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Urban Structure and Air Quality

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1. Introduction

It is an unquestionable fact that much has been done in the last decades to improve the quality of the air we breathe and live in. Policies, technology and increasing public awareness have taken us to an unprecedented level of protection. On the other hand, it is also a fact that not only our cities but also our countryside continue to show worrying and troubling signs of environmental stress, of which air pollution is one of many.

In 1900, 14% of the world's population lived in cities; fifty years later, the proportion had risen to 30%, and by 2003 to 48%; today half the world's population lives in cities and predictions are that by 2030, 60% of the population will be urban [1]. In Europe, approximately 75% of the population lives in urban areas [2]. The last two centuries have seen a transformation of cities from being relatively contained, to becoming widespread over kilometres of semi-suburban/semi-rural land with commercial areas, office parks and housing developments. People often live miles from where they work, shop or go for leisure activities. This type of urban development has been named urban sprawl, and has its origins from the rapid low-density outward expansion of the United States of America cities in the beginning of the 20th century [3]. In Europe, cities have traditionally been much more compact; however urban sprawl is now also a European phenomenon [4].

Next the scientific and policy background on the subject of this chapter is presented. Urban planning aspects related to urban structure are briefly addressed, and the issue of urban air pollution is introduced, as well as the main air pollution problems that European cities are facing. The most important research studies covering the relation between urban planning and air pollution during the last decades are then reviewed.

1.1. Urban planning

When the first cities emerged, they were created having defence in mind, resulting in compact forms of settlement. With the advent of industrialization first and transport

systems later, urban structures have changed dramatically, with an unprecedented process of urbanization that has persisted so far.

1.1.1. Urban planning perspectives

People have imagined ideal cities since ever; urban planners in particular have directed their attention to the types of urban structure that can provide a greater quality of life and environmental protection. In the 20th century, various architects have proposed radical changes in the form of the city [5]. Le Corbusier's 'Radiant City' and Frank Lloyd Wright's 'Broadacre City' represent two extremes in a broad spectrum between urban density and dispersal. Le Corbusier (1887-1965) proposed high-density urban areas, where different land uses would be located in separate districts, with distinct functions - residential, commercial areas, churches - forming a geometric pattern with a sophisticated transit system. In opposition, Frank Lloyd Wright (1867-1959) defended the need for a closer contact with nature, and defended decentralized low-density cities, composed of single-family homes on large pieces of land, small farms, light industry, recreation areas, and other urban facilities where travel needs would be almost entirely dependent on the automobile [5].

Twenty years after the mid 1970's oil crisis which incited the first search for urban forms that conserved resources, the idea of sustainability has re-emerged, due to the growing awareness of urban problems related with resources depletion, energy consumption, pollution and waste [6]. The role of urban planning in urban sustainability, namely which urban structure will provide higher environmental protection, is today still under discussion. The scope of the debate can be summarized by classifying positions in two groups: the "decentralists", in favour of urban decentralization, defending the dispersed city characterized by low population densities and large area requirements; and the "centralists", who believe in the virtues of high density cities with low area requirements, defending the compact city. Defenders of dispersal and low density development claim that low densities can be sustainable and that the quality of life within them is much higher in comparison with contained high density developments. The argument against the dispersed city is that low densities, and the consequent large area needs and land use segregation, result in a high dependence from motorized vehicles. Several authors however have associated sprawling urban development patterns with increased vehicle travel and congestion [7], increased volumes of storm-water runoff [8], loss of agricultural lands [9], and, even, increased rates of obesity in children and adult populations [10].

The compact city is characterized by high density and mixed use development, where growth is encouraged within the boundaries of existing urban areas. Those in its favour defend that urban containment will reduce the need for motorized trips, therefore reducing traffic emissions, and promoting public transport, walking and cycling [11]. It is also claimed that higher densities will help to make the supply of infrastructures and leisure services economically feasible, also increasing social sustainability [12]. Other such as [13] however, claim that the environmental benefits resulting from urban compaction are doubtful and that higher urban densities are unlikely to deliver the high quality of life that centralists promise. Although some reduction in energy consumption might be expected from

compaction, they argue that a large centralised city can often result in greater traffic congestion with fuel efficiency greatly reduced. Another important aspect mentioned is that even if vehicle emissions are reduced, they may be concentrated in the precise areas where they cause most damage and adversely affect most people [14].

1.1.2. Urban sprawl in Europe

Historically, urban dispersion rose from the struggle against the 19th century industrial cities, which were congested, polluted, and foci of crime and disease [15]. After that, the growth of cities has been driven by the growth of population; however, in Europe today there is little or no population growth, while sprawl shows no signs of slowing down. A variety of factors such as the negative environmental (pollution and noise) and social factors (poverty and insecurity) related to city cores, rising living standards, changing living preferences, and a new mobility paradigm are now driving sprawl [2, 16].

Since the mid-1950's, European cities have expanded on average by 78% whereas the population has grown by only 33%; also, more than 90% of the new residential areas are low density areas; inevitably European cities have become much less compact [4]. Figure 1 shows the European areas with higher urbanization rates, where urban land cover has been increasing between four to six times faster than the European average, and the population density in residential areas declining six times faster [17].

Figure 1. European areas with very rapid urbanization [17].

Clearly for these areas the term sprawl is well fitted. Regions of this type can be found along the Portuguese coastline, in Madrid and its surroundings as well as in some coastal regions in Spain, in the north of the Netherlands, north-western Ireland, Italy and Greece. Sprawl is particularly evident in countries or regions that have benefited from EU regional policies, such as Portugal, Ireland, and Spain.

1.2. Urban air quality

Problems regarding air pollution in urban areas have been known for millennia, but the attitude towards them was ambiguous, since they were even considered a symbol of growth

and prosperity, and the attempts to combat them were scattered and ineffective. It was only after the occurrence of a few major air pollution episodes in the 20th century (such as the Meuse Valley (Belgium) accident in December 1930 and the London December 1952 smog episode) that a greater awareness and the consequent development of air pollution policies took place.

1.2.1. Main atmospheric pollutants and sources

Atmospheric pollutants (gaseous and particulate) can be divided in primary pollutants, which are directly emitted to the atmosphere by a natural or anthropogenic emission source, and secondary pollutants, which result from primary pollutants transformation through chemical reactions highly dependent on meteorological conditions and/or solar radiation [18]. Currently, the two air pollutants of most concern for public health are surface particulate matter and tropospheric ozone, therefore receiving special attention in this review and also throughout this chapter.

There is increasing evidence that fine dust particles have deleterious effects on human health, causing premature deaths and reducing quality of life by aggravating respiratory conditions such as asthma [19]. One reason why particulate matter (PM) is of such concern is the absence of any concentration threshold below which there are no health effects. Evidence suggests that fine particulates, with an equivalent aerodynamic diameter less than 2.5 micrometres (PM_{2.5}), do most damage to human health, and that effects depend further on the chemical composition or physical characteristics of the particle [20]. Particulate matter (PM) includes as principal components sulphate, nitrate, organic carbon, elemental carbon, soil dust, and sea salt. The first four components are mostly present as fine particles, and these are of most concern for human health. Sulphate, nitrate, and organic carbon are produced within the atmosphere by oxidation of sulphur dioxide (SO₂), nitrogen oxides (NO_x) and non-methane volatile organic compounds (NMVOC); carbon particles are also emitted directly by combustion. The seasonal variation of PM is complex and location-dependent; in general, PM needs to be viewed as an air quality problem year-round [21].

