04
		Improved Conv.
		Open Loop
		Euro I - 91/441/EEC
		Euro II - 94/12/EC
		Euro III - 98/69/EC Stage 2000
		Euro IV - 98/69/EC Stage 2005
	Gasoline 1,4 - 2,0l	PRE ECE
		ECE 15/00-01
		ECE 15/02
		ECE 15/03
		ECE 15/04
		Improved Conv.
		Open Loop
		Euro I - 91/441/EEC
		Euro II - 94/12/EC
		Euro III - 98/69/EC Stage 2000
		Euro IV - 98/69/EC Stage 2005
	Gasoline >2,0l	PRE ECE
		ECE 15/00-01
		ECE 15/02
		ECE 15/03
		ECE 15/04
		Euro I - 91/441/EEC
		Euro II - 94/12/EC
		Euro III - 98/69/EC Stage 2000
		Euro IV - 98/69/EC Stage 2005

Figure 22 (Source “COPERT methodology=

The analysed pollutants are 10: NOx, N_2O, SOx, CH_4, CO, CO_2, NH_3, COVNM, Pb and particulate matter.

The warmed-up emissions are expressed, per every pollutant *i* and group of vehicles *g*, through a linear emission factor expressed in g*vehic^{-1}*km^{-1}:

$$\delta E_{base}^{i,g}\,(Vm) \qquad (2)$$

From equation (2) it may be derived the average emission factor weighed for every vehicular group thanks to the percentage N_c of the vehicles of the c category:

$$\delta E_{base}^{i} = \sum_{c} N_c * \delta E_{base}^{i,g}\,(Vm) \tag{3}$$

Other than the emission factors and the characteristics and the typologies of the car fleet, COPERT methodology takes into account the following parameters:

- Driving conditions
- Slope of the road
- Climatic condition
- Transported weight

Except for the emission factors, all the other data must be provided by the user during the creation of the input database.

Total emissions are calculated by summing emissions from three different sources, namely the thermal stabilised engine operation (hot), the warming-up phase (cold start) and the fuel evaporation. Distinction in emissions during the stabilised and warming-up phase is necessary because of the substantial difference in vehicle emission performance during these two conditions (concentrations of most pollutants during the warming-up period are many times higher than during hot operation). In that respect, total emission can be calculated by means of the equation:

$$E_{tot} = E_{hot} + E_{cold} + E_{evap} \tag{4}$$

Where:

- Hot emission is intended by convention the emissions occurring under thermally stabilised engine and exhaust aftertreatment condition. The formula to estimate hot emission, using experimentally obtained emission factors is:

$$E_{hot} = N_c * VehKm * HEF \quad (5)$$

  Where HEF stands for hot emission factor.

- Cold start emissions are calculated as an extra emission over the emissions that would be expected if all vehicles were only operated with hot engines and warmed-up catalysts. The formula for the calculation is the following:

$$E_{Cold;i\,,k} = \beta_{i,k} * N_c * VehKm * e_{hot;i,k} * (r_{Cold,hot} - 1) \quad (6)$$

  Where:

  - β is the fraction of mileage driven with a cold engine (*I* pollutant and k vehicle technology)
  - N is the number of vehicles (with c technology)
  - VehKm is the total mileage per vehicle
  - *r* is the ratio of hot emission factor and cold emission factor for pollutant *I* and vehicles of *c* technology

Copert comprehends three approaches to calculate exhaust emission (on the basis of the starting information) but the emission factors of each were all determined using Tier 3 methodology. The emission factors are derived from the results of the Artemis project that takes into account the results of comprehensive studies carried out in France, Germany, Greece, Italy, Netherlands and UK (about 3000 test per every pollutant and 1000 analysed vehicles). The analytical form of the factors is a function of the average speed and has the expression of a second-degree equation. As an example, has been reported the emission factor equation for gasoline light duty vehicles < 3.5 t:

$$CO_2\left(\frac{g}{km}\right) = 0.01104 * v^2 - 1.5312 * v + 57.789 \qquad (7)$$

2.3 Traffic situation models

To include both speed and the dynamic situation of traffic is used the ‘traffic situation modelling’. Such models refer to determined traffic situations, i.e. different conditions each one having a specific emission problem and for which the average speed may not be the best solution. Traffic situation models are usually used in local applications; this is the reason why they may be called ‘link level models’. The most useful example is the Handbook of Emission Factors (HBEFA) that associates each emission factor with a traffic situation that reflects the conditions of the section of road under consideration (e.g. ‘main road outside built-up area’). So, in such case the speed must not be given by the user, but is defined by a textual description (e.g. ‘free-flow’, ‘stop and go’) of the type of traffic situation to which an emission factor is applicable (INFRAS, 2004).

The first problem of these models is that the user may not define properly the traffic situation and this may lead to interpretation mistakes. The second one is that, although it is known that there are connections between the fundamental characteristics of the road (e.g. width, lanes), the traffic (e.g. flow, density) and the vehicles, it’s still difficult to define a well-functioning relationship with the emission factors.

2.3.1 HBEFA

HandBook of Emission Factors for Road Transport (HBEFA) is the database for vehicular emission factors in Europe. HBEFA provides emission factors (g/vehicle*km) for all current vehicle categories (passenger cars, light duty vehicles, heavy duty vehicles, buses and motor cycles), each one divided into different categories, for a wide variety of traffic situations.

The HBEFA was originally developed on behalf of the Environmental Protection Agencies of Germany, Switzerland and Austria. In the meantime, further countries (Sweden, Norway and France) as well as the JRC (European Research Centre of the European Commission) are supporting HBEFA. The handbook provides emission factors per traffic situation. For that purpose, different levels of disaggregation are being offered:

- Type of emission: “hot” emissions, cold start and evaporative emissions.
- Vehicle category
- Year
- Pollutants: CO, HC, NOx, PM, several components of HC (CH_4, NHMC, benzene, toluene, xylene), fuel consumption, CO_2, NH3 and N_2O and PM.

The methodological approach of HBEFA consists to measure real world driving patterns and classify them identifying typical traffic situations. This lead to a need of measurement programs enabling the calculation of emission factors for real world driving patterns/traffic situations and so vehicular emission have been measured in such a way that emission factors for real world driving patterns could be derived and calculation of emission factors for traffic situation results in such way identified. The methodology can be summarized in four main step:

1. Measurement of real world driving patterns to derive representative traffic situation (e.g. using GPS tracking)
2. Development of typical traffic situations based on the measured driving patterns
3. Measurement of real world emissions to generate reliable emission factors (the real HBEFA approach is not to measure the emission of all

276 traffic situation but develop a computer model to derive emission factors for traffic situations)

4. Calculate emission factors for all traffic situation using the PHEM model (PHEM is a tool abled to simulate emission factors without experiment directly emission tests on chassis dynamometer).

2.4 Multiple linear regression model

VERSIT + model is based on data that embodies a large number of emission measures covering a range of distinctive speed-time profiles and uses a large sample of vehicles that reflect the actual fleet composition. The emissions test data are obtained from chassis dynamometer tests using speed-time profiles that reflect real-world operations (Smit, 2007). Each driving cycle has been characterised by all the possible parameters (e.g. average speed, number of stops per km) and for each pollutant and vehicle category has been built an average emission values curve. So VERSIT+ should be defined as a multiple regression models based on tests on different driving cycles. In the figure below it is shown the correlation between NOx emission factors as it has been predicted by the model and NOx observed values. A dot represents the predicted and observed mean emission factor for one particular speed-time profile, with 95% confidence interval.

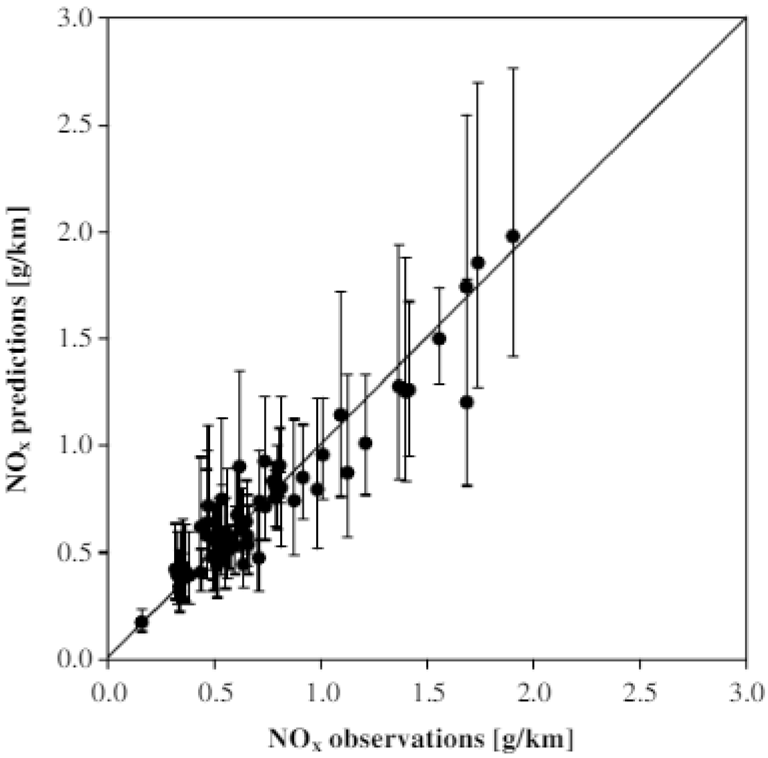

Figure 23

This type of model requires a driving pattern as the input, so by definition it may be applied only in micro-mesoscopic traffic simulations.

2.4.1 Versit+

Versit+ is a statistical emission model able to calculate real-world emission of road vehicles. Over 20,000 measurements with warm and cold engines have been taken on over 3,200 vehicles in a period of 20 years to let it work.

The vehicle categories are generally based on fuel, emission standard, injection technology, after-treatment technology and transmission (so in Versit+ the driving behaviour is not just the speed and acceleration). The negative side of this assumption is that such a detailed distinction leads to have insufficient data in some of the categories, but on the other hand automatic transmission and older injection technology will strongly affect certain emissions of these cars.

VERSIT+ micro emissions range between a − 6% and 31% compared to COPERT, and present a mean normalized bias error of 14% (taking COPERT as a reference). As explained in Smit et al. (2007), the main difference between the two models is that VERSIT+ calculates different emission factors for various traffic situations that present similar average speeds and different dynamics. VERSIT+ uses driving patterns for specific local situations (calculated by VISSIM) while COPERT 4 calculates equivalent average driving pattern

2.5 Modal models

In modal models emission factors are allocated to the specific modes of vehicle operation encountered during a trip. Different types of modal model are in use. In the simpler type of modal model, vehicle operation is defined in terms of a relatively small number of modes – typically idle, acceleration, deceleration and cruise. This type of model is indeed normally referred to as ‘modal’. A number of more detailed modal models aim to provide a more precise description of vehicle emission behaviour by relating emission rates to vehicle operation during a series of short time steps (Boulter, 2007).

2.6 Dynamic emission models

Instantaneous speed base and power based models are usually recognized by the name of dynamic emission models (not be confused with dynamic traffic assignment). In such case, emissions have been estimated through the sum of some functions, each one constituted by a group of time dependent variables. They have been measured continuously during chassis dynamometer test and stored for particular time intervals, this means that emissions derive directly from operation conditions of the vehicle at a given time. Instantaneous measurements allow both instantaneous and modal analysis and modelling, based respectively on instantaneous vehicle kinematic variables (e.g. speed and acceleration), or on more aggregated modal variables (e.g. time spent in acceleration mode, in cruise mode, etc.).

The entire mass of a pollutant *i* emitted by vehicles among an interval duration may be calculated as follows:

$$E_i(t) = \sum_j e_i\,(c_j, x_j(t)) \qquad (8)$$

Where:

J is the vehicle ID;

C_j is the category of vehicle *j*;

X_j (t) denotes instantaneous or modal variables of vehicle *j* at time *t*;

E_i $(c_j,x_j(t))$ denotes the emission of species *i* for vehicle *j* at time *t*.

The emission of species *i* of vehicle *j* at time *t* is in turn defined fixing the design characteristics of the vehicular group *c* and the cinematic mode *m* of duration of *t* by the following formula:

$$e_{base}^{i,c,m} = \int_0^t f_{base}^{i,c,m} \left(v(t), a(t)\right) dt \qquad (9)$$

So, as it was said before, it is crucial to identify different modes in function of the speed and instantaneous accelerations and collect the experimental data of e_{base} that correspond to each one of them. This is the way to fix the base function f_{base} that constitute the forecasting model that allow to assess the pollutant emissions.

The model is not exhaustive anymore as in the equation (9) are missing some important corrective functions that provide for the elements that are not currently expressed. These are:

- the slope of the road
- the cold start emission

In that way, the e_i term in the equation (8) will be expressed as the sum of various elements (in our case two):

$$e^{i,c} = e_{base}^{i,c} + e_p^{i,c} + e_{CS}^{i,c} \qquad (10)$$

As a consequence of the fact the dynamic emission models request expressively speed and/or acceleration data, it follows they need a very detailed traffic flow model that may provide data on speed, acceleration and densities.

2.6.1 MODEM

MODEM software was produced during the European Commission's DRIVE programme where emission test data were collected by laboratories of Europe forming the basis of the model. Through the statistical analysis of a large-scale survey of vehicle operating characteristics it has been developed a set of 14 driving cycles to be repeated on a chassis dynamometer. With these cycles, the emission data (relative to CO, CO_2, HC and NOx) were obtained for 150 different types of car measured on a second by second basis.

The modelling approach consists in the fact that the power of the engine determines the rate of emission, and the power itself depends upon the speed and the rate of acceleration. But for the same engine power, a low speed vehicle will accelerate at higher emission rate than a faster one. MODEM modelling establishes that the best indicators of the power demand were found to be vehicle speed and the product of the vehicle speed and acceleration (Jost P, 1992) (Figure 25Figure 24).

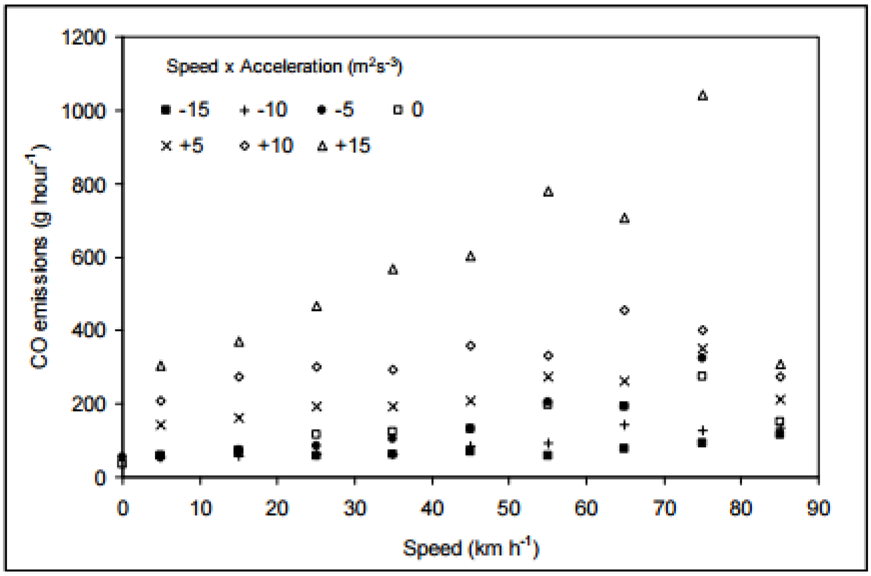

Figure 24 (Source: Transport Research Laboratory (TRL) of New Zealand)

3 Traffic modelling

A *transportation system* can be defined as a set of elements and the interactions among them that finally produce the demand that should be travel between the zones of a given study area and the provision of transportation services to satisfy this demand.

Travel demand derives from the need to access urban services in different places derived by the distribution of activities distributed all around the study area. The choices that made up the demand flows of the O-D matrix depend on the purpose of the travel and the availability of transportation modes. The characteristics of transportation services are called *level of service* and they include factors as travel time, service reliability and monetary costs.

The transportation supply component is made up of the facilities (roads, parking space, railway lines, etc.), services (transit lines and timetables), regulations (road circulation and parking regulations), and prices (transit fares, parking prices, etc.) that produce travel opportunities (Cascetta, 2009).

It's clear that a transportation system is a very complex system that is made up of a very high number of interactions. So, as a consequence of fact, there are several ways to represent the same transportation system. In the following paragraphs, some of these alternatives have been shown focusing on:

- *Traffic assignment methods*: the process of allocating given set of trip interchanges to the specified transportation system.
- *Traffic flow models*: mathematical models that formulate the relationships among traffic flows (macroscopic) or vehicles (microscopic).

3.1 Static versus dynamic modelling

Traffic assignment models simulate the interaction of demand and supply on transportation network. More in detail, path choices and flows depend on generalized path costs; moreover, demand flows themselves are generally influenced by path costs in choice dimensions such as mode and destination. There is indeed a circular dependency among demand, flows, and costs (Cascetta, 2009).

The *static assignment* represents an equilibrium configuration of the network: it means that demand, path and flows are consistent with the costs that they produce in the network. So, the cost of travel is time invariant. Static emission models aim to determine the average emissions in a certain analysis period in function of the average emissions in the evaluated period. They may be used in the assessment of emissions in stationary condition of the network (so they may be preferred in case of continuous flows instead of dynamic models for their low computation speed).

The emission computation is by definition a dynamic procedure, as it is aimed to compute the instantaneous quantity of emitted pollutant. Indeed, it's needed to approach the static emission models in a manner that is anyway dynamic: the procedure request before all the calculation of emission factors in determined time intervals (it's not rare that a static emission models had used before a dynamic emission model to calculate the emission factors). Once we have the emission factors, it is possible to assess the emission rate as a function of a unique parameter: the mean speed that represents the characteristics of the mote. Obviously, the mean speed is not the only parameter that is taken into account, but there is a series of independent explicative variables that, depending on the model used, correct the emission level obtained thanks through mean speed to obtain the final emission rate. The most diffused are the variables linked to the cold-start emissions, the longitudinal slope and the state of the engines.

Dynamic network analysis models seek to provide another, more detailed means to represent the interaction between travel choices, traffic flows, and time and cost measures in a temporally coherent manner. That is the system evolves over time through possibly different feasible states, as a result of changes in the number of users undertaking trips, path choices, supply performance and so on (Cascetta, 2009). So, dynamic process assignment models simulate the evolution of the system state considering user choices in different reference periods.