While ozone (O₃) in the upper atmosphere provides an essential screen against harmful UV radiation, at ground level it is lung irritant causing many of the same health effects as particulate matter, as well as attacking vegetation, forests and buildings. Observed effects on human health are inflammation and morphological, biochemical, and functional changes in the respiratory tract, as well as decreases in host defence functions. Effects on vegetation include visible leaf injury, growth and yield reductions, and altered sensitivity to biotic and abiotic stresses [22]. Ozone is produced in the troposphere by photochemical oxidation of carbon monoxide (CO), methane (CH₄), and NMVOC by the hydroxyl radical (OH) in the presence of reactive nitrogen oxides. The relation between O₃, NO_x and VOC is driven by complex nonlinear photochemistry, with the existence of two regimes with different O₃-NO_x-VOC sensitivity: in the NO_x-sensitive regime (with relatively low NO_x and high VOC), O₃ increases with increasing NO_x and changes little in response to increasing VOC; in the NO_x-saturated or VOC-sensitive regime O₃ decreases with increasing NO_x and increases with increasing VOC [23]. Also, in the vicinity of large nitrogen monoxide (NO) emissions,

ozone is destroyed according to the reaction $\text{NO} + \text{O}_3 = \text{NO}_2 + \text{O}_2$, generally referred as O_3 titration by NO. This situation usually takes place in heavily polluted areas, with ozone consumption taking place immediately downwind of the sources, and becoming elevated as the plume moves further downwind [24]. Ozone pollution is in general mostly a summer problem because of its photochemical nature [23].

1.2.2. Emissions and air quality trends in Europe

Emissions of air pollutants decreased substantially during the period 1990–2009 across Europe (Figure 2). PM emissions fell by 27 % for PM₁₀ and 34 % for PM_{2.5}. Emissions of the precursor gases SO_x and NO_x declined by 80 % and 44 % respectively. Emissions of ammonia (NH_3), have fallen less: only about 14 % between 1990 and 2009. It is estimated that current European policies reduced NO_x emissions from road vehicles by 55 % and from industrial plants by 68 % in the period 1990–2005 [25].

Notwithstanding the emissions decrease in Europe, the analysis of PM₁₀ concentrations since 1999 for a total of 459 European air quality monitoring stations reveals that 83 % of the stations presents a small negative trend of less than $1 \mu\text{g.m}^{-3}$ per year [25]. For ozone there is a discrepancy between the substantial cuts in ozone precursor gas emissions and the stagnation in observed annual average ozone concentrations in Europe [26]. Reasons include increasing inter-continental transport of O_3 and its precursors in the northern hemisphere, climate change/variability, biogenic NMVOC emissions, and fire plumes from forest and other biomass fires [26].

Figure 2. EU emissions of PM and ozone precursor gases 1990-2009 [25].

The target value threshold for ozone of $120 \mu\text{g.m}^{-3}$ (daily maximum of running 8-hour mean values) was exceeded on more than 25 days per year at a large number of stations across Europe in 2009 (Figure 3a). The map shows the proximity of recorded ozone concentrations to the target value. At sites marked with dark orange dots, the 26th highest daily ozone concentration exceeded the $120 \mu\text{g.m}^{-3}$ threshold, implying an exceedance of the threshold and the number of allowed exceedances by the target value [25]. The EU limit and target values for PM were exceeded widely in Europe in 2009, as evidenced in Figure 3b. The annual limit

value for PM₁₀ was exceeded most often (dark orange dots) in Poland, Italy, Slovakia, several Balkan states and Turkey. The daily limit value was exceeded (light orange dots) in other cities in those countries, as well as in many other countries in central and western Europe.

Figure 3. a) Twenty-sixth highest daily maximum 8-hour average ozone concentration; b) Annual mean concentration of PM₁₀ recorded at each monitoring station in 2009 [25].

Across Europe, the population exposure to air pollution exceeds the standards set by the EU (Figure 4). For ozone there has been considerable variation along the period 1997-2009, with 14% to 61% of the urban population exposed to concentrations above the target value. In 2003, a year with extremely high ozone concentrations due to specific meteorological conditions, the exposure was higher. Regarding PM₁₀, in the period 1997-2009, 18 to 50% of the urban population was potentially exposed to ambient air concentrations higher than the EU limit value set for the protection of human health [25].

Figure 4. Percentage of the EU urban population potentially exposed to air pollution exceeding acceptable EU air quality standards [25].

1.3. Integrating urban planning and air quality

Since the world's cities are the major consumers of natural resources, the major producers of pollution and waste, and the focus of most other human activities, various governments

realised that much of the sustainable debate has an urban focus. Solving the problems of the city would be a major contribution to solving the most pressing global environmental problems, since it is in cities that we find the greatest concentration of population and economic activity, and it is in cities that the crucial long term and often irreversible decisions on infra-structure investments (related to energy supply and waste treatment) are made. After the Brundtland Commission report [27] the notion that the natural environment should become a political priority, and the pursuit of sustainable development received a remarkable attention. In many countries there have been profound changes in policies and in political and popular attitudes, as the commitment to the sustainable development idea has increased. The question now is which urban form or structure will be likely to deliver more environmental benefits or will be less harmful to the human health and the environment. The most important work conducted in the field in the last two decades is reviewed next.

1.3.1. Data analysis studies

Much of the technical arguments for compact cities have revolved around the allegedly lower levels of travel, and hence lower levels of fuel consumption and emissions, associated with high urban densities. [28, 29] have related fuel consumption per capita to population density for a large number of cities around the world, and found a consistent pattern with higher densities associated with lower fuel consumption. [30] compared a group of world cities over the period 1980 to 1990 regarding its land use and transport characteristics. The study demonstrated the importance of urban density in explaining annual per capita auto use, with annual kilometres travelled per capita strongly inversely correlated with urban density. Similar conclusions emerged from [11], which found a clear inverse correlation between total distances travelled per week and population density. People living at the lowest densities were found to travel twice as far by car each week in comparison to those living at the highest densities.

The studies by [28, 29] have been criticised for focusing on the single variable of density, when other factors are likely to be important in explaining travel behaviour. [31] argues that household income and fuel price are important determinants of such behaviour, making it difficult to clearly identify the link between density and fuel consumption.