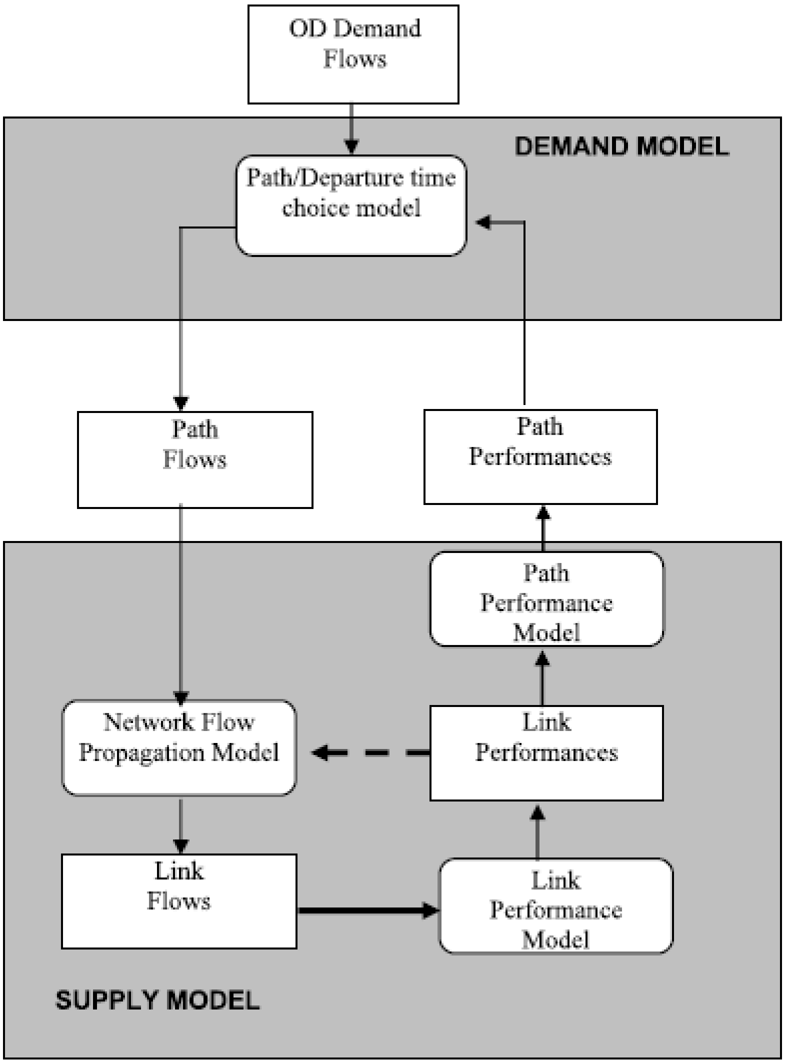

Figure 25

The simplifications induced in the static traffic assignment do not allow the system's internal behaviour to be represented and consequently it is impossible to represent phenomena that belong to highly congested urban road systems like the creation, propagation and dissipation of queues. Additionally, is not possible to reproduce effects caused by nonstationary demand or supply (e.g. demand peaks in rush hours). It becomes evident that these procedures are inadequate as explanations of influences on travel choices and as measures used to evaluate impact when deciding how to develop policies for managing transportation systems, how to fund transportation system improvements, and how to measure environmental impacts related to system wide travel (Kross, 2011).

3.2 Traffic simulation model types

The formulation of supply, demand and equilibrium assignment and their level of complexity depend on the type of supply system concerned. Transport services and corresponding supply models may be divided into two main classes: continuous and discrete.

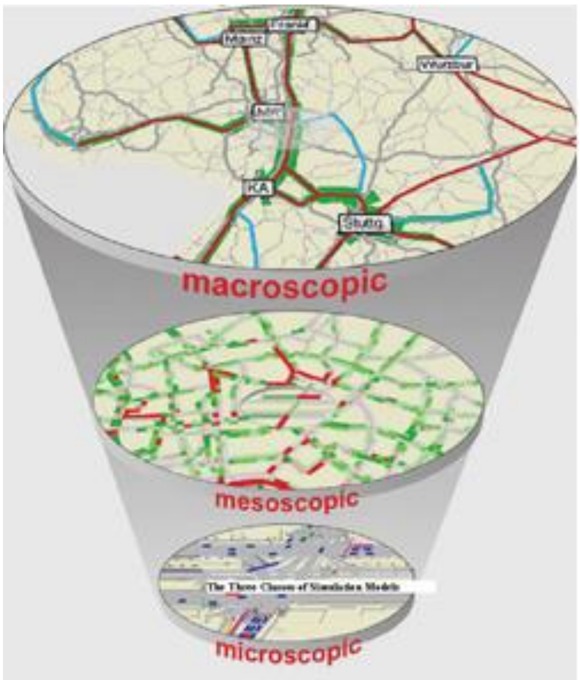

Figure 26

The first traffic flow model proposed in the 1950 represented traffic flow basing on the analogy with the lines of water flow in rivers. In that way, the model attempt to classify the average behaviour of a system instead the behaviour of a specific vehicle. The evolution of the variables in time is modelled using partial differential equations (today modern models utilize hyperbolic partial differential equations). This approach to modelling vehicle flow is called *macroscopic*.

Macroscopic models may be divided according to their representation of space, assuming that time is always treated continuously. In *space-continuous* models the state variables are defined at each point in space. On the other side, *space-discrete* models: the basic variables affecting link performance, such as density or speed, do not vary along the link.

The need to obtained a more detailed level to understand particular part of the traffic system under study, has led to develop algorithms and software that describe the actions and reactions of the vehicles in a traffic state in a way that is as close as possible to the reality. This kind of models are called *microscopic*. Indeed, microscopic models describe traffic at the level of individual vehicles and their interaction with each other and the road infrastructure. Normally this behaviour is captured in some set of rules of behaviour which determine when a vehicle accelerates, decelerates, changes lane, but also how and when vehicles choose and change their routes to their destinations (Burghout, 2005). Path choice, decisions to accelerate or change lanes, behaviour at intersections, and so on, of each individual vehicle, are generally explicitly modelled.

Mesoscopic models are halfway between macroscopic and microscopic models taking the aggregate level approach of macroscopic models and the individual interactions of the microscopic ones. Mesoscopic models normally describe the traffic entities at a high level of detail, but their behaviour and interactions are described at a lower level of detail. The working paradigm of mesoscopic models is that vehicles are grouped into cells that they share with other vehicles having the same behaviour. The cells traverse the link, and the speed of vehicles is determined by the cell, not by the individual drivers'.

<table>
<tr><th rowspan="2">Flow Representation</th><th colspan="2">Performance functions</th></tr>
<tr><th>AGGREGATE
(explicit capacity)</th><th>DISAGGREGATE</th></tr>
<tr><td rowspan="2">CONTINUOUS</td><td>MACRO-SIMULATION</td><td rowspan="2">•</td></tr>
<tr><td>space discrete | space continuous</td></tr>
<tr><td>DISCRETE</td><td>MESO-SIMULATION</td><td>MICRO-SIMULATION</td></tr>
</table>

Figure 27

4 Analysis of pollutant emissions on a link

To analyse the results of different approaches and methods to obtain the emitted pollutant on a network link, it has been used a small network that it will be called "Example".

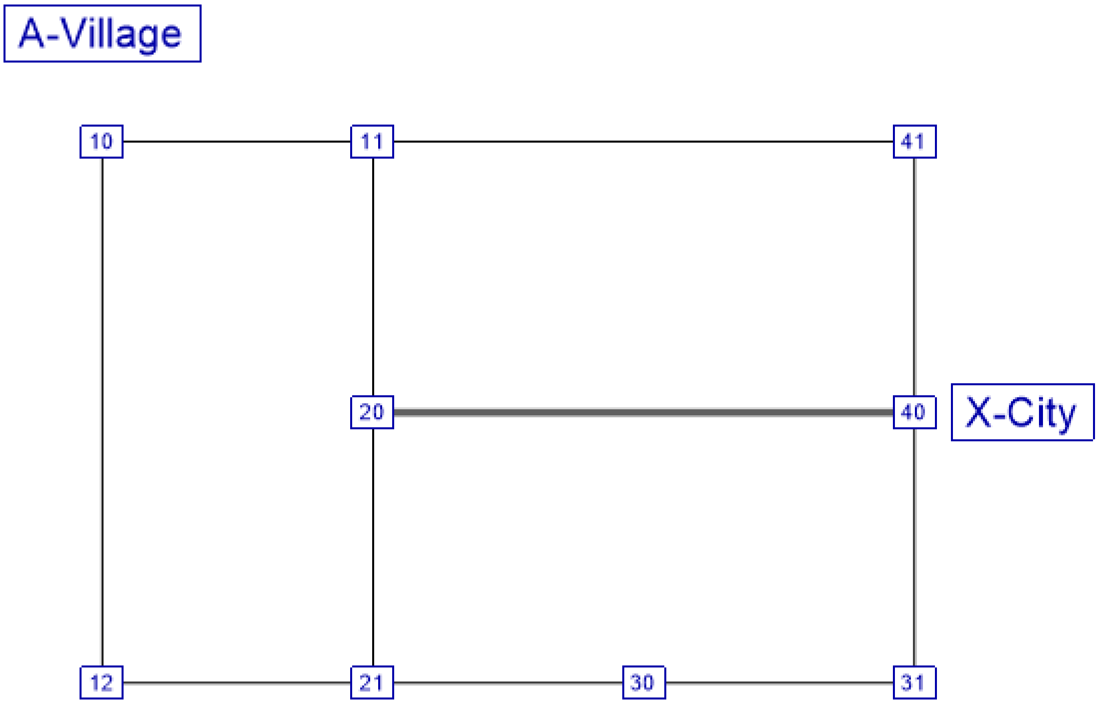

Figure 28 – Network representation

The demand is that defined by the pictures below that shows the O-D matrices (one for car "CAR" transport system and one for heavy vehicles "HVeh") how has been set in the model.

2 x 2			100	200
	Name		A-Village	X-City
		Sum	0.00	2000.00
100	A-Village	2000.00	0.00	2000.00
200	X-City	0.00	0.00	0.00

Figure 29 – CAR O-D matrix

2 x 2			100	200
	Name		A-Village	X-City
		Sum	0.00	200.00
100	A-Village	200.00	0.00	200.00
200	X-City	0.00	0.00	0.00

Figure 30 – Hveh O-D matrix

Both the transport systems' flows start from 5:30 a.m. until 7:30 a.m. and are distributed as represented in the following picture.

	From day	FromTime	To day	ToTime	Weight	Share	Percentages total
1	1	05:30:00	1	06:30:00	33.000	33%	33%
2	1	06:30:00	1	07:30:00	67.000	67%	100%

Figure 31 – Time series

4.1 Case 1: HBEFA macrosimulation (static traffic assignment)

As it has been said the HBEFA is a traffic situation model. This implies that for working it needs a definition of the traffic situations that actually occur in the network for every link (so a combination of road type, speed limit and service levels as well as the vehicle types). In a particular way Visum calculates emissions allowing the user to take into account three important elements:

- Traffic situation
- Volumes
- Fleet composition

For a HBEFA-based emission calculation, it has first been necessary to define fleet composition. The fleet composition can be chosen among one of those that are stored in the HBEFA database. Selecting the “Fleet compositions” entry in the “Network” menu it is in fact possible to select one or more of the transport systems that make up the entire composition, and the “country” (in this case “Germany”) and the “reference year” (2016) in which the base emissions have been calculated. In the study case the fleet composition has been created as follow:

It is then possible to associate to every fleet composition created a demand segment and a volume attribute that means the base attribute on which the final emission factors will be calculated.

It’s also possible to define the basic elements of the HBEFA procedure and the definition of the traffic situations. For what concerns the basis tab, it allows the user to define if the emissions are calculated statically or dynamically and the pollutants that the procedure will take into account to assess final emissions factors.

Instead the traffic situation tab allows the user to select a link attribute for the determination and the way it may be determined the LOS (it may be chosen the link attribute that defines the Level of Service and the expected values for that attribute or the class limits). In the study case the options have been set as follows:

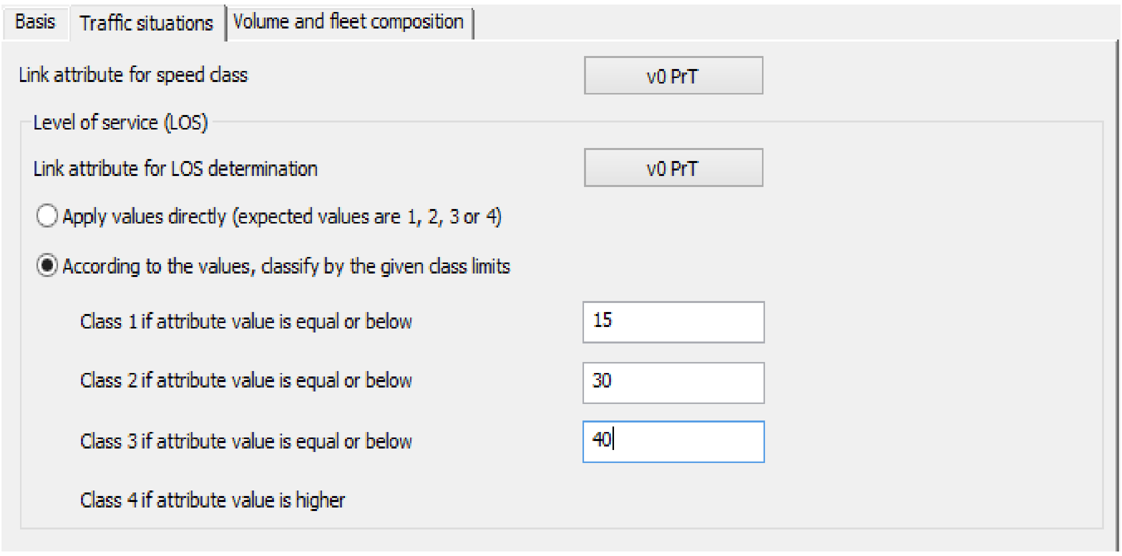

Figure 32

At this point all the HBEFA parameters have been fixed and a procedure sequence with a static traffic assignment may be launched. Visum provides several procedures for PrT assignment. In the current case, it has been chosen the Equilibrium assignment that distributes the demand according to Wardrop's first principle ("Every road user selects his route in such a way, that the impedance on all alternative routes is the same, and that switching to a different route would increase personal travel time"). The state of equilibrium is reached through a multi-step iteration process based on an incremental assignment as the starting point.

The obtained equilibrium situation has been the following:

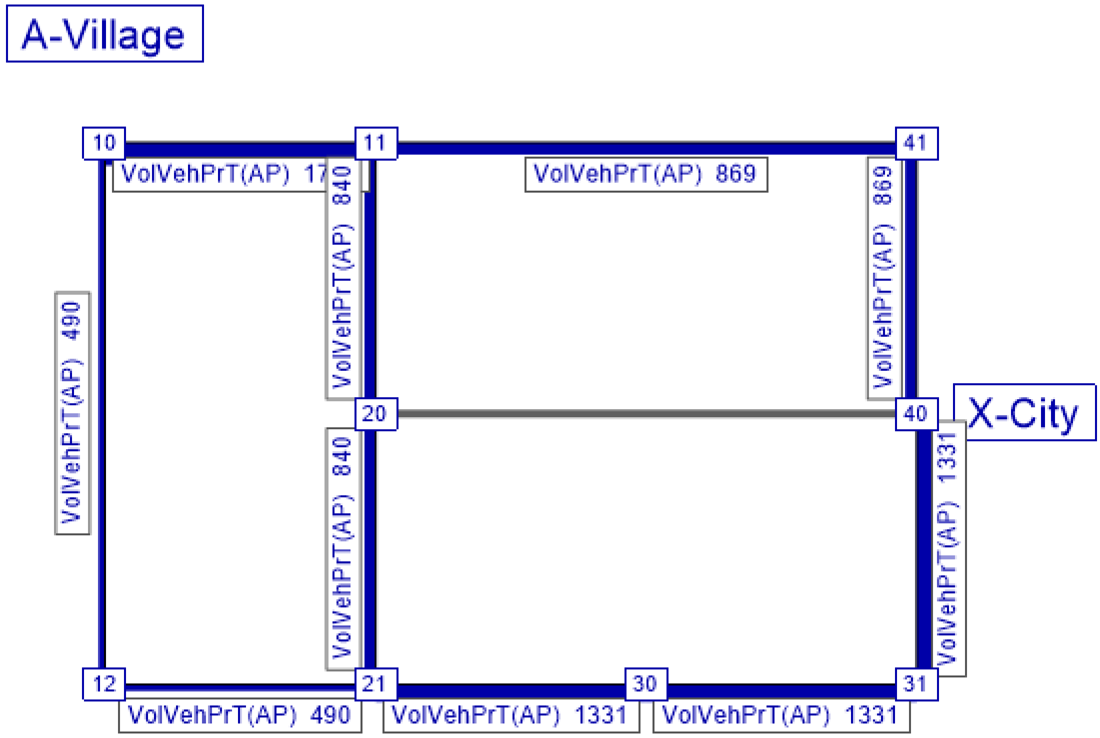

Figure 33

The resulting emission obtained with the HBEFA emission calculation model have been represented through the creation of 4 new User Defined Attributes determined as the numbers obtained through the ratio among the HBEFA emission rates and 60 that is the number of minutes in an hour (as the results are referred to an hour). The creation tab is shown below.

Thanks to the customizable bars of Visum graphic parameters editing it was possible to edit 4 different bars (one for each new User Defined Attribute) and consequently to show how the minute average emission rates change from link to link.

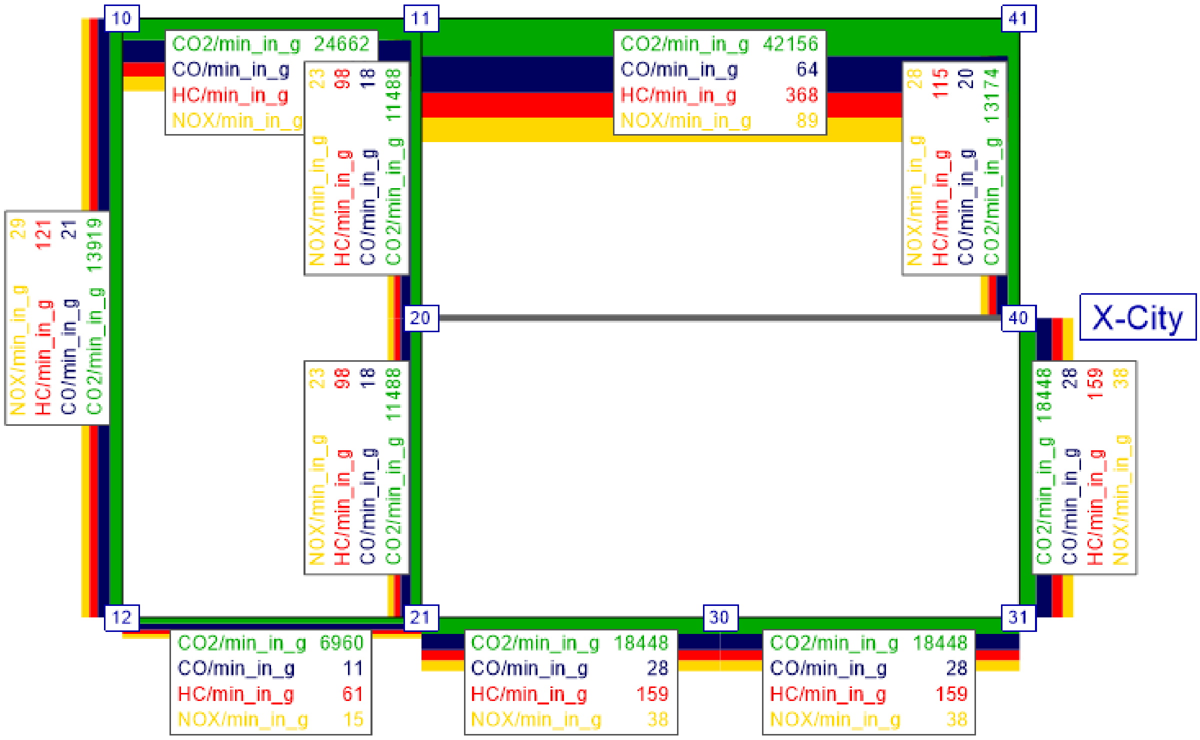

Figure 34

It may be seen that all the final emission results are referred to the entire analysis period. This let the static traffic assignment not to be the ideal way to calculate the pollutant mass. But in the case of very big network this has been used and in such case the final result is divided by time intervals number to obtain a more useful one. So the first value of F. table 1 that describe the emission rate of the link that goes from node 10 to node 11 may be divided into 120 (number of minutes in a 2 hours simulation). The reference values for that link will be:

- 24.6 Kg/Km per CO_2 (value in the table divided by 120 and by the length of the link)

- 0.0095 Kg/km per CO
- 0.0065 Kg/Km per NOx

4.2 Case 2: COPERT macrosimulation (dynamic traffic assignment)

COPERT model is an average-speed emission model and so it works on functions that make the emission factor for a certain pollutant and a given type/category of vehicles depends on the average speed during a trip.

To better reproduce the reality, it has been analysed the implementation of the COPERT model in a fist-order dynamic macroscopic traffic simulation model developed by SISTeMA that has been called TRE.

TRE models the traffic behaviour via a model implementing the Kinematic Wave Theory (KWT) based on cumulative flows (Newell, 1933) which implements on each link the macroscopic flow paradigm of representing vehicles as a partially compressible mono-dimensional fluid, and through its network extension which requires a node model to propagate flow states among adjacent links involving priority rules and the approach to address it on the network is the GLTM (General Link Transmission Model, Gentile, 2008). It performs a dynamic network loading according to the route choice provided in input as node-splitting rates.

TRE problem formulation is composed by two alternating models:

- The node model that gets as an input the sending flow from the upstream links, the turn probabilities, the node turn priorities and the receiving flows
- The link model that gets as an input the link current instant inflow and outflow and return the sending flow and potential receiving flow.

TRE uses the TDE as a base for its internal data structures. TDE is the data model library used by SISTeMA to store the transportation data. Implementing COPERT model in TRE the problem has obviously been that of link the categories defined by ARTEMIS to that define in TDE.

There is a set of TDE table that let the user to define the externalities and associate vehicle categories to the defined externalities:

TABLE NAME	CONTENTS	EXAMPLES
EXTE	Contains the externalities identification names.	CO (carbon monoxide), CO_2 (carbon dioxide), NOx (mono-nitrogen oxides)…
VEID	Contains vehicles categories identification (with reference to speed and slope).	HDV Gasoline >3,5 6 RT petrol Conventional 50_0
VEHE	Contains the function ID yielding the emission factor (exte/km) in terms of SPED (km/h)	('CAR_Gasoline_cc < 1.4 l_ECE 15-01__','FC',26071)
TSVE	Contains the number of vehicles of the vehicular fleet for each externality-vehicle code.	('PC','CAR_Gasoline_All capacities_ECE 15-01__',5250)

Moreover, it's possible (and necessary) to insert into the "Function" table all the mean-speed functions as they have been defined by ARTEMIS project (in which the mean speed is indicated with "xx" string). As an example a function has been reported (function for *CAR_Gasoline_cc < 1.4 l_Euro 4* category):

$$(136 - 1.65 * xx + 0.03 * xx^2)/(1 + 0.026 * xx + 0.0002 * xx^2) \quad (11)$$

Once defined the externalities and linked the transport system (TSYS) created in Visum to the COPERT categories is possible to launch the simulation.

After starting TRE will be shown the configuration graphical user interface (GUI). The graphical interface shows the complete list of parameters of TRE and for each of them shows the specified value in the file *CommandLineTDE.csv*. For parameters not specified in the configuration file the default value is displayed. Also, parameters are grouped into different thematic sections (DataSource, RouteChoice, Control…) in order to facilitate the identification.

There is a specific section ("Externalities") that contains all the settings related to the estimation of the transport externalities. The figures below show the parameters contained in the Externalities tab of TRE graphic user interface and their setting in the current study case.

Name	Type	Unit	Validity	Default	Description
MIES	Int32	km/h	≥0	1	minimum speed in externality function computation
MAES	Int32	km/h	≥0	100	maximum speed in externality function computation
SSTE	Int32	km/h	≥1	1	speed step in externality function computation
NSPE	String			EVEL	name of the speed in externality function expressions

Figure 35 – Externalities parameters

Finally, after setting all the other TRE parameters (in this case the values for a correct dynamic traffic assignment have been modified), the simulation is ready to start. So, what will be done is a dynamic traffic simulation on the "Example" network and then the computation of externalities rates on the base of the mean speeds just calculated and the externalities parameters previously set.

It has been selected the link 1 from node 10 to node 11 and the elements (emission rates by minutes) have been summed up by columns to obtain the total emission rates in the reference period.

	CO	**CO2**	**FC**	**HC**	**NOX**	**PM**
	...	...	...	...	...	...
	2.096	191.89	68.652	0.259	1.129	0.046
	2.096	191.89	68.652	0.259	1.129	0.046
	2.096	191.89	68.652	0.259	1.129	0.046
	2.096	191.89	68.652	0.259	1.129	0.046
	2.096	191.89	68.652	0.259	1.129	0.046
Total	**200.123**	**18316.99**	**6553.244**	**24.747**	**107.819**	**4.348**

Figure 36 – link 1 from node 10 emission rates

To compare the results obtained with those observed after using HBEFA model, it has been effected the ratio among the results to see how the orders of magnitude were different. The results are those that follow:

tre		hbefa		Ratio
1746.425	CO2	2221.491	CO2	1.272022
10.316	Nox	4.588992	CO	0.444842
19.13	CO	3.417175	Nox	0.178629
2.348	HC	0.320254	HC	0.136394

Figure 37

The results are perfectly coherent with the emissions' research literature that states in general the resulting emissions obtained with the CO_2 HBEFA emission calculation model are higher than those computed with COPERT" (Borge, 2012).

4.3 Case 3: EnViVer microsimulation

EnViVer is an odd-on module for Vissim, which is based on the VERSIT+ exhaust emissions model from TNO: it gets possible to determine pollutant emissions based on vehicle trajectories and other information from PTV Vissim. As it said (par. 2.4.1) Versit+ emission model is capable of modelling emissions, like NO_x, particle matter and CO_2, for any type of car (vehicle types are used to assign additional properties such as fuel type or pollutant class to each vehicle). For this reason, info about the behaviour of cars (speed-time profile) is required. This info is available from traffic simulation software that in the case is Vissim.

To reproduce the same situation of the previous points it has been considered only the link that goes from node 10 to node 11. The input vehicles in Vissim are located at the start of every link that enters the Vissim network and define the absolute vehicle volume per hour.

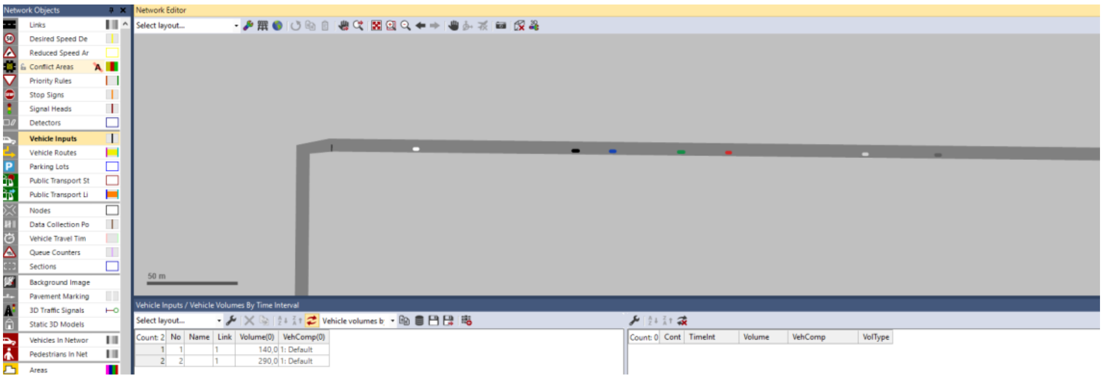

Figure 38 – Vissim Snapshot

After the simulation the software produces a .fzp file that contains information related to the simulation (simulation second), traffic (speed, vehicle type number) and link (link gradient). The .fzp is all that EnViVer requests to assess traffic emissions.

Once imported the .fzp file it remains only to link every "vehicle input category" as it was previous defined in Vissim to the ones defined by EnViVer (defined according to Versit+ categories). The obtained results are listed below:

Application version: 4.5.5 [Release date: 11/02/2016]
VERSIT+micro version: TNO Versit+micro [Release date: 6-9-2016]
Licenced for: university la Sapienza - university la Sapienza, Mariano Biasella
[illegible] Guido Gentile

Emission

CO_2	NO_X	PM_{10}
1709.813 kg	2987.315 g	456.493 g
855.275 kg/h	1494.301 g/h	228.345 g/h
207.155 g/km	361.933 mg/km	55.307 mg/km

Figure 39 – EnViVer Output

The results obtained with static traffic assignment, dynamic traffic assignment and microsimulation are finally the ones that follow:

Copert		hbefa		EnViVer	
1746.425	CO2	2221.491	CO2	1709.813	CO2
10.316	Nox	3.417175	Nox	2.987	Nox
19.13	CO	4.588992	CO	-	-
2.348	HC	0.320254	HC	-	-

Figure 40

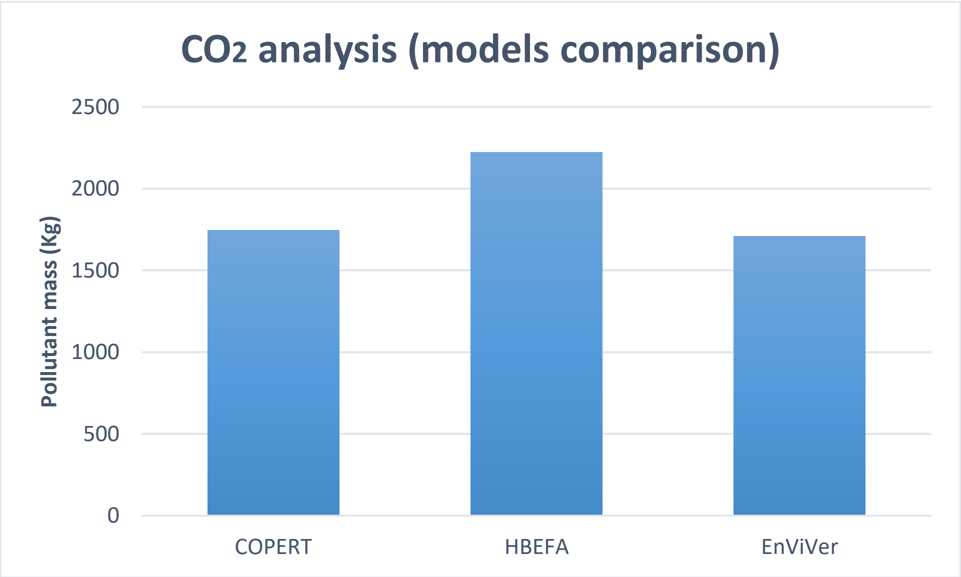

Figure 41

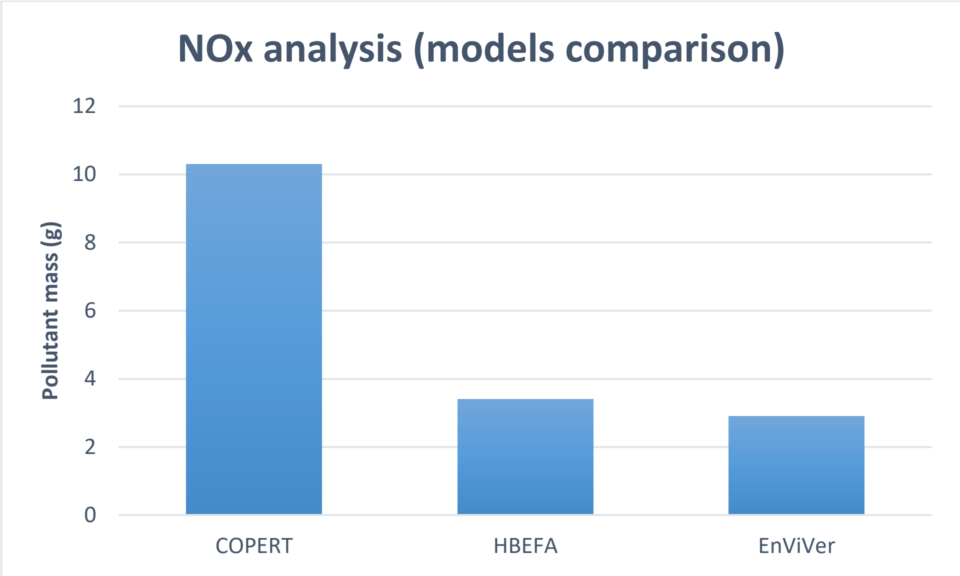
NOx analysis (models comparison)
Pollutant mass (g)
0
2
4
6
8
10
12
COPERT
HBEFA
EnViVer

Figure 42

5 DTAlite

DTALite is a mesoscopic DTA simulation software that has been developed to provide transportation planners a rigorous and above all fast traffic network modelling tool. In fact, DTAlite adopts a new software architecture and algorithm design to facilitate the most efficient use of emergent parallel (multi-core) processing techniques and exploit the unprecedented parallel computing power newly available on both laptops and desktops (Xhou, 2014).

DTALite's four major modelling components include:

1. Time-dependent shortest path finding
2. Vehicle/agent attribute generation, which combines OD demand matrices with additional time-of-day departure time profiles to generate trip
3. Dynamic path assignment module which considers major factors affecting agents' route choice or departure time choice behaviour (e.g. different types of traveller information supply strategies, road pricing strategies etc..)
4. A class of queue-based traffic flow models that can accept essential road capacity reduction or enhancement measures (e.g. work zones, incidents, etc…)

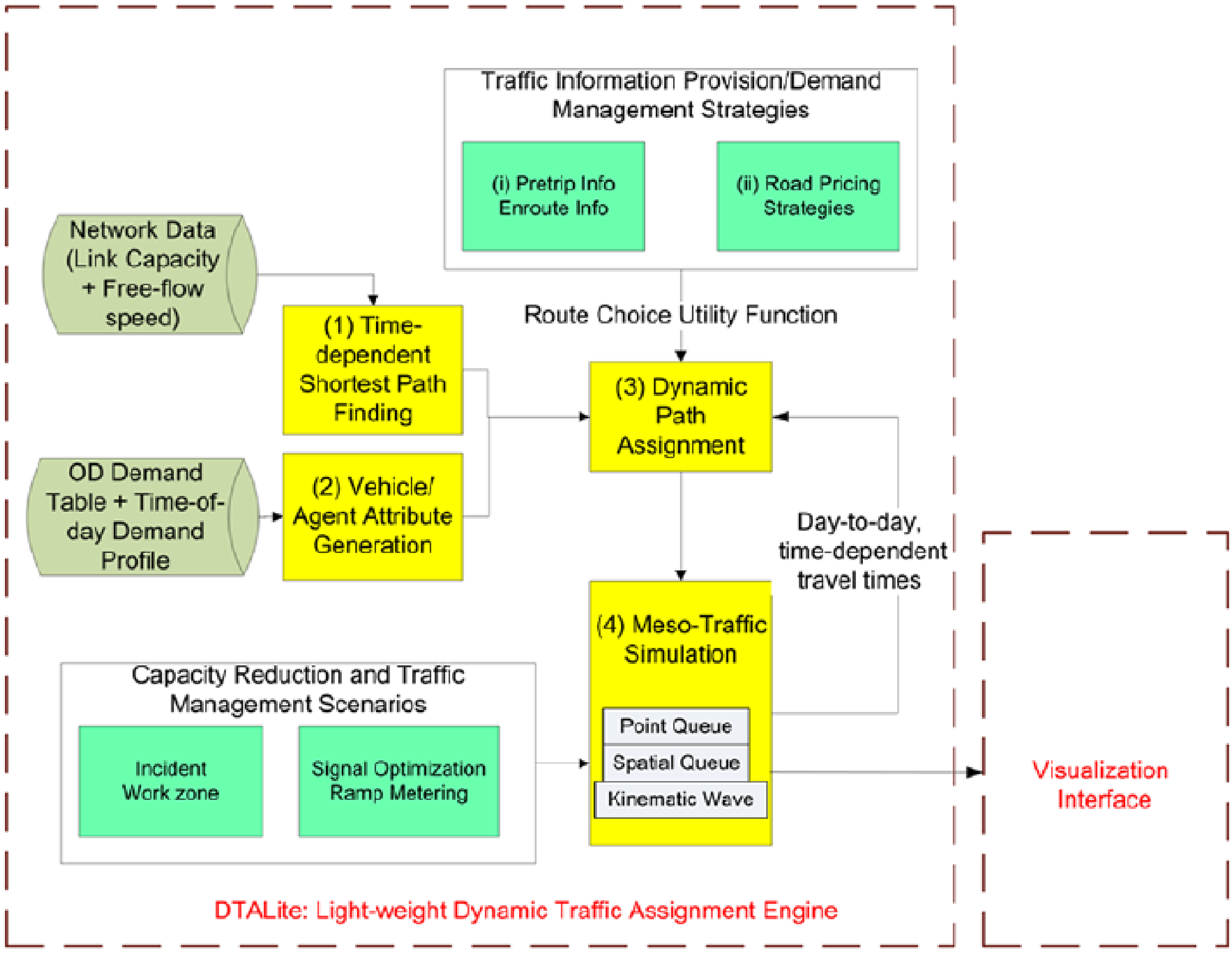

Figure 43 – DTALite software system architecture

A simulation-assignment DTA model needs to read time-dependent OD matrices and the assign vehicles to different paths based on link travel time. In particular, way a vehicle is moved across a link by a link traversal model that involves a speed-density relationship and outflow capacity constraints (determined by link properties) and then moved between links at the node by a node transfer function. To capture queue formation, spillback, and dissipation, DTALite uses a number of computationally simple but theoretically sound traffic queuing models to track waves' propagation. By doing so, traffic simulation in DTALite only requires a minimal set of traffic flow model parameters, such as outflow, inflow capacity, and storage capacity constraints, as illustrated in Figure 44 (Xhou, 2014).