While several additional studies [32-35] have related travel behaviour, traffic, energy consumption and emissions with land use patterns, only few were found relating land use with air quality, i.e., with atmospheric pollutant concentrations. [36] examined the relationship between the degree of sprawl and ozone levels for 52 metropolitan areas in the United States. While there was evidence regarding the association between lower population densities and higher vehicle miles of travel, only moderate evidence was found relating sprawl and increased ozone levels. [37] analysed the impact of changes in land area and population on per capita exposure to motor vehicle emissions, concluding that infill development has the potential to reduce motor vehicle emissions yet increasing per capita inhalation of those emissions, while sprawl has the potential to increase vehicle emissions

but reduce their inhalation. [38] explored the implications of sprawl for air quality through the integration of data on land use attributes and air quality trends recorded in 45 of the 50 largest US metropolitan regions. The results of this study indicate that urban form is significantly associated with both ozone precursor emissions and ozone exceedances. Overall, the most sprawling cities experienced over 60% more high ozone days than the most compact cities.

Most of the above work relied on empirical studies to provide descriptive comparisons of current cities and to find evidence that certain types of urban forms are correlated with desirable levels of energy consumption and emissions. These approaches integrate the land use and transport aspects of urban form, but lack the extra step that translates energy efficiency into indicators of air quality, via pollutant concentrations.

1.3.2. Numerical modeling studies

As just mentioned, several empirical and modelling studies integrate land use and transport issues and its relation with urban structure, however, few were found that explore the connection to air quality and human exposure. Conclusions from most of the studies done so far have been harmed by the lack of knowledge about the complex path between an initial action for the reduction of atmospheric emissions and the final benefit in terms of air quality and human exposure [39]. Health effects of air pollution are the result of a chain of events, going from the release of pollutants leading to an ambient atmospheric concentration, over the personal exposure, uptake, and resulting internal dose to the subsequent health effect. It is important to make a distinction between concentration and exposure; concentration is a physical characteristic of the environment at a certain place and time, whereas exposure describes the interaction between the environment and a living subject, referring to an individual's contact with a pollutant concentration.

Emissions reduction conducts to changes in atmospheric pollutant concentrations, but those changes will have different spatial and temporal magnitudes and signs, due to differences in emissions, weather patterns and population exposed to pollution according to the time of the day, day of the week or month of the year, and also according to the population age structure (children, adults and elderly suffer different effects due to their different respiratory frequencies). Exposure is the key factor in assessing the risk of adverse health effects, since high pollutant concentrations do not harm people if they are not present, while even low levels may become relevant when people are present [19].

Recent advances in computer technology have allowed the integration of land-use and traffic models with air quality models; these modelling tools assume a particular importance to the subject under study, since they allow the integration of the most important variables that have to be analysed. One of the earliest investigations in this field was carried out for Melbourne in [39]. The authors developed a framework for linking urban form and air quality, integrating land use, transport and air quality models, and the results of the study shown that any of the several strategies designed to deliberately channel and concentrate additional population and industry into specific zones, when supported by simultaneous

investments in transport infrastructure, will deliver environmental and efficiency benefits that consistently outperform those associated with the “business-as-usual” approach.

Through the application of dispersion and photochemical models, [40] concluded that compact cities with mixed land uses promote a better air quality when compared with dispersed cities with land use segregation. A subsequent study, conducted by the same team [41], investigated the influence of urban structure on human health, estimating the human exposure to atmospheric pollutants. Results reveal that the compact city presents more people exposed to higher pollution levels due to the existent high population densities. [42] investigated the potential effects of extensive changes in urban land cover, in the New York City (NYC) metropolitan region, on surface meteorology and ozone concentrations. Results from the study suggest that extensive urban growth in the NYC metropolitan area has the potential to increase afternoon temperatures by more than 0.6°C leading to increases in episode-average ozone levels by about 1–5 ppb, and episode-maximum 8 h ozone levels by more than 6 ppb. [43, 44] investigated the effects of urban sprawl on road traffic, air quality and population exposure for the German Ruhr area. The sprawl scenario produced a temperature increase of about half a degree over significant portions of the domain, including beyond the area where the land use changes were implemented. The combination of increased temperature and emissions yielded ozone concentration pattern changes, from -1.5 to $+4.5 \mu\text{g.m}^{-3}$.

2. Case study presentation

In the report “Urban sprawl in Europe” [2], Porto urban area is identified as one of the top ten European cities where sprawl is growing faster. In the last decades, the Porto area has experienced an accelerated process of land occupation, with the urban area increasing at much faster rates than the population. Also, according to the air quality reports for Portugal’s Northern region, the assessment of pollutant concentrations measured in the air quality monitoring network shows that Porto metropolitan region presents a poor air quality, with ozone thresholds and PM10 limit values exceeded [45]. It seems therefore that the Porto region is an interesting and challenging case to be studied in the framework of the topic urban structure and air quality.

The region selected for the analysis is showed in Figure 5 and includes 21 municipalities, with a total area of almost 240 000 hectares. The Porto municipality constitutes the study region’s centre around which a first metropolitan ring is formed by the municipalities of Matosinhos, Maia, Gondomar and Vila Nova de Gaia; the municipalities of P. Varzim, V.N. Famalicão, Lousada, Felgueiras, Penafiel, M. Canavezes, C. Paiva and S.J. Madeira can be considered part of a peripheral ring, while the remaining intermediate municipalities constitute a second metropolitan ring.

2.1. Patterns of urban growth and change

This section explores the path of the recent urban expansion in the Porto area. For that purpose the process of urban growth in this area is analysed in detail, with the use of two digital Corine Land over (CLC) maps – CLC90 and CLC2000.

Figure 5. Study region, including 21 municipalities.

The CORINE (COordination of INformation on the Environment) programme of the European Commission includes a land cover project – CLC - [46] intended to provide consistent localized geographical information on the land cover of the Member States of the European Community. CLC is a standardised land cover inventory derived from satellite imagery for 24 countries, with 250 m resolution. For Portugal, CLC 1990 (CLC90) was produced with satellite images from 1985 to 1987, depending on the region, while CLC2000 concerns the year 2000. The two datasets are here analysed for the study region, in order to produce a thorough characterization of the land use evolution in the period between 1987 and 2000. Figure 9 presents the study region land cover maps for 1987 and 2000, resulting from the processing of CLC90 and CLC2000 data, respectively. To obtain a clearer picture of the land cover, the 44 CLC classes were grouped in 5 large categories: 1) artificial surfaces; 2) agricultural areas; 3) forests and shrub areas; 4) other non-artificial surfaces (areas of little or no vegetation, and inland and coastland wetlands); 5) water bodies.

Figure 6. Study region land cover maps for 1987 and 2000.

The land cover maps reveal the expansion of artificial areas throughout the study region, mainly occupying land previously dedicated to agriculture, due to its proximity to the already existent urban areas. In order to have a clearer picture of the magnitude and nature of this growth, Table 1 presents the numbers behind the maps, including the total area for each of the four large land use categories and corresponding share (%) for each dataset, as well as the magnitude of the change between 1987 and 2000. Furthermore, artificial surfaces area is analysed with more detail by looking at its composition: continuous urban fabric; discontinuous urban fabric; industrial or commercial units; other artificial surfaces. From 1987 to 2000, built-up land uses increased 41.5%, around 13 000 new hectares have become artificial during this period, with urbanized land rising from 13% to 18% of the total area of the region. The analysis by municipality shows that the largest artificial surface increases are particularly observed outside the urban centre confirming the previous assertions about the existence of urban sprawl processes in the region. Municipalities in the first metropolitan ring around Porto reveal the largest absolute increases of artificial surfaces. Municipalities outside the first metropolitan ring, with very low shares of urbanised areas in 1987 presented the highest growth rates between 1987 and 2000. As expected, Porto municipality presents the highest percentage of artificial land uses, with 91.5% of the total area in 2000 (83% in 1987). As urbanization advanced, many non-urban hectares disappeared: agriculture land loss represents more than half of the entire non-urban losses (12820 ha); forest and shrub areas come next with 26%.

Land uses	CLC90 (1987 data)		CLC2000		Change	
	hectares	%	hectares	%	hectares	%
Artificial surfaces	30908.2	12.9	43727.9	18.3	+12819.7	+41.5
Continuous urban fabric	3369.0	10.9	4059.2	9.3	+690.2	+20.5
Discontinuous urban fabric	23583.0	76.3	32895.0	75.2	+9312.0	+39.5
Industrial or commercial units	2719.9	8.8	4973.1	11.4	+2253.2	+82.8
Other artificial surfaces	1236.3	4.0	1800.7	4.1	+564.3	+45.6
Agricultural areas	101350.1	42.3	93766.2	39.1	-7584.0	-7.5
Forests and shrub areas	101598.7	42.4	98319.4	41.0	-3270.3	-3.2
Other non-artificial surfaces	5750.4	2.4	3784.9	1.6	-1965.4	-34.2
TOTAL AREA	239598.4	100	239598.4	100	-	-

Table 1. Study region land cover data for 1987 and 2000.

A more detailed analysis of the new artificial uses between 1987 and 2000 reveals little changes in the urbanization trends. The discontinuous or low density urban fabric ranks first for both years, summing around 75% of the total artificial area. While in 1987 continuous urban fabric was the second land use category, with 11% of the total artificial area, in 2000 the industrial and commercial units took over the second place. This land use category showed the highest growth rate between 1987 and 2000 (83%), followed by other artificial surfaces (46%). The discontinuous urban fabric is the first in terms of area growth, representing 73% of the new artificial areas. The land use category compact or continuous urban fabric showed the lowest growth.

Evidence therefore suggests that Porto region is undergoing a process of urban sprawl; to further confirm it, it is important to look at the relation between the artificial areas growth and the population growth in the same period. Making use of the population data and of the residential area, obtained through the sum of continuous and discontinuous urban fabric, the residential density (number of residents per residential square kilometre) was calculated for 1987 and for 2000 (Figure 7), for a limited group of municipalities with available data for 1987 and 2000 simultaneously.

Figure 7. Residential density calculated for 1987 and 2000 for a group of municipalities in the study region.

A trend towards lower residential densities is observed, revealing that the population growth has lost importance as an explanatory factor of the urbanization process, while the generalization of dispersed urban patterns has risen. An important sprawl process in the region is the proliferation of new industrial and commercial areas. Extensive industrial areas and mega commercial structures punctuate the Porto region, with the traditional tendency of locating commercial uses within the urban fabric rapidly fading. There is no longer a real mixture of uses; instead, commercial activities are now segregated and concentrated in large portions of land orientated to commercial and leisure activities.

2.2. Mobility and attractiveness

In metropolitan areas, the need for daily-travel or commuting is a reality steaming from the progressive distancing between residential areas and work and study areas. Hence, in a study whose aim is to link urban structure with emissions and air quality, it is essential to look not only at the number of residents per municipality but also at the population flow between municipalities. It was therefore necessary to characterize the commuting characteristics of the region and the relative attractiveness/ repulsiveness of each municipality in the study area. For that purpose, a study from the National Statistics Institute [47] for the year 2001 was the main source of data. The study demonstrates the existence of important commuting movements in the Porto Metropolitan Area, through the analysis of the main interaction axis and the accounting of workers and student's flows between municipalities. Of great significance are the interactions between Porto, the centre of the region, and the municipalities of the first metropolitan ring; these interactions are strongly unbalanced in favour of Porto [47]. The mentioned study compiled the rates relating the number of individuals entering/ exiting a

given municipality with the number of individuals residing in the municipality. The described data was processed and attraction and repulsion rates re-calculated for the municipalities in the case study region. It was assumed that the study region acts as a tight zone, and the possible interactions between it and the surrounding areas are not considered. As an example, Figure 8 presents the data for Porto municipality, with a net attraction rate of 38.2%.

These attraction and repulsion rates are essential for the definition and construction of the urban development scenarios for the region since, in order to determine the total amount and distribution of atmospheric pollutant emissions in the study region, it is necessary to consider not only the number of inhabitants or residents per municipality but also the flow between municipalities.

Figure 8. Porto main entering and exiting movements and attraction and repulsion rates for 2001.

2.3. Air quality levels

Portugal's northern region, in accordance to the established in the Air Quality Framework Directive (96/62/EC), was classified [48] in two zones (Interior North and Coastal North) and four agglomerations (Coastal Porto, Braga, Vale do Ave and Vale do Sousa). Since 2005, the air quality monitoring network covers all the zones/agglomerations, with a total of 24 stations in 2006, the large majority of them (15) located in Coastal Porto due to the high number of inhabitants.

Figure 9 shows the air quality monitoring stations for which PM₁₀ daily legal requirements were not fulfilled [49]. High PM₁₀ concentrations are measured in urban and suburban monitoring stations; regarding the daily limit value the number of annual exceedances goes well beyond the allowed 35. As a result of these exceedances, and accordingly to the determined in the Air Quality Framework Directive, the Northern Region of Portugal is currently under the obligation of developing and implement Plans and Programs for the Improvement of the Air Quality [49].

Figure 9. Monitoring stations not fulfilling PM10 legal requirements for daily LV + MT in 2001-2006 in the study area (the red line indicates the allowed number of daily exceedances) (data from [49]).

The analysis of ozone measured data shows that concentration values are higher outside the urban centre of the region, i.e. outside Porto municipality. Nevertheless the ozone information threshold is exceeded in the majority of the monitoring stations, and often along a high number of hours per year. Concerning the seasonal occurrence of exceedances, ozone limit values are generally higher between April and September, while for PM10 high concentrations have been found both in summer and winter.

3. Setup of the urban air quality modelling system

This section describes the meteorological (MM5) and chemical (CAMx) numerical models, used in the atmospheric simulations for the Porto study region. Both models are freely available, and have been extensively used and validated worldwide, being subject of constant improvement and update. These facts, together with the good performance of the models obtained for different regions, including the present study region, justify their selection. Moreover, these models are ready to be applied in long-term simulations with acceptable computing times.

Figure 10. Simplified scheme of the MM5-CAMx modelling system.

Figure 10 presents a simplified scheme of the MM5-CAMx modelling system applied to the simulation of the atmospheric flow and air quality in the study region.