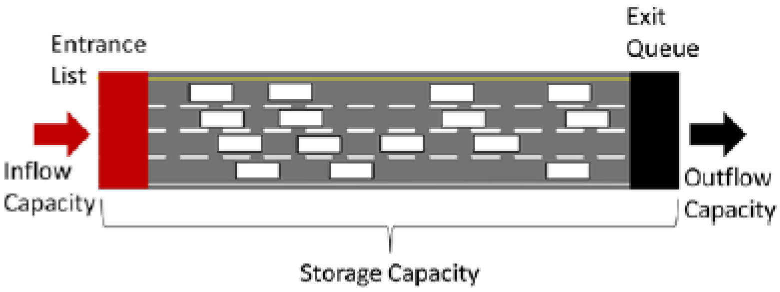

Figure 44

In DTALite has been implemented the Newell's solution (that use cumulative flow counts), the point queue model and the spatial queue model to describe the queuing phenomena. By imposing an outflow capacity constraint on each link, a point queue model aims to capture the effect of traffic congestion at major bottlenecks but not the queue spillback and the consequent delay due to storage capacity (Figure 45 – Point queue model).

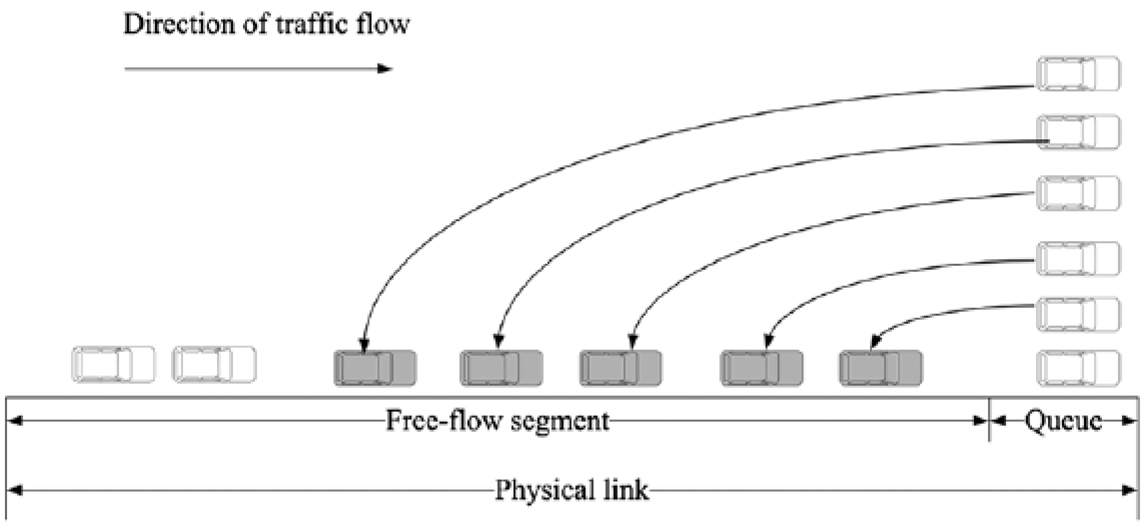

Figure 45 – Point queue model

For calculating transfer flow from link *l* to link *l+1* has been used the following formula:

$$q_{l,t} = Min(v_{free} * k_{l,t}, cap_{l,t}^{out}) \qquad (12)$$

Adding the storage capacity constrain as follows the spatial queue model has been enhanced:

$$q_{l,t} = Min(v_{free} * k_{l,t}, cap_{l,t}^{out}, (k_{jam} - k_{l+1,t}) * \Delta x) \qquad (13)$$

Where $(k_{jam} - k_{l+1,t}) * \Delta x$ is the physical space availability at downstream link *l+1*.

The most thorough of the models is the Newell's simplified Kinematic wave model, which is built upon the assumption of a triangular flow-density relationship. In Figure 46 is represented the cumulative number of vehicles moving into a link (A(t)) and the cumulative outflow vehicles (D(t)) and V(t) that is the number of vehicles in vertical queue.

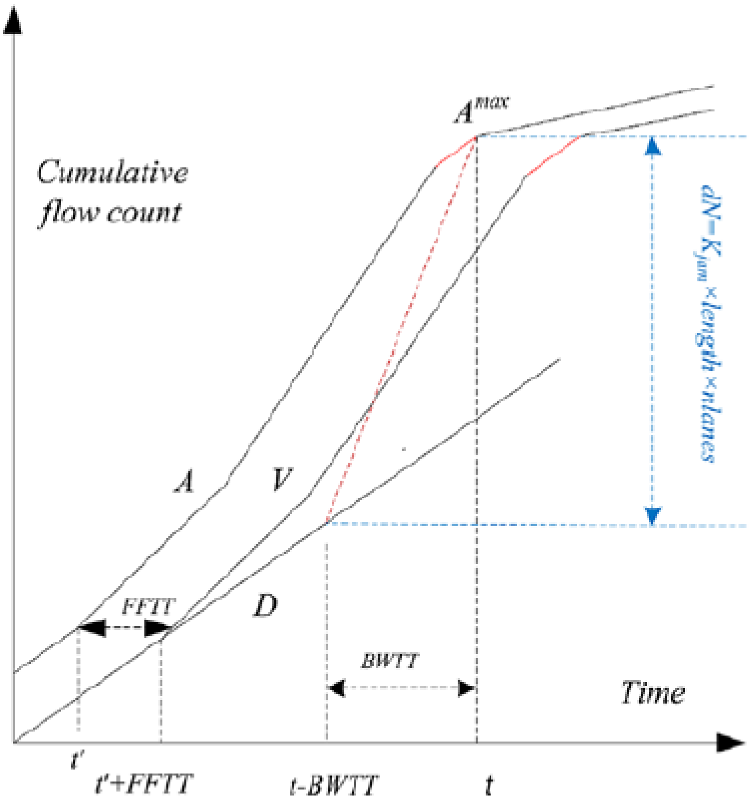

Figure 46

From the node management side, the proposed DNL model load agents into the network at the origin node using a loading buffer (rather than being loaded directly into link l=1). Three different models have been developed (origin node, merge node, and signalized intersections) to allocate capacity at merge junctions, while diverge junctions did not require special treatment because the paths for agents traveling through the network are known.

DTALite works as an executable file that needs to let the simulation start only CSV input files that collect all the supply and demand information. All the input data and their relationships are represented in the following picture:

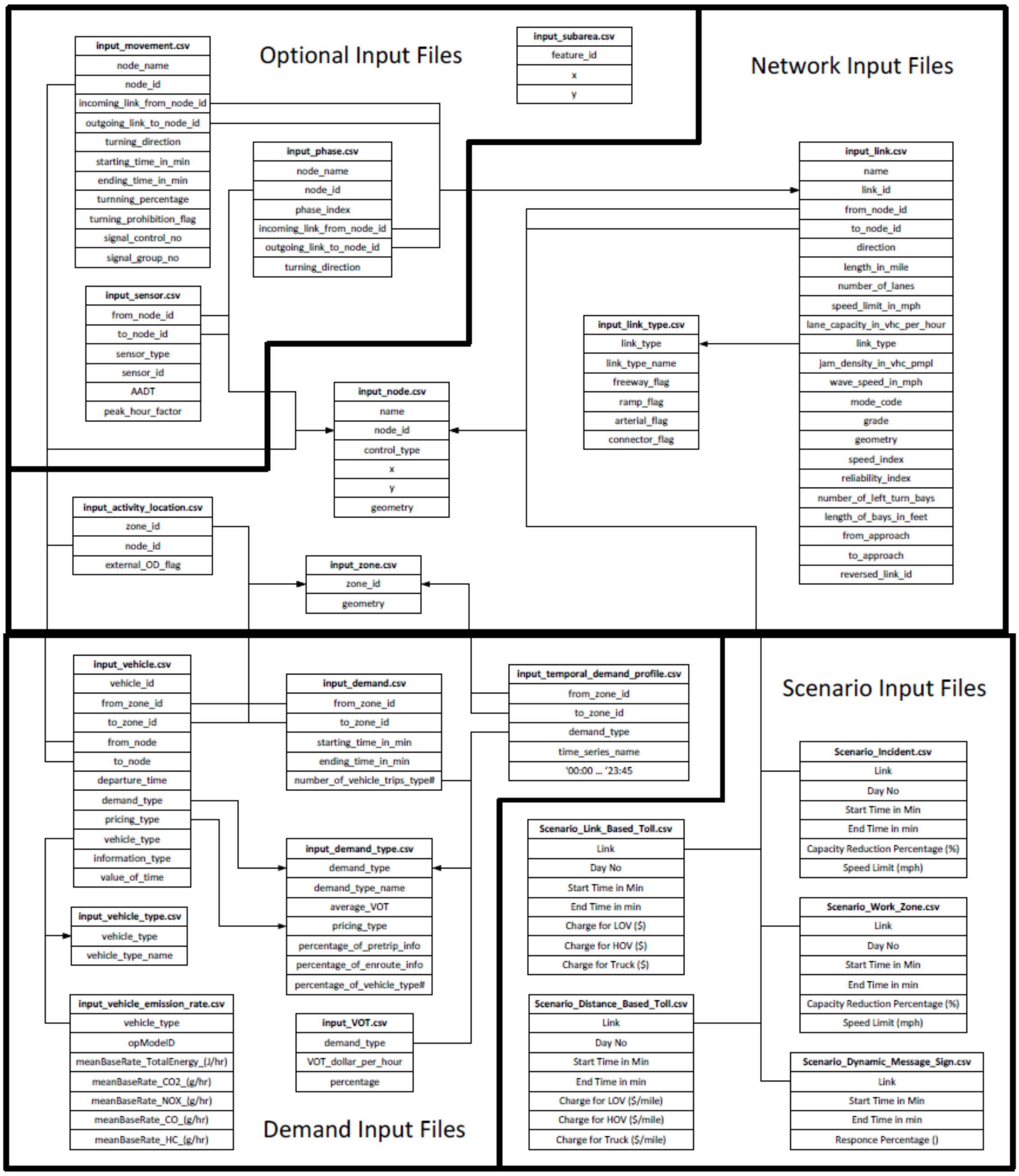

Figure 47

At this point takes over the central point of the thesis work. In fact it has been thought to develop a visum add-in to obtain a mesoscopic DTA simulation directly from Visum. As it has been said all DTALite needs are .csv input files that describe the network and demand, so it has been written a code that automatically create all the input files that DTALite requests (in the format it requests). It's important to say that is possible to do this kind of constructing a network data set for DTAlite from all the software that have a base structure that consist of nodes, links, centroids, and connector layers (e.g. TransCad and Cube). Thanks to the editing of a Pyhton script template (aimed to link the .NET code to Python code), it has been possible to write the add-in entirely in .NET (even if the developing of a Visum add-in requests Pythone code).

During the code writing there's been an issue that is important to mention. Something came up when it has been defined a time-dependent demand profile. In fact, setting to 1 the "apply_additional_time_dependent_profile" it is possible to use it and define for each time interval the proportion of demand. First of all it has been declared the variable "resTime" in a way to obtain the entire value major or equal to the number set as the initial instant of the simulation.

Then, tanks to "OverlappingTime" function (defined in utility module of TDE), it has been possible to build the "buckets" and the exact percentage of demand that they contain.

This allows to define the demand as represented by the following chart (that exactly corresponds to Visum "Example" demand distribution).

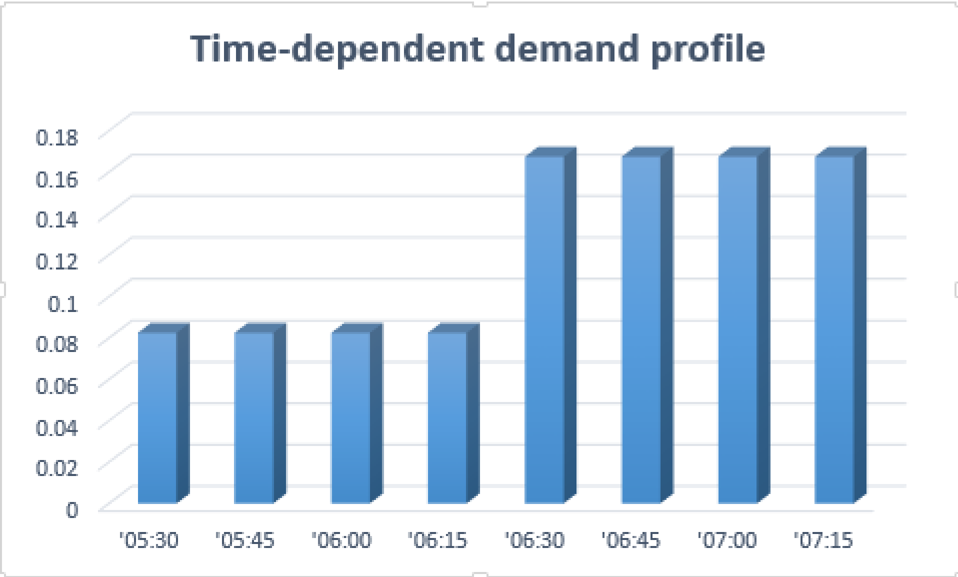

Figure 48

There has been also another recurrent problem: the definition of the unit of measure. This because DTALite software works with distances defined in miles and speeds define in mph, so it has been needed a particular attention to convert the measure that instead in Visum were defined in kilometres (distances) and kmh (speed).

The conversion from the length in kilometres to the length in miles was done through the factor 0.00062 and from the speed limit in kmh to the same one in mph through the factor 2.24 to let DTALite work with the correct measures.

5.1 Emissions modelling in DTALite

The definitional files for vehicle emission modelling are:

- Input_cycle_emission_factor.csv

- Input_vehicle_emission_rate.csv
- Input_base_cycle_faction_of_OpMode.csv

In the study case the files have been provided by Dr. Chris Frey's team at NCSU that contain data belonging to MOVES lite. In particular, 23 different operational modes have been defined (each one corresponding to a different driving cycle). In "input_base_cycle_fraction_of_OpMode.csv" the percentages of *vehicle_type* that belong to each *operational mode* have been established. In input_vehicle_emission_rate.csv the emission factor per every pollutant have been defined on the basis of cycle average speed (distinguished for vehicle type and age of vehicle). In "input_vehicle_emission_rate.csv" the mean base rate per pollutant (g/hr) have been specified (distinguished for operational modes and vehicle types).

As the previous cases, only the results related to link 1 (10->11) have been reported (the emission results have been stored in output_linkTDMOE.csv file). For a qualitative analysis, it will be shown only the sum of the emission rates related to the examined pollutant, but it's important to say that, as DTAlite works as a mesoscopic traffic simulator the instantaneous results are different from each other (unlike TRE emission results).

Time stamp in min	**CO2**	**Nox**	**CO**	**HC**
…	…	…	…	…
446	6.924782	1.281412	0.724302	0.637931
447	7.006625	1.264235	0.690761	0.79503
448	5.813265	1.529456	0.97475	0.597816

449	6.435039	1.378084	0.79431	0.753881
450	0	0	0	0
	4002.974	110.0098	65.84558	72.42866

Figure 49

6 Catania: study case of an application on a real network

For checking the validity of the DTA simulators previously introduced, it has been deemed the case of a real network taken from a contract of SISTeMA s.r.l. for Famas System s.p.a. and Università degli studi di Catania.

The transport system model has been built and calibrated starting from census data, map books and pre-existent mobility data. Furthermore, the model has been calibrated with the average traffic measures (flows and link speeds) to generate a new forecast of the real time traffic states in a few minutes.

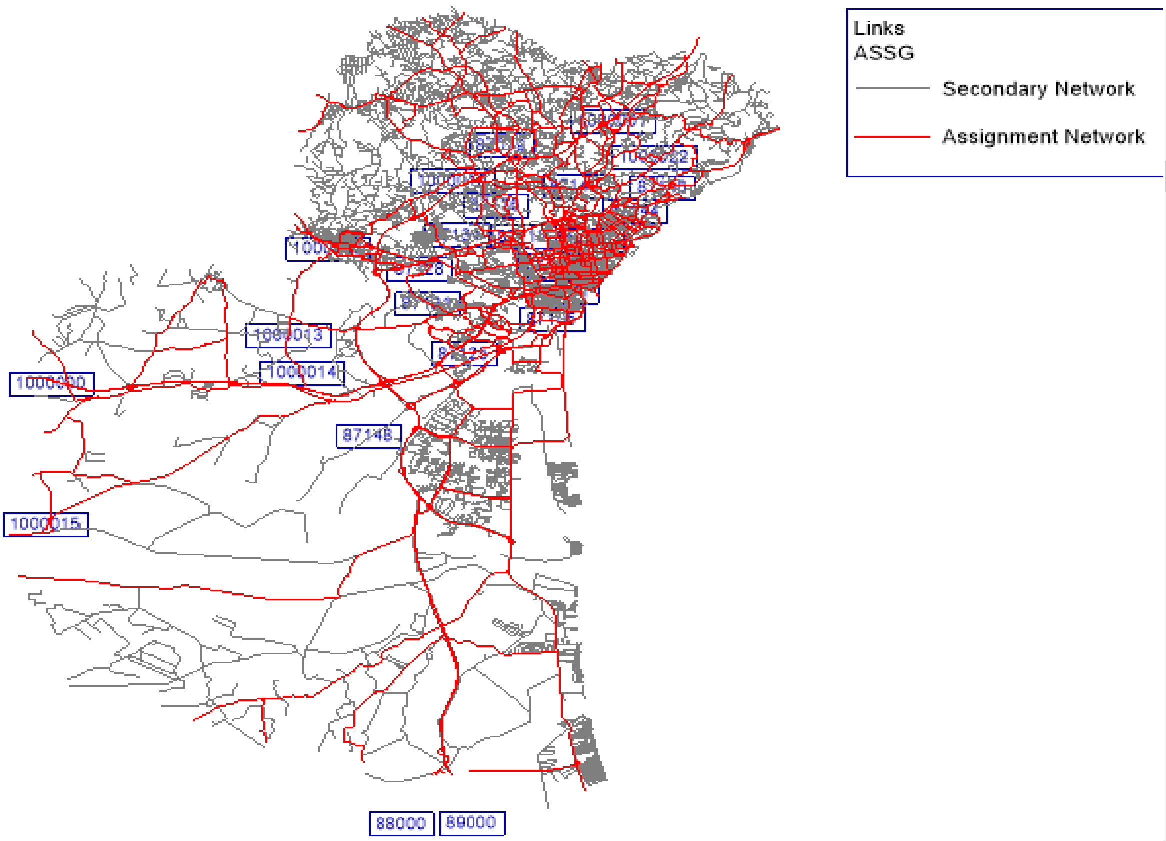

Figure 50 – Catania Visum network

The network has been defined as it has been shown in Figure 50, with 20285 nodes, 89 zones and 50424 links. It is clearly visible from the picture that less than a half of them (17528) is signed as part of primary network and so has been selected in the network that has to be simulated (links marked with ASSG=1). To exploit the computational power of DTALite software the network has been reduced to let the available PC do the simulation without any difficulties. This was done simply cutting the network with the *subnetwork generator function*. To use that function a west zone of the town has been chosen (corresponding to Lineri suburb) and a static demand assignment has been executed in order to obtain a new O-D matrix for the new generated network.