3.1. MM5 meteorological model

The PSU/NCAR mesoscale model was developed at the Pennsylvania State University and the National Centre for Atmospheric Research (NCAR). The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modelling system [50]. The MM5 modelling system software is freely provided and supported by NCAR, therefore it is widely used internationally [51, 42]. The MM5 is a three-dimensional non-hydrostatic prognostic model that simulates mesoscale atmospheric circulations. Important features in the MM5 modelling system include: (i) a multiple-nest capability; (ii) non-hydrostatic dynamics; (iii) a four-dimensional data assimilation capability; (iv) increased number of physics options; and (v) portability to a wide range of computer platforms [52]. The program numerically solves the pressure, mass, momentum, energy and water conservation equations; it presents different parameterization schemes for clouds, planetary boundary layer and diffusion, moisture, radiation, and surface. MM5's nesting capability allows the consideration of several domains in a single simulation or in consecutive simulations; therefore, the first domain can present a more regional dimension with a coarser mesh, while the next domain will cover a smaller area but with a higher resolution.

Since MM5 includes several parameterizations, users can choose among the multiple options of model physics and parameterization schemes; some are based on the scale of the motion, such as the cumulus parameterizations, while others are dependent on users preferences, such as the planetary boundary layer (PBL) schemes [53]. Based on previous MM5 applications for the West Coast of Portugal, namely by [54], the chosen MM5 physical options include: Grell cumulus scheme for the coarser resolution domain and no cumulus parameterization for the smaller grids, RRTM radiation scheme, Reisner-Graupel moisture scheme, MRF BPL scheme for the coarser resolution domain and Gayno-Seaman PBL scheme for the smaller grids. The used land surface model is the five-layer soil model. The initial and boundary conditions are from the National Centre for Environmental Predictions (NCEP) global 1-degree reanalysis data, updated every 6-hours [55].

The MM5 modelling system has two types of land use data with global coverage available from the United States Geological Survey (USGS): 13-category, with a resolution of 1 degree, 30 and 10 minutes; and 24-category, with a resolution of 1 degree, 30, 10, 5 and 2 minutes, and 30 seconds. The USGS 24-category data is referred to 1990, and some of the components are originated from a dataset compiled in the 1970s [52]. This data was compared with the data from Corine Land Cover 2000 [56], and it was possible to conclude that the land use in the study area is weakly represented in the USGS24 original dataset: in CLC2000, Porto and the surrounding municipalities are presented as a large urban area, while in USGS24 the urbanized area is much more restricted and concentrated over Porto. Therefore, the USGS24 default land use data was replaced by CLC2000 data in the present study.

3.2. CAMx air quality model

The Comprehensive Air quality Model with extensions (CAMx) was developed by ENVIRON International Cooperation, from California, United States of America. CAMx [57] is an Eulerian photochemical dispersion model that allows the integrated “one-atmosphere” assessment of gaseous and particulate air pollution over many scales ranging from sub-urban to continental. CAMx simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids. The Eulerian continuity equation describes the time dependency of the average species concentration within each grid cell volume as a sum of all of the physical and chemical processes operating on that volume [58]. The nested grid capability of CAMx allows cost-effective application to large regions in which regional transport occurs, yet at the same time providing fine resolution to address small-scale impacts in selected areas [58]. The CAMx chemical mechanisms are based on Carbon Bond version 4 and SAPRC99.

CAMx requires input files that configure each simulation, define the chemical mechanism, and describe the photochemical conditions, surface characteristics, initial/boundary conditions, emission rates, and various meteorological fields over the entire modelling domain. Preparing this information requires several pre-processing steps to translate “raw” emissions, meteorological, air quality and other data into the final input files for CAMx. Some changes have been performed over the last years in order to implement MM5-CAMx system for Portugal [59].

The MM5-CAMx pre-processor generates CAMx meteorological input files from the MM5 output files, including land use, altitude/pressure, wind, temperature, moisture, clouds/rain and vertical diffusivity. The vertical structure in CAMx will be defined from the MM5 sigma layers, and therefore will vary in space, also vertical layer structures can vary from one grid nest to another. Topographic and land use information is also provided by the MM5 model through the MM5-CAMx pre-processor.

In this study initial concentrations and hourly boundary conditions were created from output concentration files from the LMDz-INCA chemistry-climate global circulation model [60] for gaseous species, and from the global model GOCART [61] for aerosols.

Finally, pre-processors are also used to calculate the hourly variation of emissions from point and area sources, respectively. The processing of the atmospheric emissions is described in the following section.

3.3. Atmospheric emissions processing

Emission inventories are crucial ingredients to successfully simulate atmospheric pollutants concentrations, although including substantial uncertainties related to the spatial and temporal allocation of emissions, as well as the chemical speciation [62, 63]. Besides the

degree of completeness of the inventory and the quality of the emission factors, the accuracy of the inventory's temporal and spatial patterns is of major importance for successful air quality modelling. The Portuguese National Inventory Report (NIR) [64] compiles total annual quantities of atmospheric emissions, which are assigned by municipality and SNAP (Selected Nomenclature for sources of Air Pollution) category. For air quality modelling purposes it is therefore necessary to further spatially disaggregate emissions to the model's grid cell resolution level. In previous air quality studies for Portugal [62, 65] the NIR was disaggregated at the sub-municipality level using data given by Census 2001, concerning population and fuel consumption [66].

In the present study a new methodology is designed and implemented using spatial surrogates to disaggregate national emission totals onto a spatially resolved emission inventory, which can be used as input for any air quality model domain over Portugal. A spatial surrogate is a value greater than zero and less than or equal to one that specifies the fraction of the emissions of a particular country, in this case Portugal, which should be allocated to a particular grid cell of the air quality model domain of interest [67]. Typically, some type of geographic characteristic is used to weight the attributes into grid cells in a manner more specific than a simple uniform distribution. In this study, based on the methodology described in [68], CLC2000 land use data in combination with national statistics (for population, industry and agriculture employment) are applied as spatial surrogate variables for disaggregating non-point emission sources over Portugal. The surrogate value is calculated as the ratio of the attribute value in the intersection of the country and the grid cell to the total value of the attribute in the country.

The methodology developed and applied is now described. First, point source emissions were allocated on the air quality domain of interest. Next, non-point emissions, for each SNAP category, were spatially distributed using specific quantitative spatial surrogate data, based on statistics from the National Statistics Institute (INE), and other source specific activity data, and on CLC2000 data for Portugal. The emissions considered in the present study concern the following atmospheric pollutants: NO_x , NMVOC, CO, NH_3 , PM10 and PM2.5. The first step consisted in disaggregating population according to land use. Population density data are available in Portugal at the sub-municipality level, or commune. The size of communes in Portugal is very heterogeneous, ranging from 4 ha to 42500 ha; hence this level of spatial resolution is insufficient for air quality modelling purposes. Moreover, a certain commune may contain, for instance, parts of dense urban nucleus, agricultural land with some sparse population, and natural vegetation areas with very little or no population. CLC2000 gives useful geo-referenced information for disaggregation, since its geographic database provides information that is spatially much more detailed than the commune limits. Different population densities were attributed to different land cover categories, following the methodology described in [69]. The methodology was then applied to the Portuguese inland territory, with population and employment statistics given by CENSUS 2001 [70] being disaggregated over the CLC2000 and emissions disaggregated with population density using GIS. This procedure is illustrated in Figure 11 for NO_x emissions from non-industrial combustion (SNAP2).