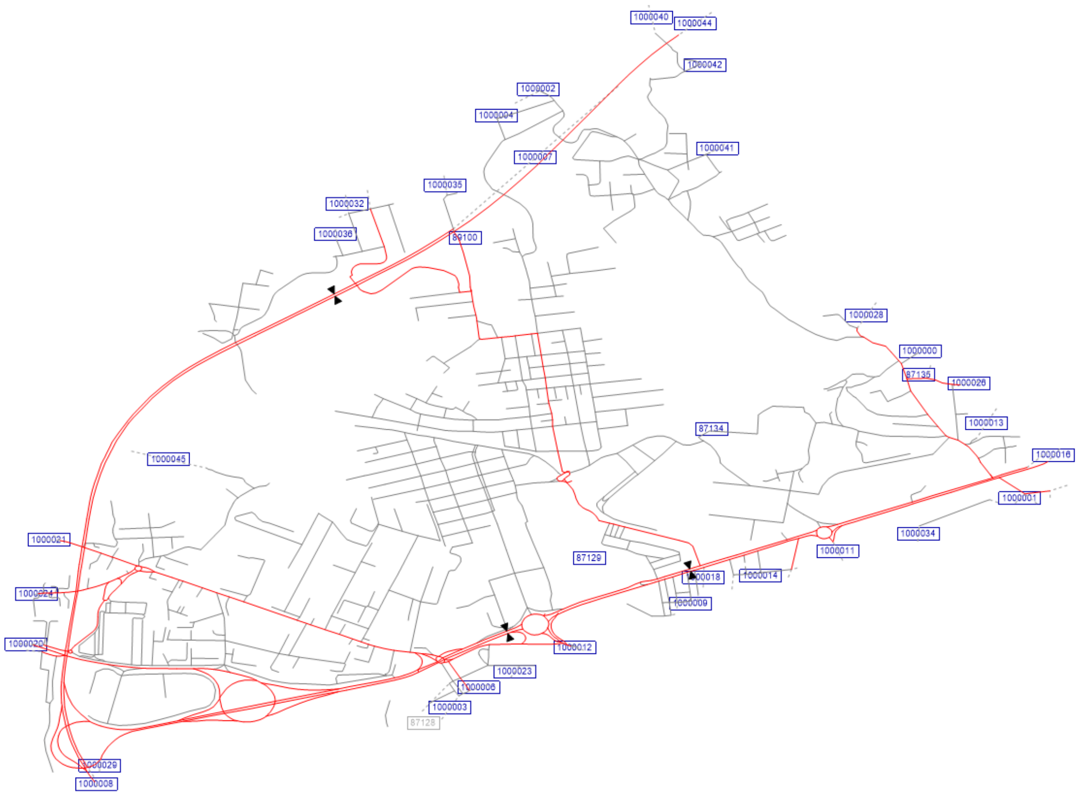

Figure 51 – Subnetwork (Lineri suburb)

Regarding the demand side 6 matrices have been defined (three for each day-type): 2 for light vehicles (“LEGGERI_DTYP1_BK0” or “LEGGERI_DTYP2_BK0”) and 1 for heavy vehicles (“PESANTI_DTYP1” or “PESANTI_DTYP2”). Furthermore, the matrices designed for light vehicles are divided into 2 matrices: one that goes from 00:00 to 14:00 and the other that goes from 14:00 to 23:59.

In the following paragraph the reference day type will be DTYP1, so the reference matrices will be those indicated with identification numbers equal to: 10, 20 and 30.

To evaluate the efficiency of the two exanimated models the developed network has been tested with TRE software (that, as it has been said it implemented with COPERT functions to assess emissions) and then with DTALite (implemented with MOVES functions).

In particular way two link have been chosen to this aim: the first (link=924401745; fnod=617589712) and the second (link=807434336; fnod=617570611).

6.1 DTALite-TRE model simulation comparison (analysis of emission on the total network)

The first value it was taken into consideration was the total time spent on the network by vehicles. This because this value is the only one that let to obtain a qualitative analysis about the differences between the two simulations. The results were the following:

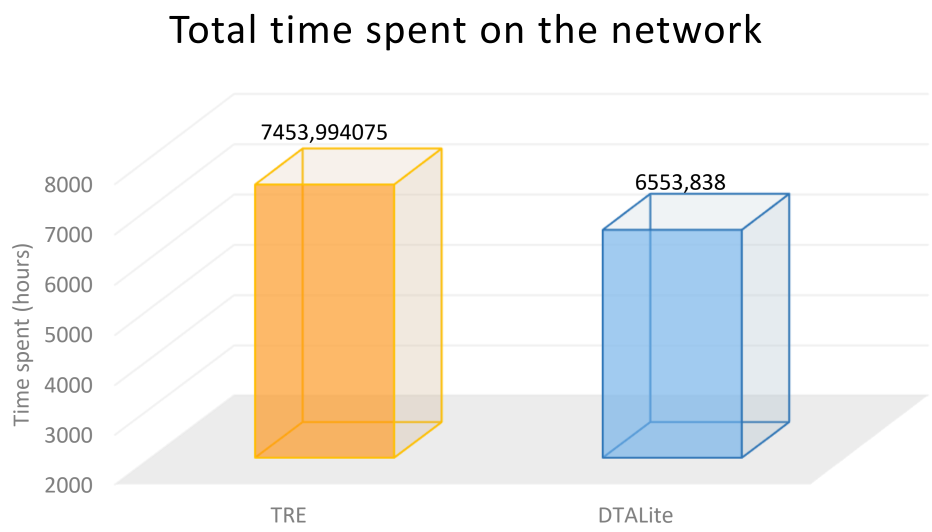

Figure 52

Once assimilated this result, it was possible to proceed with emission analysis. The first value it was analysed was that relative to carbon dioxide.

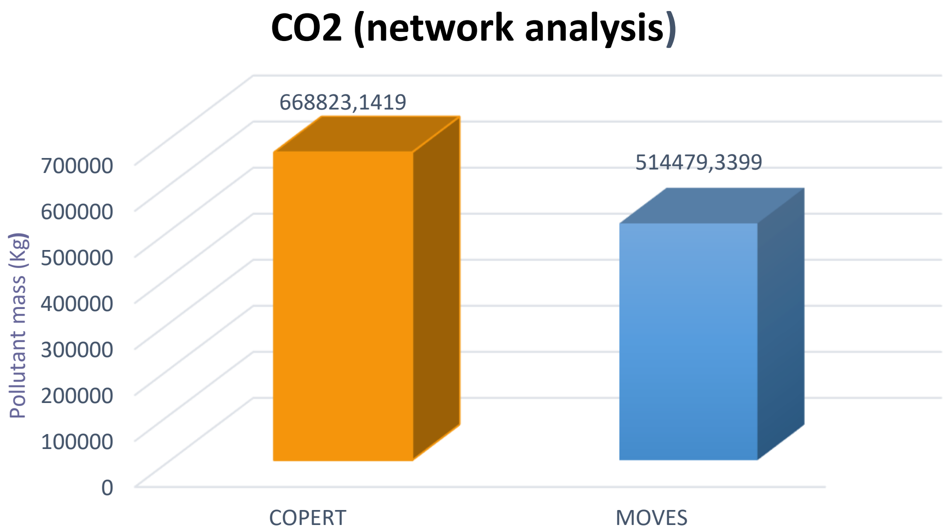

Figure 53

This was an expected result, because carbon dioxide is dependent from fuel consumption that is supposed to be higher, in absence of congestion, where travel time spent by vehicles on the network is higher too.

The second analysis was relative to carbon monoxide emissions.

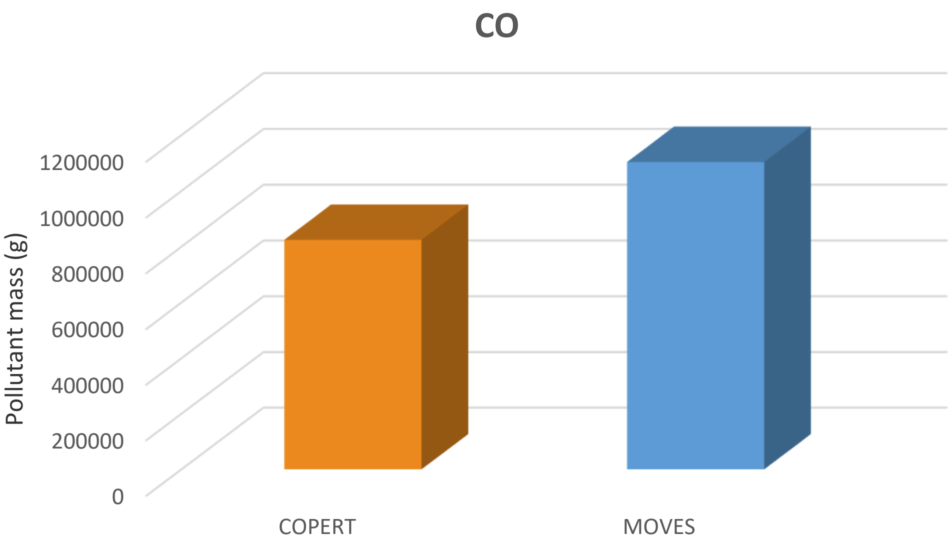

Figure 54

In that case was obtained an unusual result. In fact, result outcome from MOVES result higher then COPERT ones, where travel times results were the opposite.

Series results relative to hydrocarbons and nitrogen oxides outcome immediately very different one from the other.

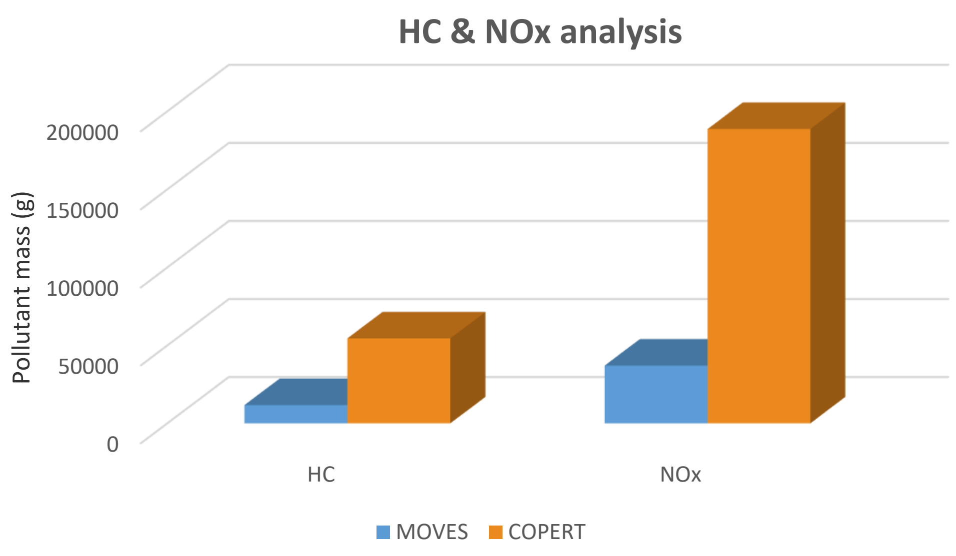

Figure 55

While the results relative to hydrocarbons were unexpected, the results relative to nitrogen oxides were instead not. This because in COPERT guidelines is expressly written that nitrogen oxides values are not yet reliable.

To understand better what happened in pollutant mass estimation, it was done an analysis for two links of the network, and emissions were forecasted there.

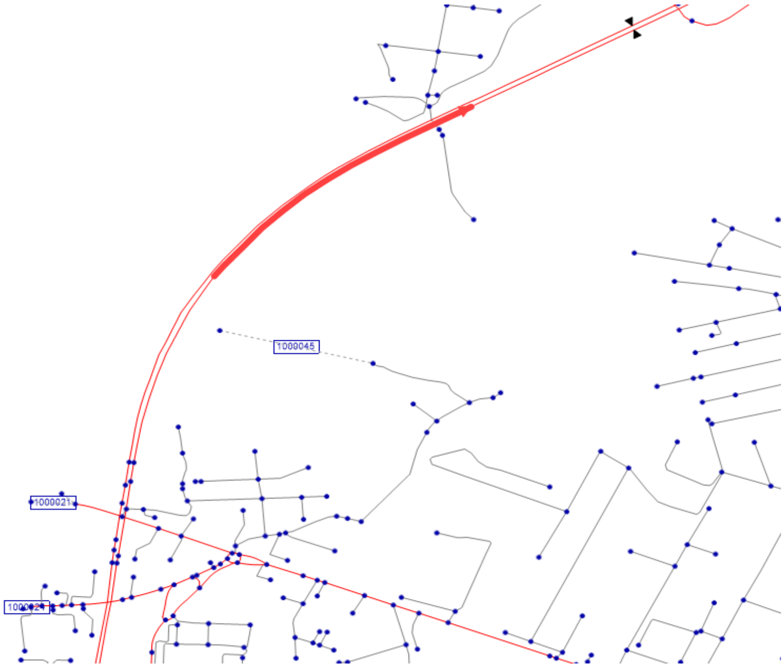

Figure 56 - link=924401745

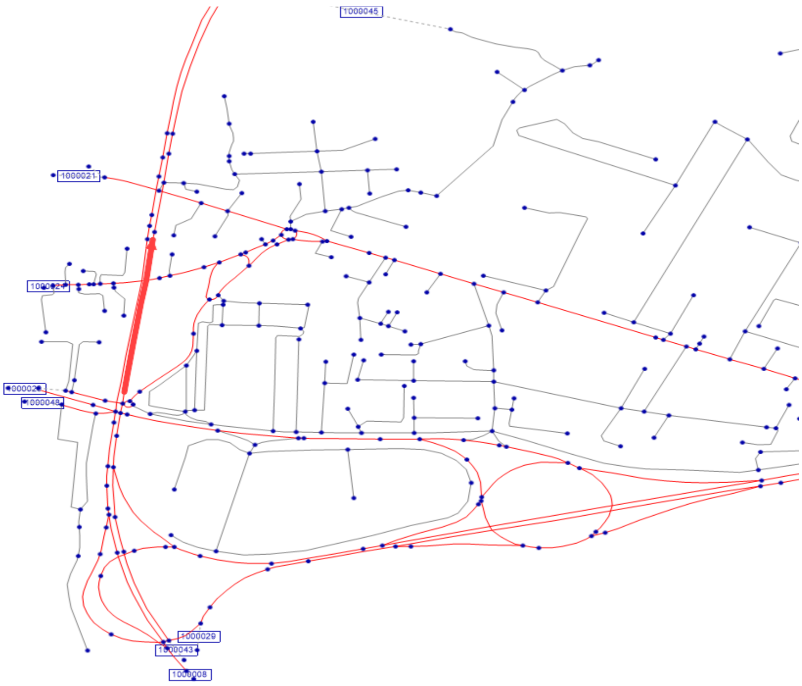

Figure 57 - link=807434336

The links are both situated on E45 road (*Tangenziale Est)*. That because the high flows roads are the only places where flows, speeds and levels of service are comparable (and thus it has been possible to focus the attention on the differences among the two emission models).

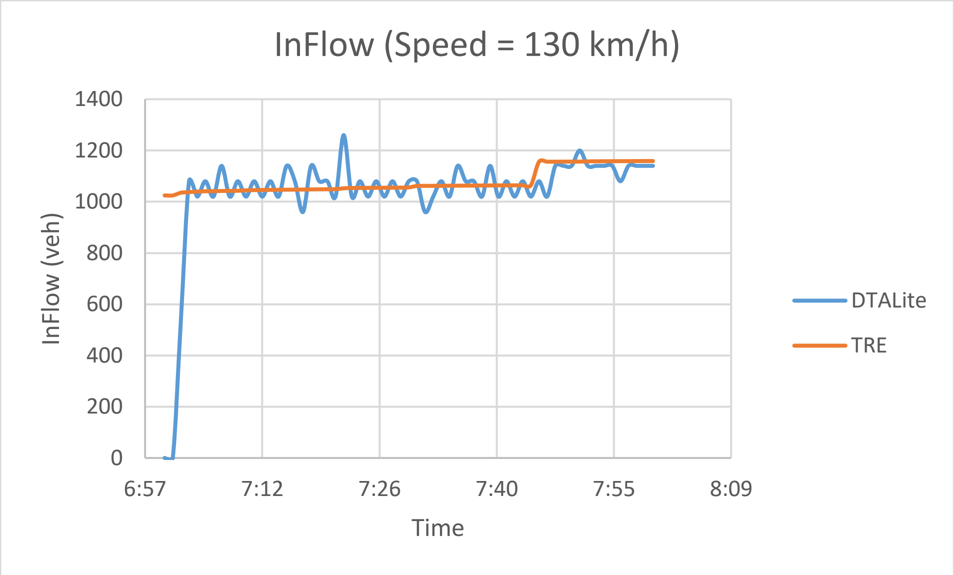

Figure 58 – InFlows on link=924401745

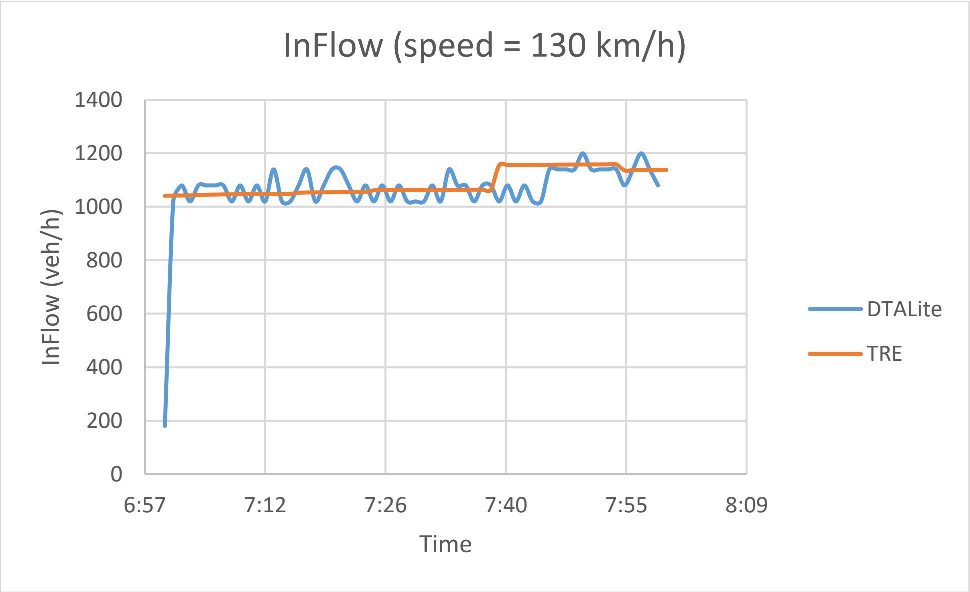

Figure 59 – InFlows on link= link=807434336

6.2 DTALite-TRE model simulation comparison (analysis of emissions on two links)

In order to show the differences between the emission models (Copert used by TRE and Moves used by DTALite) under analysis, the emission quantities of each pollutant matter by both emission models has been plotted in charts that have on the x axis the time (in the same way it was done in the *Inflows charts*).

6.2.1 Analysis on carbon dioxide

Carbon dioxide is the element that pays the major attention from the environmental agencies. Cars and trucks account for nearly one-fifth of all US emissions, emitting around 24 pounds of carbon dioxide (www.ucsusa.org, s.d.), and it could be generally said that the CO_2 emissions are numerically the highest among the exhaust gasses. This is the reason why the carbon dioxide emission factor advertising (e.g. 132 g/km CO_2) has now become common practice among car manufacturers.

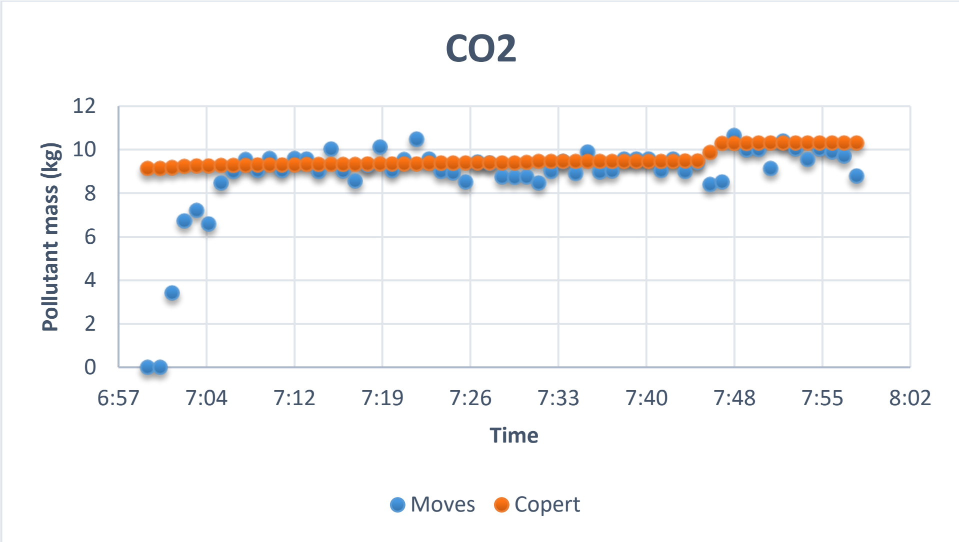

Figure 60 - link 924401745

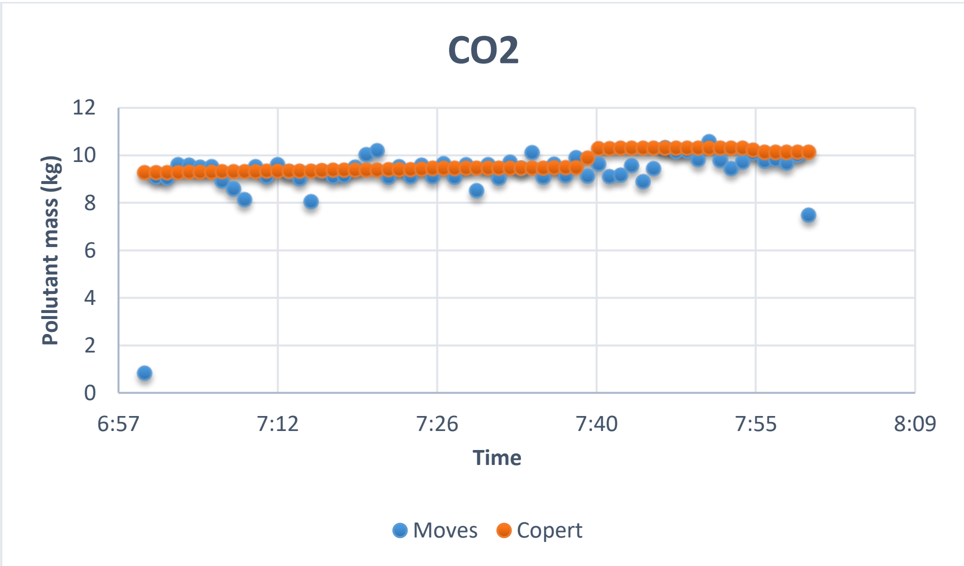

Figure 61 - link 807434336

6.2.2 Analysis on carbon monoxide

Carbon monoxide (CO) is produced in the incomplete combustion of carbon-containing fuels. The largest anthropogenic source of CO is vehicle emissions.

This is the reason why the scientific researches makes strong efforts to better represent the carbon monoxide as they currently are.

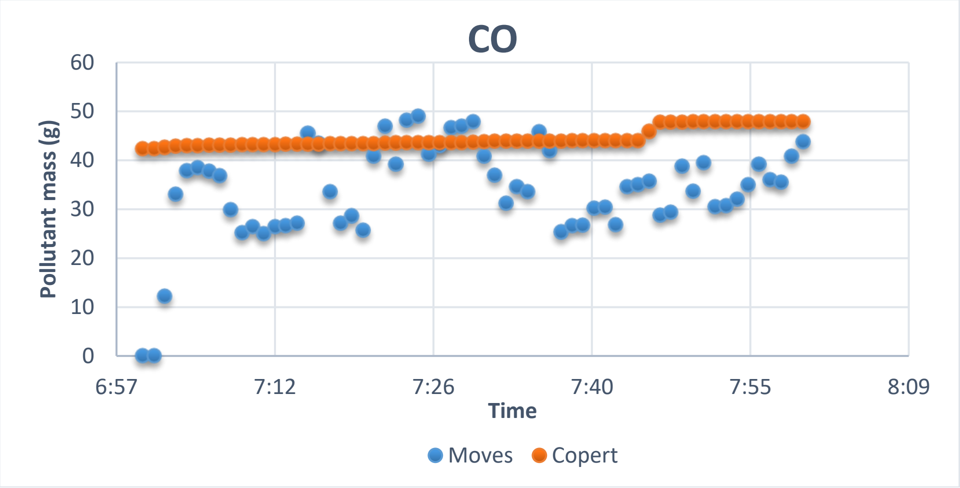

Figure 62 – link 924401745

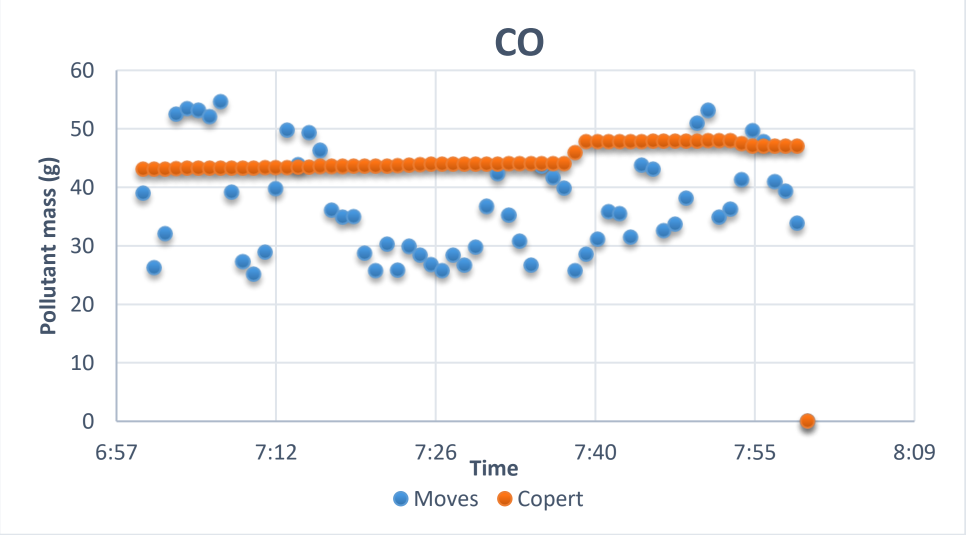

Figure 63 - link 807434336

6.2.3 Analysis on hydrocarbons

Hydrocarbons are a class of burned or partially burned fuel. Thanks to the validation studies conducted in research (e.g. (Kousoulidou, 2010)), the results are supposed to be reliable and closed to the reality.

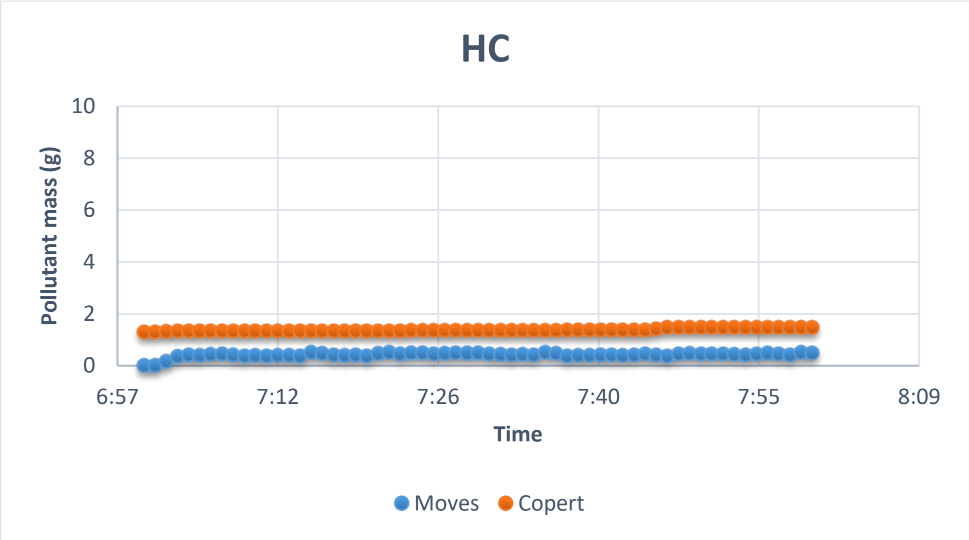

Figure 64 - link 924401745

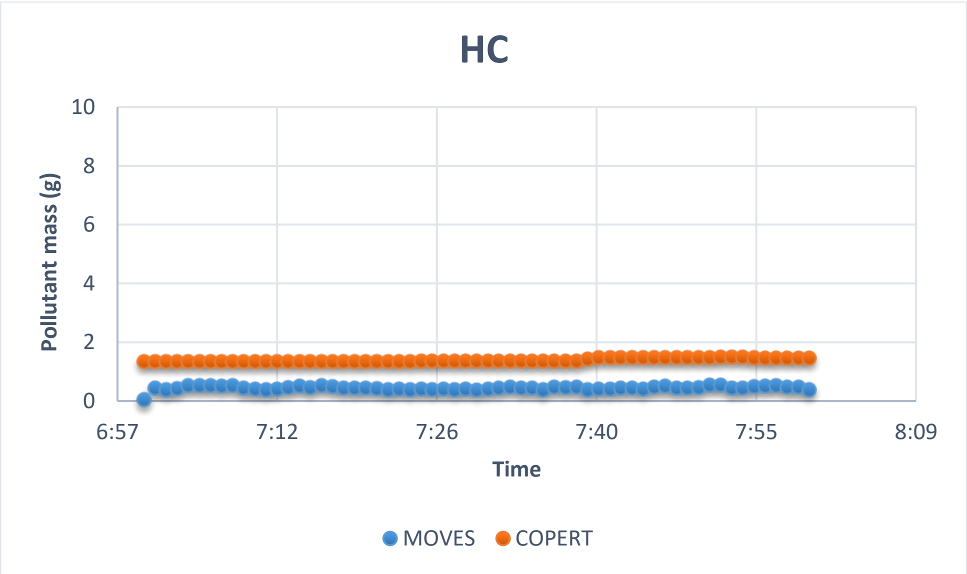

Figure 65 - link 807434336

6.2.4 Analysis on nitrogen oxides

Uncertainty in Vehicle NOx emissions within Air Quality Assessments is a spread topic in scientific research. COPERT guidelines declare that NOx emitted mass are not supposed to be precise quantities rather an indication assessment of the pollutant mass.

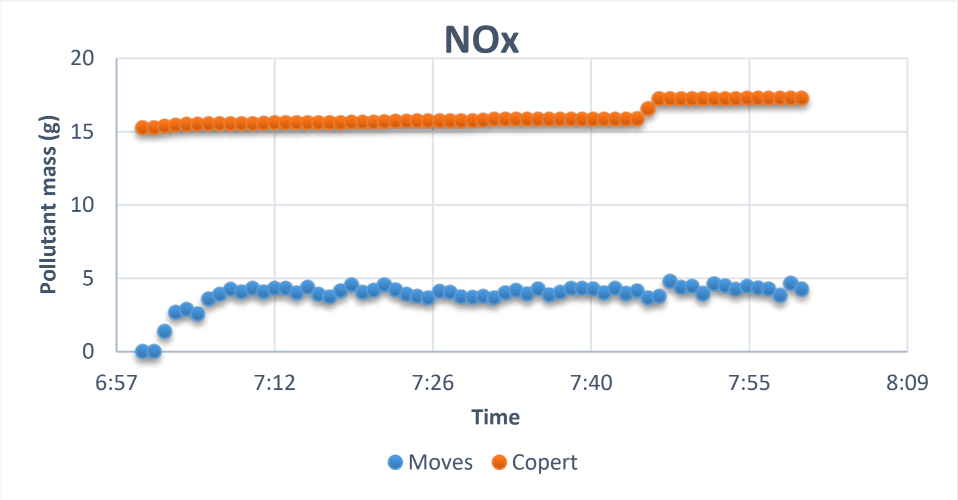

Figure 66 - link 924401745

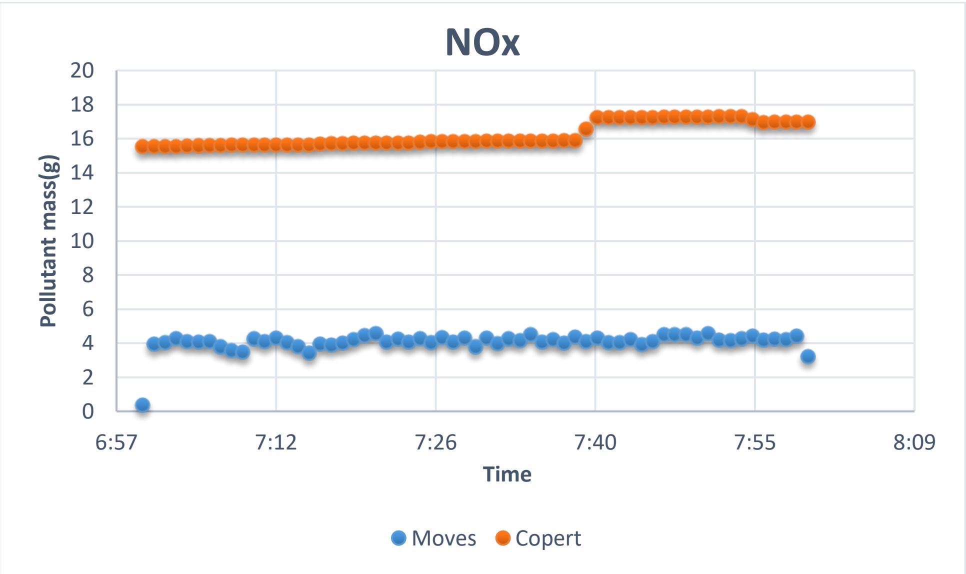

Figure 67 - link 807434336

6.2.5 Congestion case (pollutants emissions comparison)

To analyse the emissions in case of congestion it has been created a bottleneck downstream the link *924401745* reducing the capacity of the successive link from 4000 veh/h to 860 veh/h. The congestion situations are obviously different from one to the other: using TRE software (macrosimulation) the queue quickly forms, while using DTALite the vehicles are able to travel much closer each other for a while and so, for the first 20 minutes, there is no congestion on the link (even if the vehicles reduce their speeds).

So, basically using TRE there is immediately a hypercritical segment on the link and, consequently, the emissions are highest than those of the situation in free flow speed. Instead using DTALite there is no spillback in the first 20 minutes and that means the emissions are supposed to be similar to those viewed in the previous case until 7:20 a.m. After the time stated a spillback forms and the emissions sharply go up. In the following charts have been shown the trends of the emissions on the link *924401745* in the range of 7 a.m. to 8 a.m.