Figure 11. Spatial allocation of NO_x emissions from SNAP2 for domain 3: a) Input data: emissions at municipality level; b) CLC aggregated classes; c) calculated population for each grid cell of the domain; d) gridded emissions at 1 km resolution.

The same procedure was followed for disaggregating emissions for the remaining SNAP categories, except for SNAP7, since the NIR distinguishes road transport emissions in two sub-categories: motorway emissions and non-motorway emissions. Non-motorway emissions were spatially distributed using the population disaggregated over the CLC2000 data as described above. Motorway emissions were disaggregated over the national motorway network, again using GIS.

For the biogenic emissions a bottom-up approach was used. The methodology for Portugal is described in [71], and requires the knowledge of the temperature, solar radiation and forest area density. For the CAMx simulations, biogenic emissions are given as isoprene and monoterpenes.

As the NIR provides annual emission totals, time-varying profiles were developed describing variations in monthly (12-element), daily (2-element, weekday and weekend) and

hourly (24-element) anthropogenic emissions, transforming time-averaged man-made emissions into hourly fluxes. The information to construct representative and meaningful temporal profiles was taken from National official statistics (energy, industrial production, transport, etc).

3.4. Case study domain definition

For the meteorological simulation, the MM5 capability of doing multiple nesting is used, and the model is applied for four domains, using the two-way nesting technique. Figure 12 shows the model domain setup and the location of the meteorological stations to be used in the validation process: domain 1 (D1) at 27 km resolution covering the Iberian Peninsula and France; D2 at 9 km resolution over Portugal; D3 at 3 km resolution over NW Portugal; and D4 with 1 km resolution over Great Porto Area.

Figure 12. Simulation model domains.

Table 2 summarizes the corresponding grid configurations. Considering previous research studies performed for NW Portugal [72], 25 unequally spaced vertical levels are used in order to optimize the simulation through the increase of vertical resolution near the surface.

Domain	No. of cells in x-direction	No. of cells in y-direction	Z levels	Resolution (km)
D1	91	77	25	27
D2	63	81		9
D3	45	51		3
D4	51	51		1

Table 2. MM5 domains configuration.

Regarding the air quality simulations, CAMx is applied for three domains, slightly smaller than the corresponding MM5 domains, using its two-way nesting capability: domain 1 (D1) at 9 km resolution covering Portugal; D2 at 3 km resolution over NW Portugal; and D3 with

1 km resolution over Great Porto Area. Table 3 summarizes the corresponding grid configurations. Considering previous research studies performed for Portugal [59], 17 unequally spaced vertical levels are used.

Domain	No. of cells in x-direction	No. of cells in y-direction	Z levels	Resolution (km)
D1	40	70	17	9
D2	35	41		3
D3	38	38		1

Table 3. CAMx domains configuration.

4. Urban development scenarios

This section presents the development and characterization of two different and opposite urban development scenarios - SPRAWL and COMPACT - in terms of land use and population. The first represents the continuation of the trend observed in the last decades, and can be described as a business-as-usual scenario; the second symbolizes the rupture with the current situation through urban containment. In addition, the reference situation corresponding to the year 2000, now on referred as BASE, is also presented for comparison purposes.

4.1. Land use

The development of the two land use scenarios, was performed over the original CLC2000 land use map, through the alteration of land use type parcels, using the ArcGis software. The SPRAWL scenario corresponds to the business-as-usual scenario, representing the continuation of the last decades trend, with urban areas continuing to expand at much faster rates than population, and urban development spreading throughout the study area, by filling up existing gaps and expanding the boundaries of existing urban areas. All the new residential areas (or urban fabric) take place in the form of discontinuous urban fabric. This urban sprawl scenario results in the smearing out of the region’s inhabitants over a large area, thus effectively simulating the sprawl-related growth process. The urban development process in the period 1987-2000 was analysed for each municipality separately and replicated for SPRAWL; the original CLC2000 land use map was changed through the creation of new artificial surface areas, which replaced natural and semi-natural areas. The combined SPRAWL land use from each municipality resulted in a new land use map for the study region presented in Figure 13, side-by-side with the BASE map (CLC2000). The built-up area (artificial surfaces) was increased from 18% to 25% of the total area; a number that can be considered realistic given current trends and the fact that in 1987 the share was 13%. The artificial areas expansion took over agricultural and forested landscapes located in the proximity of already existent urban areas.

Figure 13. Study region land cover maps for a) BASE and b) SPRAWL scenario.

The land cover maps reveal the expansion of artificial areas not only in the urban centre of the region (Porto, Matosinhos, Gondomar and Vila Nova de Gaia), but also throughout the entire study region. Table 4 presents the comparison between the BASE and the SPRAWL scenario in terms of the total area for each of the 4 large land use categories, and sub-categories, and corresponding share (%), as well as the magnitude of the change.

Land uses	BASE		SPRAWL		Change	
	hectares	%	hectares	%	hectares	%
Artificial surfaces	43727.9	18.3	60139.2	25.1	+ 16411.3	+37.5
Continuous urban fabric	4059.2	9.3	4059.2	6.7	0	0
Discontinuous urban fabric	32895.0	75.2	44647.7	74.2	+11752.7	+35.7
Industrial or commercial units	4973.1	11.4	9571.7	15.9	+4598.6	+92.5
Other artificial surfaces	1800.7	4.1	1860.6	3.1	0	0
Agricultural areas	93766.2	39.1	83201.4	34.7	-10564.8	-11.3
Forests and shrub areas	98319.4	41.0	92472.9	38.6	-5846.5	-5.9
Other non-artificial surfaces	3784.9	1.6	3784.9	1.6	0	0

Table 4. Study region land cover data for the BASE and SPRAWL scenario.

In comparison with BASE, in the SPRAWL scenario built-up land uses increase 37.5%. Agricultural areas present the largest decrease, representing now less than 35% of the total area of the region; forest and shrub areas continue to be the dominant land use in the region, with a share around 39%. Regarding the composition of artificial surfaces, the continuous urban fabric loses importance, with no additional areas of this type being created, representing now less than 7% of the artificial surfaces. Discontinuous urban fabric presents the largest increase, almost 12 000 hectares; industrial and commercial units continue the growth trend verified between 1987 and 2000, with the highest relative growth, almost doubling its presence in the study area.

In COMPACT the totality of urban growth is accommodated within already existent urban areas, i.e., no additional artificial surfaces are created. The only land-use changes implemented in this scenario concern limited changes from discontinuous to continuous urban fabric (around 40 hectares). Therefore, no spatial representation of the COMPACT scenario is presented here, since it coincides with the BASE maps.