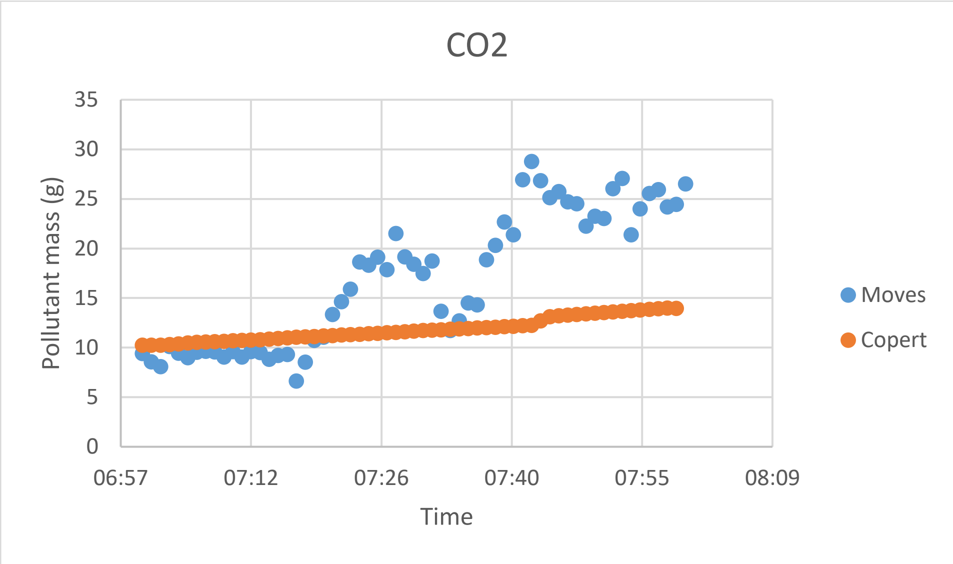

Figure 68

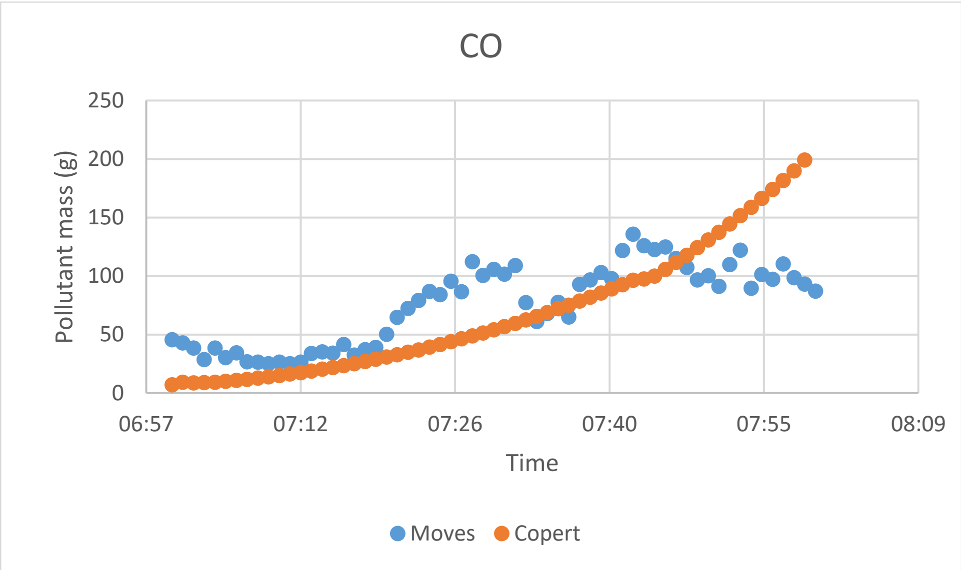

Figure 69

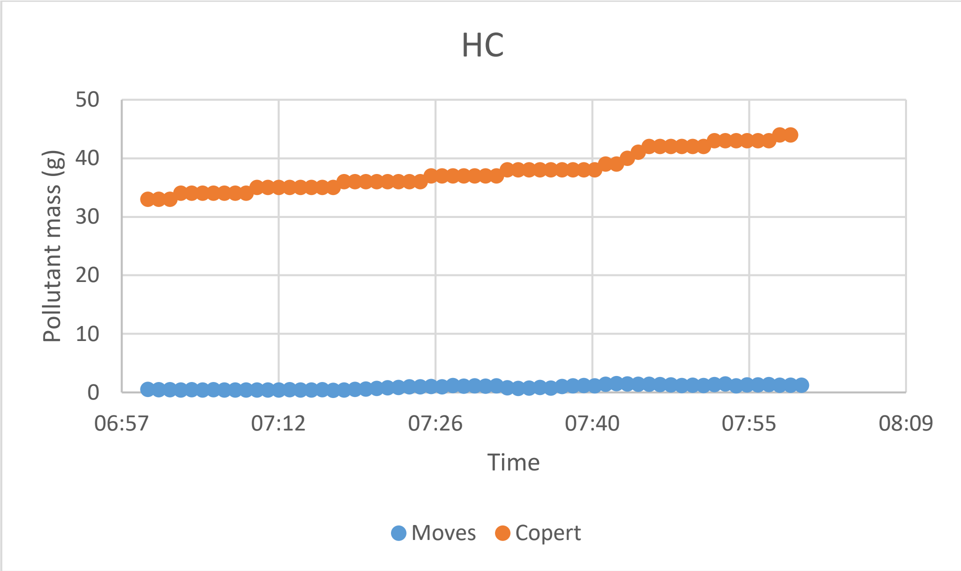

Figure 70

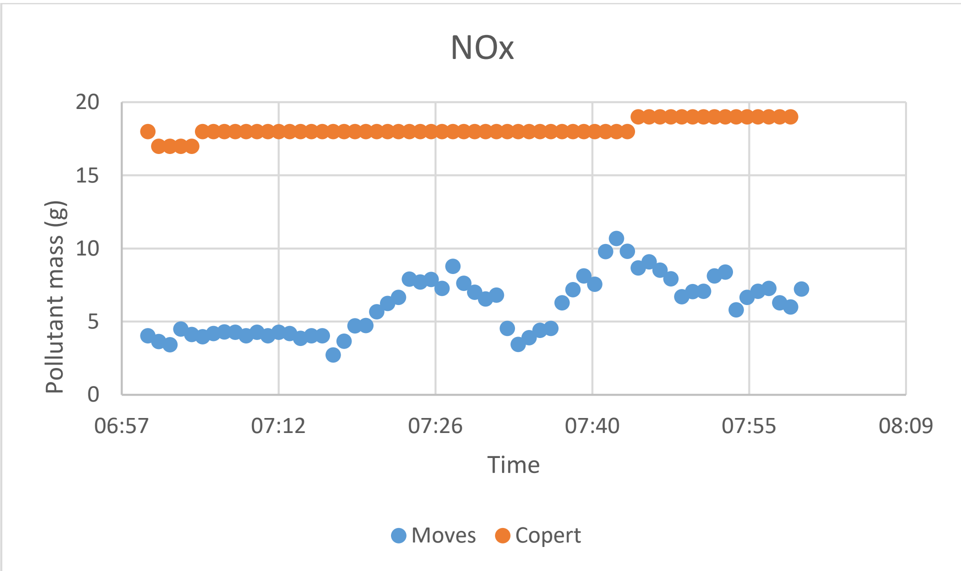

Figure 71

It is possible to see in all four charts that the spots relating to *Moves* do not constantly grow. This phenomenon is supposed to be linked to the formation of queue: until 7:40 the queue grows and decrease and finally settled (7:45) probably occupying the entire road. Unfortunately, as the data referred the hypercritical segment of the link are not available, it’s not possible to validate that consideration.

7 Dispersion models

Air pollution models are computer programs that use mathematical algorithms to simulate how pollutants in the ambient atmosphere disperse and, in some cases, how they react in the atmosphere based on knowledge of the emission characteristics (stack exit velocity, plume temperature, stack diameter, etc.), terrain (surface roughness, local topography, nearby buildings) and state of the atmosphere (wind speed, stability, mixing height, etc.). Such models are routinely used in environmental impact assessments, risk analysis and emergency planning, and source apportionment studies. In highly polluted cities such as Athens, Los Angeles and Mexico, regional scale air quality models are used to forecast air pollution episode.

The concentration of emitted pollutants over the soil level may pass from a low level to a high level in relationship to the variation of the conditions of the *planet boundary layer* (PBL) that is the lowest layer of the troposphere where wind is influenced by friction. The thickness (depth) of the PBL is not constant. At night and in the cool season the PBL tends to be lower in thickness while during the day and in the warm season it tends to have a higher thickness. The two factors that explain this phenomenon are the wind speed and thickness of the air as a function of temperature. Strong wind speeds allow for more convective mixing.

It's very important to define the PBL because wind is turbulent and gusty within that layer (because of surface friction from vegetation and topography causes turbulent eddies and chaotic wind patterns to develop).

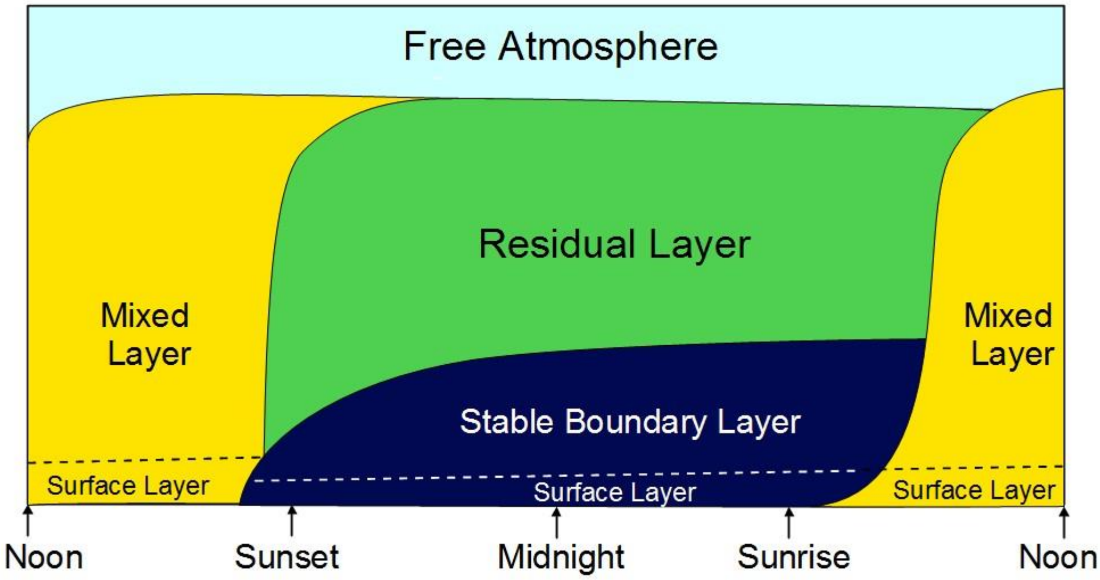

Figure 72

As it is shown in Figure 72 the PBL could be divided into several layers:

- the surface layer (SL) that reaches about 200 m high. In this layer, the fluxes of momentum, heat and moisture are assumed to be independent of height and the Coriolis effect is generally negligible (Zannetti, 1990). In that layer the turbulent phenomena prevail over molecular phenomena.
- The transition layer (TL) from 20 m to 2 km (indicated in the figure as Residual Layer). The top of the boundary layer is the longer influences the dependent variables through the turbulent transfer of mass (Pielke,

1984). In that layer, molecular motion can play a role in the transfer of mass and energy.

In a general way it's possible to declare that the dispersions mechanisms of the pollutants in the atmosphere are influenced by the following factors:

1. Meteorological factors (e.g. speed and direction of wind, temperature etc…)
2. Turbulences generated by vehicular flows
3. Roads characteristics

To simulate the pollutant dispersion in the Planetary Boundary Layer have been proposed three different approaches. In the following paragraphs, each one of them has been deepened.

7.1 Eulerian models

Eulerian models are used to describe dispersion phenomena that are based on the mass conservation law for a reference system in built with the earth. Two main hypothesis are declared: the isotropy of the pollutant and the fact that the variables are composed by a deterministic part and a random part.

The Eulerian approach comes from the conservation of mass of a single pollutant species of concentration C(x,y,z;t).

$$\frac{\partial C}{\partial t} = -\mathrm{u} \cdot \nabla \mathrm{C} + \nabla \cdot \mathrm{K} \cdot \nabla C + S \qquad (13)$$

Which derives from the conservation of mass equation law with the addition of the term $\nabla \cdot \mathrm{K} \cdot \nabla C$ where K is a turbulent diffusivity tensor and S that is the total rate of addition (or removal) of the pollutant species.

Assuming that the wind is blowing towards the positive x-axis, the previous equation become:

$$u\frac{\partial}{\partial x}C = \frac{\partial}{\partial z}\left(K_z\frac{\partial}{\partial z}C\right) + \frac{\partial}{\partial y}(K_y\frac{\partial}{\partial y}C) \tag{14}$$

It's important to say that generally the speed that appears in the conservation of mass law is the sum of two components: the "average" and the "fluctuating" components. The equation (14) is particularly efficient because in its form only the "u" part of the velocity (the "average") appears, that is the one resolvable using measurements or meteorological models.

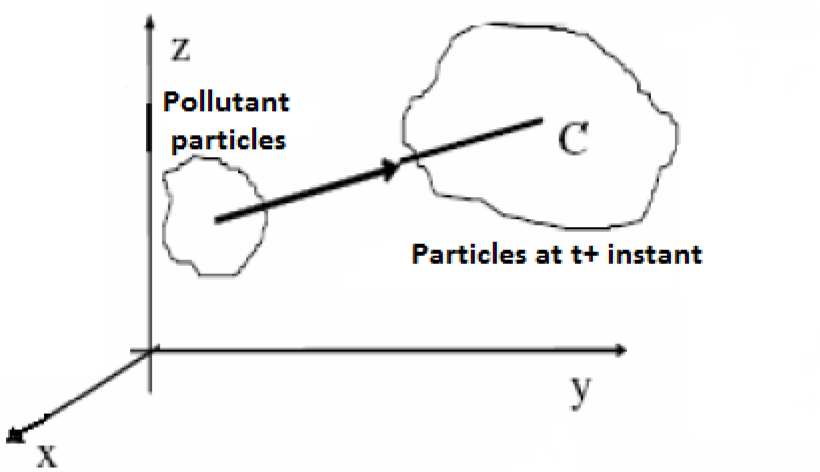

Figure 73

7.2 Lagrangian models

In the Lagrangian models the fluid is considered as a continuous means and the particles as material points that follow the fluid motion. The concentration of a generic matter that belongs to a portion of atmospheric fluid of volume V may be assessed with the sum of all the particles contained in the same volume. As is not possible to determine with exact precision the position of the particles, this is made thanks a probabilistic description of the trajectories.

The major shortcoming of this technique is the forced assumption of a constant wind speed and direction throughout the PBL (while wind shear plays an important role). Another problem of Lagrangian box models is the difficulty in comparing their outputs (i.e., time-varying concentrations along a trajectory) with fixed (Eulerian) air quality monitoring data (Zannetti, 1990).

An analytic method to solve the Langrangian model is the three-dimensional Langevin equation:

$$u'(t + \Delta t) = u'(t)R(\Delta t) + u''(t) \quad (14)$$

Where U_i is the turbulent velocity, R is the autocorrelation coefficient at time lag Δt and u'' is a random component.

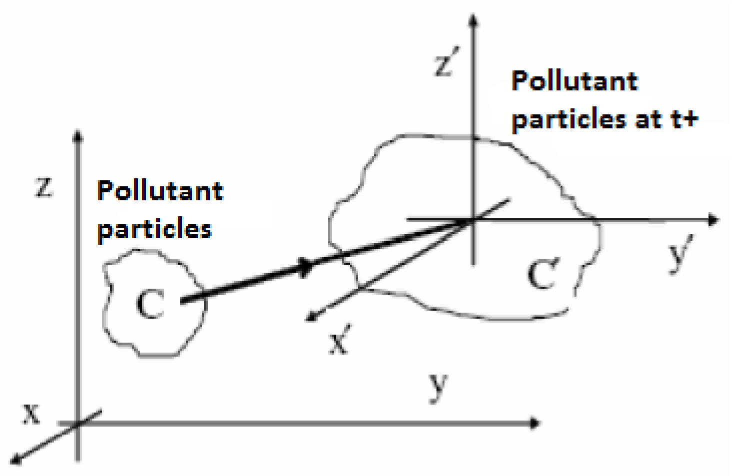

Figure 74

The most used Lagrangian photochemical model has been developed is the TRACE model (Tran, 1981). TRACE uses a two-dimensional wall of cells moving along a specified trajectory to simulate the transport of a plume parcel from a source to a receptor. The TRACE model solves numerically the following set of coupled, nonlinear, partial differential equations (conservation of mass)

$$\frac{\partial Ci}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial Ci}{\partial z}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial Ci}{\partial y}\right) + R_i + S_i + D_i \qquad (14)$$

Where Ci is the concentration of the i-th species; K_y and K_z are the eddy diffusion coefficients in the crosswind and vertical direction, respectively; R_i is the rate of chemical transformation of the i-th species; S_i is the rate of emission of the i-th species along the trajectory; and D_i is the rate of the deposition of the i-th species.

7.3 Gaussian models

At present, Gaussian plume model is the most widely used model for point source emission predictions. It describes the dispersion around a single source in an open and homogeneous terrain under steady-state conditions.

Gaussian plume model uses a realistic description of dispersion, where it represents an analytical solution to the diffusion equation for idealized circumstances. The model indeed assumes that the atmospheric turbulence is both stationary and homogeneous. In reality these conditions result satisfied only in rural condition and so a very high number of developed Gaussian Plume model were thought (Abdel-Rahman, 2008).

The Gaussian dispersion equation can be written as:

$$C(x,y,z) = \frac{Q}{2\pi\pi_y\sigma_z u}\exp\left(-\frac{{y_r}^2}{2\sigma_y^2}\right) * \exp\left(-\frac{(h_e - z_r)^2}{2\sigma_z^2}\right) \qquad (15)$$

where C is the concentration, Q is the emission rate of the pollutant from the source, u is the wind speed which defines the direction x. y is the horizontal distance perpendicular to the wind direction, z is the vertical direction, h_e is the effective height of the plume (considering the additional height Δh to which the hot gases rise above the physical height of the source h); i.e., H = h + Δh, and σy & σz are the parameters of the normal distributions in y and z directions, usually called the dispersion coefficients in y and z directions respectively. A definition sketch of the plume dispersion is shown in figure.

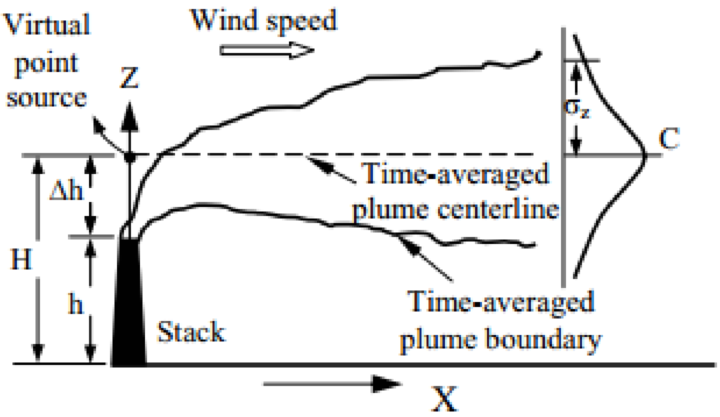

Figure 75

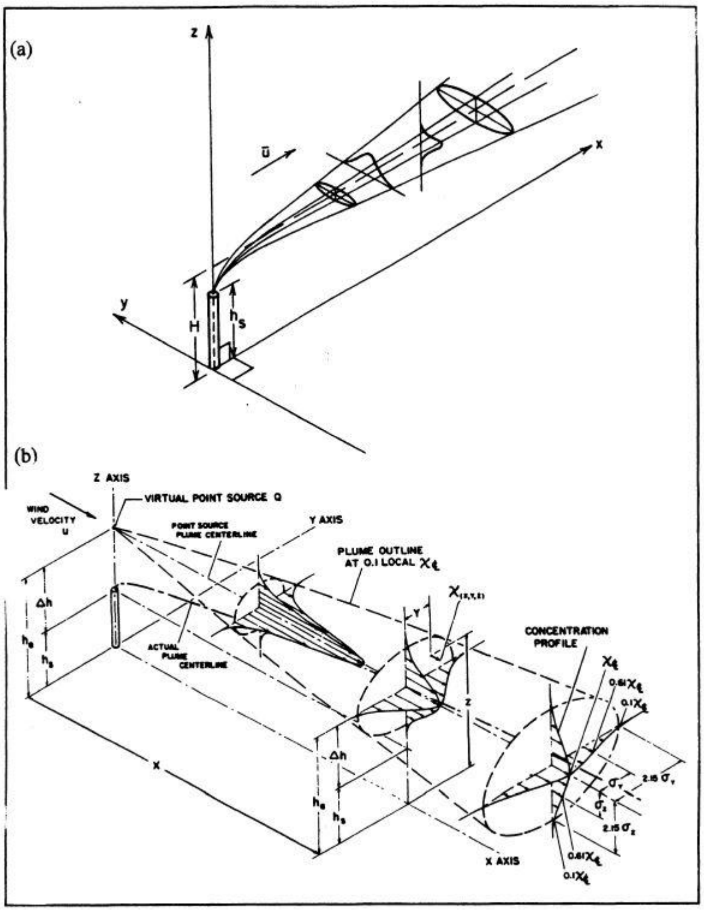

Figure 76

The problems of the gaussian models are the physical meaning of some of the parameters that implies strong long term approximations and the fact that concentrations are computed as spatial averages in three-dimensional cells (this means that relating the diffusion coefficients K to standard atmospheric measurements is difficult).

To overcome these limitations, the segmented plume approach and the puff approach were defined. Both methods break up the plume into a series of independent elements that evolve in time as a function of temporally and spatially varying meteorological conditions.

7.3.1 Segmented plume model

The guassian dispersion equation is not valid anymore when the situation become non-stationary and/or non-homogeneous. To treat that problem, the segmented Gaussian plume models have been developed.

In the segmented plume approach, the plume is broken up into independent elements (plume segments or sections) whose initial features and time dynamics are a function of time-varying emission conditions and the local time-varying meteorological conditions encountered by the plume elements along their motion (Zannetti, 1990).

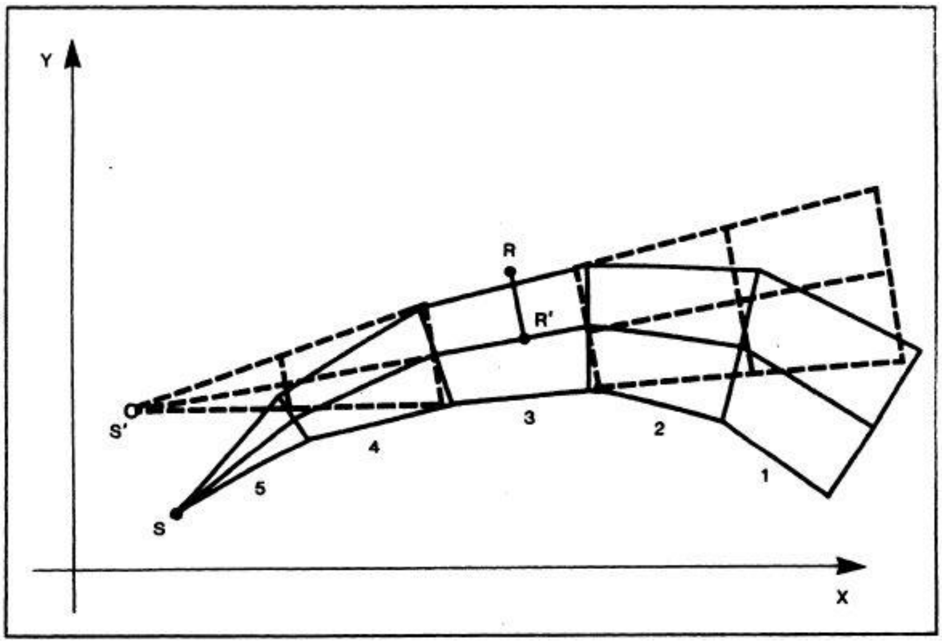

Figure 77

7.3.2 Puff models

Puff models have been developed to treat nonstationary emissions in nonhomogeneous dispersion conditions as well. Moreover, puff models have the additional feature of being able to simulate calm conditions.

The Gaussian puff model assumes that each pollutant emission of duration Δt injects into the atmosphere a mass $\Delta M = Q*\Delta t$, where Q is the time-varying emission rate. The center of the puff containing the mass ΔM is advected according to the local time varying wind vector. If, a time t, the center of a puff is located at $p(t)=(x_p, y_p, z_p)$, then the concentration due to that puff at the receptor $r=(x_r, y_r, z_r)$ can be computed using the basic Gaussian puff formula

$$C(x,y,z) = \frac{Q}{2\pi\pi_y\sigma_z u}\exp\left(-\frac{(xp-xr)^2}{2\sigma_y^2}\right) \quad (16)$$

$$* \left\{\exp\left(-\frac{(yp-yr)^2}{2\sigma_z^2}\right) * \exp(-\frac{(zp-zr)^2}{2\sigma_z^2})\right\}$$

It's important to say that integrating the previous equation, the general Gaussian plume formula is obtained.

Zannetti has proposed a mixed methodology that combines the advantages of both the segment and puff approaches for realistic and cost-effective simulation of short-term plume dispersion phenomena using the Gaussian formula.

7.4 Empirical models

Furthermore, there is a class of models called *empirical* that were developed on the basis of experimental observations of the main variables that affect the dispersion phenomena. The mathematical formula usually requests a careful calibration with statistical procedures. The evident limit of such models is that they can be used only in the context in which were thought or at most in the contexts that are not very different from that.

One of the most used is the *Canyon model*. The Canyon model is an empirical model that allow the user to determine the pollutant level in an urban canyon. The literature has proved that the pollutant concentrations in a canyon depend on

- the geometric characteristics of the canyon that are principally described by the height of the buildings (H) and the width of the canyon
- the atmospheric conditions represented by the mean speed of the wind at the ground level and at buildings' roofs.

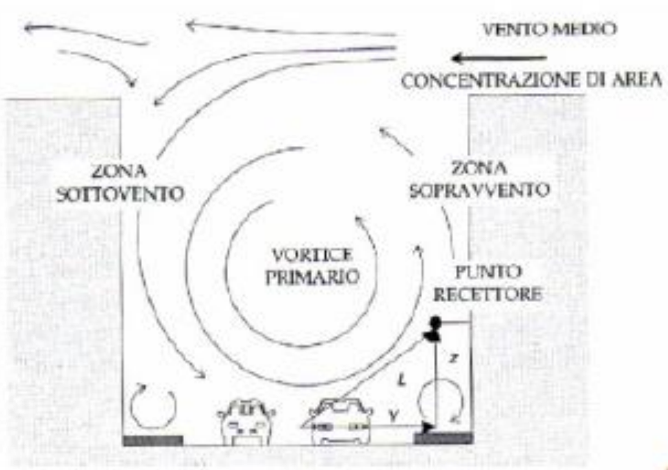

Figure 78

8 Conclusions

The aim of the thesis work was to evaluate the effectiveness of the average-speed emission models used with macroscopic simulation in opposition to the same model type applied to mesoscopic simulation. As it was previously written, currently macroscopic simulation is the more used, and what the work wants to assess is if the macroscopic models, in spite all the simplifications that their use implies (respect to the mesoscopic), are able to reproduce with reliability and accuracy the pollution levels over a road on a network.

The main problem linked to mesoscopic simulation is the high memory consumption required. In fact, the need to obtained a more detailed level to understand particular parts of the traffic system under study, has led to develop more complex algorithms that can describe the actions and reactions of the vehicles in a traffic state in a way that is as close as possible to the reality and, as a consequence of the fact, a more complex software architecture. This entailed a problem for the study case even before starting: it has been required a reduction of the network (from 50424 links to 2290*)* and in spite of that, a 32 GB ram computer was needed to run the simulation.

By analysing the results obtained in the simulations it is clearly visible from the plots (Figure 60 - link 924401745 to Figure 63 - link 807434336) that in the case of the CO_2 and CO analysis, there was a very good correlation among the pollutants emissions collected by COPERT (and so by doing a macroscopic simulation) and by MOVES (mesoscopic simulation). As it was said carbon dioxide is the element that has become increasingly important (for the public opinion as for by the environmental agencies), and this results in the equations used by COPERT that prove reliable values close to those given by the mesoscopic simulation (and that, for this reason, are supposed to be very close to the real situation). The correlation between carbon monoxide forecasted emission were not as good as what was seen in the case of carbon dioxide. But going more in depth in the literature review was found the carbon monoxide predicted by MOVES is a really sensitive value, and a little variation in speed or acceleration could led to an higher variation in the final estimated pollutant mass (and so results were perfectly coherent with what we could expect).

Instead, NOx and HC emissions outcome immediately different COPERT ones from MOVES ones (e.g. Figure 66 - link 924401745) even if the hydrocarbons to a lesser extent. Hydrocarbons emissions are very low compared to nitrogen oxides ones (their percentage ratio goes from 300% to 600%) and so, even if the emission calculated by COPERT could be the triple of those calculated by MOVES, actually their difference has never been greater than 1.5 grams.

The above considerations are represented in the following charts, where the ratio of the averages per hour of each pollutant have drawn on.

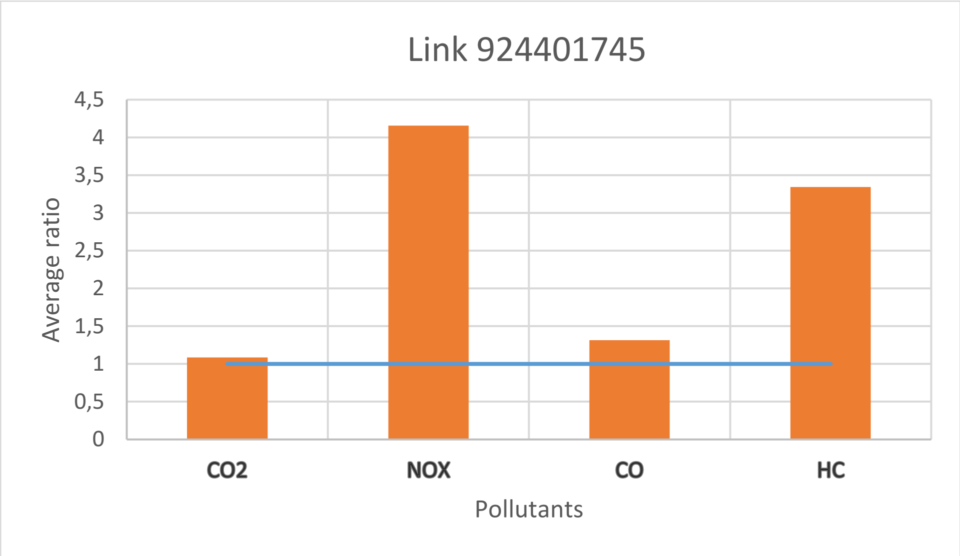

Figure 79

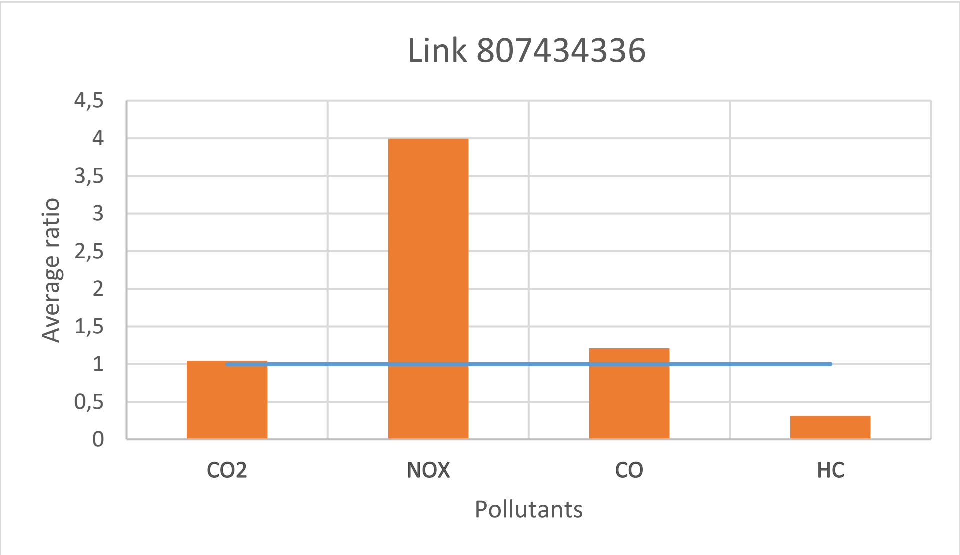

Figure 80

A different conclusion has been reached reading results obtained in a congested situation. After creating a bottleneck indeed, the macroscopic simulation results outcome different from the mesoscopic ones and consequently pollutants emissions are expected to be different.

While in macroscopic simulation there is immediately a segment of the link in hypercritical condition, in mesoscopic simulation there is no spillback in the first 20 minutes (because DTALite is able to represent vehicles that travel closer each other) and that means the emissions are similar to those viewed in the case of free flow. But after the time stated a spillback forms and the emissions go up (due to stop and go phenomena).

So, in the case of spillback, emissions calculated through macroscopic simulation could be underestimated and so, if it has been requested a well-founded estimate for a link or for a zone it’s better to use the mesoscopic simulation even at the cost of losing the speed and all the advantages of the macroscopic simulation.

9 Appended tables

ID	FromNode	ToNOde	co2	Nox	HC	Fuel Cons
1	10	11	2490395	3934.593	504.6831	592664.4
1	11	10	0	0	0	0
2	11	20	1192389	1883.863	241.6397	283764.7
2	20	11	0	0	0	0
3	20	21	1192389	1883.863	241.6397	283764.7
3	21	20	0	0	0	0
4	20	40	0	0	0	0
4	40	20	0	0	0	0
5	21	30	2419094	10197.76	553.5919	328472.6
5	30	21	0	0	0	0
6	30	31	2419094	10197.76	553.5919	328472.6
6	31	30	0	0	0	0
7	31	40	2419094	10197.76	553.5919	328472.6
7	40	31	0	0	0	0
8	11	41	4153622	6562.335	841.7389	988479.1
8	41	11	0	0	0	0
9	40	41	0	0	0	0
9	41	40	1298007	2050.73	263.0434	308899.7
10	10	12	2453411	16627.8	623.9044	89415.74
10	12	10	0	0	0	0
11	12	21	1226706	8313.902	311.9522	44707.87
11	21	12	0	0	0	0

F. table 2

timestamp_in_min	CO2_per_mile	NOX_per_mile	CO_per_mile	HC_per_mile
330	16.59572	0.533512	0.28788	0.5599
331	12.61068	0.704401	0.426709	0.593275
332	11.267717	0.789271	0.466691	0.517506
333	14.425414	0.614987	0.342028	0.510597
334	14.237359	0.622994	0.377978	0.642483
335	14.285443	0.620928	0.37263	0.644024
336	14.276219	0.621337	0.374585	0.615815
337	11.759068	0.755838	0.479946	0.630331

338	12.552289	0.707644	0.432619	0.593224
339	11.259614	0.789842	0.472236	0.517499
340	11.23259	0.791698	0.499995	0.597292
341	21.381712	0.413057	0.210652	0.562185
342	12.521228	0.709394	0.441583	0.620032
343	11.209817	0.793252	0.494163	0.597221
344	11.559722	0.768459	0.46729	0.619726
345	12.709808	0.699009	0.394716	0.488325
346	16.419502	0.539173	0.318309	0.691522
347	19.541134	0.451957	0.228135	0.607782
348	11.183569	0.795109	0.505778	0.597206
349	11.240147	0.791161	0.486673	0.543967
350	10.189366	0.8736	0.509973	0.468319
351	11.23702	0.791397	0.481354	0.544047
352	17.095179	0.517647	0.296257	0.643918
353	11.196411	0.794221	0.505587	0.597272
354	19.747492	0.447238	0.218857	0.582561
355	12.658857	0.701769	0.378475	0.486692
356	15.400366	0.575968	0.318403	0.519036
357	9.280225	0.959865	0.603285	0.499064
358	11.287452	0.787884	0.482462	0.517425
359	10.380984	0.85674	0.499935	0.508049
360	16.411552	0.53942	0.323864	0.693011
361	14.358067	0.617826	0.364726	0.5892
362	12.544913	0.708061	0.438358	0.593241
363	12.582518	0.705986	0.412542	0.566572
364	11.281201	0.788338	0.462419	0.490733
365	12.575928	0.706363	0.438466	0.593324
366	14.229988	0.623304	0.387403	0.66928
367	11.800487	0.753214	0.462613	0.581276
368	11.20025	0.793951	0.49621	0.570609
369	11.142118	0.798029	0.530178	0.650516
370	11.199537	0.793977	0.499969	0.597216
371	15.309846	0.579321	0.35672	0.642031
372	19.575365	0.451163	0.238195	0.634285
373	10.145348	0.877279	0.557747	0.57474
374	11.512877	0.771532	0.463836	0.677787
375	12.560412	0.707199	0.436158	0.621333
376	19.511251	0.452592	0.250807	0.687428
377	19.642197	0.449615	0.233633	0.607803
378	12.660062	0.701708	0.396983	0.540198
379	12.271469	0.724765	0.417904	0.428718
380	9.0829	0.980298	0.598175	0.531472

381	14.101942	0.628908	0.430401	0.775578
382	12.620127	0.703895	0.418815	0.539865
383	11.213477	0.793005	0.48642	0.545403
384	15.418906	0.575257	0.357583	0.617546
385	10.899905	0.815448	0.515616	0.656514
386	10.982771	0.810422	0.501499	0.505885
387	11.200153	0.793938	0.49073	0.570595
388	19.292709	0.4577	0.275047	0.740602
389	11.552403	0.768938	0.467569	0.618071
390	12.203824	0.727909	0.441895	0.607751
391	12.474413	0.711676	0.417569	0.65126
392	11.65694	0.761295	0.439786	0.690942
393	10.45483	0.85035	0.524191	0.653532
394	10.763046	0.825281	0.484246	0.65527
395	11.119108	0.798104	0.453454	0.691398
396	8.712299	1.021528	0.648547	0.588885
397	11.51173	0.76996	0.432021	0.721752
398	12.491226	0.709285	0.422924	0.749807
399	10.406256	0.85287	0.515092	0.70796
400	10.13448	0.875528	0.49568	0.630194
401	9.013058	0.986224	0.605983	0.647871
402	7.800108	1.140139	0.736414	0.640695
403	11.553499	0.76688	0.398607	0.624024
404	9.757805	0.908796	0.499964	0.64717
405	8.905243	0.997232	0.605602	0.631045
406	10.34733	0.85704	0.490781	0.615581
407	7.297696	1.218676	0.755273	0.570042
408	10.184292	0.870508	0.473587	0.597474
409	9.401452	0.943105	0.531971	0.670731
410	8.107873	1.095046	0.646246	0.585227
411	7.201623	1.235018	0.806301	0.565551
412	8.029144	1.105384	0.64891	0.617162
413	6.69639	1.328877	0.863854	0.498718
414	6.345395	1.402425	0.932113	0.545256
415	8.497098	1.043213	0.584209	0.622619
416	9.635674	0.919092	0.491104	0.591443
417	8.366767	1.059535	0.583081	0.512806
418	8.254176	1.075042	0.629127	0.526154
419	9.197344	0.962107	0.486642	0.599909
420	7.442479	1.192888	0.708383	0.535955
421	7.712152	1.15122	0.691464	0.534698
422	6.216866	1.430152	0.921542	0.549803
423	8.258945	1.073999	0.619394	0.520125

424	6.904399	1.286701	0.783589	0.553841
425	8.486485	1.043421	0.535968	0.597216
426	7.475392	1.187623	0.7118	0.551752
427	5.929879	1.499607	0.960771	0.602472
428	7.449301	1.19186	0.696076	0.521985
429	7.447734	1.191127	0.684441	0.633128
430	6.868532	1.291861	0.777451	0.697161
431	5.643132	1.577333	1.07891	0.568758
432	6.168875	1.440304	0.897375	0.640103
433	7.598104	1.167354	0.67762	0.617996
434	6.639787	1.337088	0.802249	0.602258
435	6.23891	1.424609	0.881739	0.55218
436	8.513753	1.040255	0.542211	0.584448
437	6.320005	1.404905	0.85007	0.660579
438	7.535102	1.176646	0.65797	0.653828
439	6.774673	1.310304	0.765069	0.59727
440	5.64111	1.575649	0.996412	0.694465
441	5.97336	1.488475	0.97203	0.648556
442	5.775689	1.538724	0.952036	0.645189
443	6.191293	1.435167	0.917444	0.629088
444	7.332024	1.20869	0.672039	0.682266
445	6.421212	1.381751	0.776463	0.683522
446	6.924782	1.281412	0.724302	0.637931
447	7.006625	1.264235	0.690761	0.79503
448	5.813265	1.529456	0.97475	0.597816
449	6.435039	1.378084	0.79431	0.753881
450	0	0	0	0

F. table 3

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