4.2. Population

The population of the study region has been increasing; however, this increase has not been uniform along the region, with municipalities growing at different rates and even decreasing in Porto municipality. From 1991 to 2006 the study region population increased from 1.86 million people in 1991 to 2.07 million in 2006 (11.3% growth); the rate of growth however has decreased from around +1% per year in 1991-2001, to 0.2% per year, in 2001-2006. In the 25-years period under analysis, in Porto municipality population presented a decrease of 27%; an important feature of this decrease is that its rate has been accelerating: in the period 1981-1991 the rate was around -0.8%, in 1991-2001 the rate increased to -1.3%, and in 2001-2006 around -1.8% [56].

Considering the previous population evolution, both scenarios are developed for a population of 2.2 million people, corresponding to an increase of 220'000 inhabitants (13% increase) in relation to the base year 2000, in what can be considered a 20-year period. This population increase is differently distributed through the municipalities, according to the land use scenario. Since the SPRAWL scenario corresponds to the perpetuation of the past 20 years trend, the population will change accordingly in each of the municipalities, presenting the same growth rates as observed between 1991 and 2001. In the COMPACT scenario however, the trend is interrupted; Porto municipality attracts new residents, and its population is increased. The remaining cities will continue to attract people, but at a smaller rate than the verified in the last years (and therefore also in SPRAWL). Figure 14 presents the population observed in 1991 and 2000, and considered in SPRAWL and COMPACT. In COMPACT all the municipalities present a growth in their population, but at a smaller rate than the verified for SPRAWL. The exception is Porto, with more inhabitants than those in 2000, but still less than those registered in 1991.

Figure 14. Population for the SPRAWL and COMPACT scenarios and its comparison with the population in 1991 and 2000.

The population in each municipality is distributed over the land use data for BASE, COMPACT and SPRAWL, according a disaggregation methodology described in §3.3. SPRAWL presents the lowest population density (maximum values are below 9000 inhab.km⁻²), while BASE and COMPACT show a similar situation, but higher densities are found in the later with maximum values of 11 000 inhab.km⁻² in comparison with 10 000 inhab.km⁻² in BASE. This data is fundamental for the further determination of the population affected by air pollutants concentrations in each of the studied scenarios.

4.3. Emissions

As a result of the population growth and the land use changes established for each urban development scenario, new emission totals have to be calculated, as well as their spatial distribution. Atmospheric pollutants emissions for the BASE situation were the basis for estimating the scenarios emissions. New emissions were recalculated for each scenario considering the new population in each municipality, and also land use changes. Emission rates per inhabitant per municipality were kept equal to the BASE rate, as well as emission rates per land use type per municipality.

Land use differences are particularly important for three emission categories - mobile, agriculture and biogenic sources -, therefore these will be given particular attention in the next sections.

4.3.1. Road transport emissions

Since road transport emissions are highly dependent not only on population distribution but mainly on the mobility of the population, ideally a traffic model should be applied to simulate the effect of urban sprawl on traffic volumes and their spatial distribution. These modelling techniques fall out of the scope of the present work and therefore are not used. Here, to calculate transport emissions resulting from land use changes, a methodology is developed taking into account the population growth, the urban area expansion and the mobility attractiveness/repulsion rates between municipalities. These three factors influence emissions and are considered as follows:

- i. The growth of the population causes an increase in the number of trips. For each municipality it was assumed that the emissions are proportional to the number of trips, which in turn is proportional to the number of residents.
- ii. The growth of the urban area causes an increase in the mean distance from home to employments and leisure destinations. The residents in new urbanized areas find themselves more distant from locations where most employments are concentrated, while the residents in already existent urban areas will find possible employment and leisure destinations in the newly built areas in the periphery. For each municipality it was assumed that the emissions are proportional to the mean travel distance, which in turn is proportional to the urban area's radius. For example, in SPRAWL Maia's urban area increases by a factor of 1.4; therefore the mean travelled distance increased by a factor of $1.4^{1/2}=1.185$; in COMPACT the factor is 1 since no urban growth was verified.

- iii. An additional factor related to attraction/repulsion rates between municipalities has to be considered since traffic emissions are not only dependent on the population and urban area, but also on the mobility of people between municipalities. The attraction/repulsion rates calculated for BASE, presented in §2.2 are maintained and used for both scenarios.

The distribution of emissions between municipalities is very different for both scenarios, as illustrated in Figure 15, which presents CO yearly emission totals for non-motorways road transport emissions for each municipality and for the entire study area. Resulting emissions are higher for SPRAWL, which are 19% higher than the BASE emissions, while COMPACT emissions are only 4% higher. The largest differences between scenarios are found for Porto (25% lower than the BASE emissions for SPRAWL, and 30% higher for COMPACT), Matosinhos (+38% for SPRAWL, +8% for COMPACT), Vila Nova de Gaia (+20% for SPRAWL, -2% for COMPACT) and Maia (+56% for SPRAWL, +9% for COMPACT).

Figure 15. Study region SNAP7 (non-motorways road transport) CO emissions for BASE, COMPACT and SPRAWL, for each municipality and for the entire study area.

Regarding the spatial distribution of emissions, Figure 16 presents SNAP7 non-motorway CO grid emissions at 1 km resolution for SPRAWL and COMPACT. For both scenarios, emissions are concentrated in the Porto, Matosinhos, Maia, NW Gondomar and Vila Nova de Gaia municipalities; however COMPACT presents a greater concentration of emissions, as a result of the urban containment, and therefore higher emission rates.

4.3.2. Agriculture emissions

New emissions for the agriculture category were recalculated considering the new agricultural area in each scenario, with emission rates per agricultural area per municipality kept equal to the BASE rates. Since the COMPACT scenario presents no changes in agricultural area in relation to the BASE, emission totals, as well as their spatial distribution are the same. As a result of the transformation of agricultural areas into artificial land use, agriculture emissions were reduced by almost 10% in SPRAWL.

Figure 16. SNAP7 (non motorway road transport) CO grid emissions at 1 km resolution for a) SPRAWL and b) COMPACT.

4.3.3. Biogenic emissions

Biogenic emissions were calculated for the forested areas according to the methodology previously described in §3.3. Differences in relation to BASE result from the conversion of forested areas to artificial areas, and also from temperature changes induced by land use changes; these only take place in the SPRAWL scenario, since in COMPACT, the forest land use are not changed in relation to BASE. Therefore, as a result of land use changes biogenic SPRAWL emissions are lower when compared to BASE (and COMPACT): 20% lower for monoterpenes and 16% lower for isoprene.

4.3.4. Total emissions

The above presented methodology results on different emission totals for both scenarios. Figure 17 shows emission totals for the study region for SPRAWL and COMPACT as well as for BASE.

Figure 17. Study region total NMVOC, NH₃, NO_x, PM and CO emissions for BASE, SPRAWL and COMPACT.

Figure 18. Spatial allocation of CO, NMVOC, NO_x and PM₁₀ total emissions at 1 km resolution for a) SPRAWL and b) COMPACT

Lower emissions are obtained for BASE and higher for SPRAWL; SPRAWL emissions are around 9% to 17% higher than BASE emissions (for NH_3 and NMVOC, respectively), while COMPACT emissions are 4% to 6% higher (for NH_3 and NMVOC, respectively).

Figure 18 shows the spatial distribution of CO, NMVOC, NO_x and PM10 gridded emission totals for the 1 km resolution domain for SPRAWL and COMPACT. COMPACT emissions are more concentrated over Porto municipality and present higher emission rates per grid cell; SPRAWL presents more scattered emissions throughout the simulation domain, and therefore lower emission rates. Emissions of NMVOC constitute an exception, because they are highly related with the port activity in Matosinhos, and therefore present higher values for this municipality in both scenarios.

5. Atmospheric modelling results

Aiming to provide a thorough analysis of the air quality impacts of different urban land use scenarios, the atmospheric simulation of BASE and scenarios is performed for a one-year period, covering a wide range of air pollution conditions. The meteorological year of 2006 was chosen for simulations since it is considered an “average” year, as opposed to others such as 2003 and 2005, which were abnormally dry and/or warm [73, 74]. Meteorological differences between the two scenarios, and between each of the scenarios and BASE, will stem solely from land use changes since the meteorology is the same. The air quality simulations were performed with meteorological inputs given by the respective MM5 annual simulation and emissions described in §3.2 and §4.3 for BASE and for the scenarios, respectively.

5.1. Meteorological modelling

5.1.1. BASE simulations

For BASE the simulation was performed with land use data from 2000 since no data was available at the time for 2006. In order to evaluate the model performance, modelling results were compared with data from Porto/Pedras Rubras meteorological station, located in the municipality of Matosinhos. Figure 19 shows the time-series comparison of surface temperature and wind components for observed and BASE simulated values.

Concerning temperature, simulated values follow the distribution of the observed ones; a general under-estimation of temperature is visible, especially for the higher temperatures registered at the end of May / beginning of June, July and August. Simulated wind components present a smaller variability when compared with observed ones, but also follow the observed trend.

The MM5 skill was also evaluated through the application of the quantitative error analysis introduced by in [75] and widely used in model validation exercises:

Figure 19. Observed and BASE (1km resolution) time-series comparison of surface a) temperature, b) zonal wind component and c) meridional wind component, at Porto/Pedras Rubras meteorological station.

$$E = \left(\sum_{i=1}^N (\phi_i - \phi_{iobs})^2 / N \right)^{1/2} \quad (1)$$

$$E_{UB} = \left(\sum \left[(\phi_i - \phi_0) - (\phi_{iobs} - \phi_{0obs}) \right]^2 / N \right)^{1/2} \quad (2)$$

$$S = \left(\sum_{i=1}^N (\phi_i - \phi_0)^2 / N \right)^{1/2} \quad (3)$$

$$S_{obs} = \left(\sum_{i=1}^N (\phi_{iobs} - \phi_{0obs})^2 / N \right)^{1/2} \quad (4)$$

The parameter E is the root mean square error (rmse), E_{UB} is the rmse after the removal of a certain deviation and S and S_{obs} are the standard deviation of the modelled and observed data. If ϕ_i and ϕ_{iobs} are individual modelled and observed data in the same mesh cell, respectively, ϕ and ϕ_{obs} the average of ϕ_i and ϕ_{iobs} for some sequence in study, and N the number of observations, then the simulation presents an acceptable behaviour when $S \approx S_{obs}$, $E < S_{obs}$ and $E_{UB} < S_{obs}$. In addition to these parameters the correlation coefficient was also determined for each simulation.

Figure 20 presents the statistical analysis of BASE 1km resolution simulations, for Porto/Pedras Rubras. For temperature the correlation coefficient obtained is 0.9, with S/S_{obs} also near 1, and E/S_{obs} below 0.5. As expected, wind components results are not as good as for temperature, with lower correlation coefficients and higher errors. The meridional wind component is better simulated than the zonal one. Overall, the meteorological simulation reveals a good performance for the three meteorological variables, with statistical parameters presenting a reasonable behaviour.

Figure 20. BASE statistical parameters for surface temperature, and zonal and meridional wind components for Porto/Pedras Rubras meteorological station.

5.1.2. Scenario simulations

As for BASE, the SPRAWL and COMPACT meteorological simulations are performed for 2006 meteorological year, using the land use data produced according to the procedure described in §4.1. Since for COMPACT the land use is very similar to that of BASE (the only change concerned the conversion of a few hectares of discontinuous urban fabric to continuous urban fabric), meteorological results from COMPACT only present very small temperature differences in relation to BASE. Therefore, from now on, and for meteorological purposes, no distinction is made between BASE and COMPACT.

Taking into consideration that the most widely recognized meteorological effect of urbanization is the urban heat island effect and because of the recognized influence of urban temperatures on ozone formation, hereafter the meteorological analysis will be focused on surface temperature. SPRAWL meteorological simulations produced a domain-averaged annual temperature increase of approximately 0.4 °C. This is attributed to the increased share of built-up areas in the domain, which convert incoming radiation to sensible heat rather than to latent heat (evaporation), owing to the limited water availability in artificial

surfaces characterized by impervious materials. However, in some regions and for certain time-periods differences between scenarios reached significantly higher values than the average.

Figure 21 presents the differences between COMPACT and SPRAWL annual simulations for hourly surface temperature, at Porto/Pedras Rubras meteorological site, with 1 km resolution. Although the land use in Porto/Pedras Rubras was not changed, there were temperature differences as high as 2.5°C between the two simulations. These differences indicate that changes in meteorological parameters are not necessarily confined to the cells where the land use pattern was modified. Also, higher differences are found in the summer months, i.e., from April to September, since higher temperatures are also reached, and therefore meteorological differences are enhanced. While temperature increases would be expected with increasing urbanization, due to the urban heat island effect, temperature decreases are also verified. Local temperature increases in grid cells with modified land use could have lead to higher wind speeds and increased instability which downwind can lead to areas of increased vertical mixing and decreased surface temperatures.

Figure 21. Hourly surface temperature differences between SPRAWL and COMPACT for Porto/Pedras Rubras meteorological site for 1-km resolution.

To illustrate the spatial extent of effects of land use changes in temperature, the average afternoon (12:00 – 18:00) temperature differences for July are shown in Figure 22. For July, average afternoon temperature differences range from about -1.2°C to +1.4°C, with largest increases occurring over Vila do Conde, Maia, Matosinhos, Porto and Gondomar, i.e., municipalities in the first metropolitan ring, which present some of the largest urban expansion. The observed changes are consistent with the substantial increases in urban surfaces across large parts of the model domain, and the spatial pattern of the temperature changes generally matches the area of increased urbanization. This is quite evident for the coastal part of Vila do Conde, NE Matosinhos and SE Vila Nova de Gaia.

The temperature differences obtained as a result of land use changes are consistent with previous research by [42, 44], although these authors conducted research only for episodic air pollution situations. Although not presented, the SPRAWL scenario with its increased urban land cover also had a noticeable effect on surface layer winds across the metropolitan region, generally leading to a slight increase in wind speed.

Figure 22. July differences between SPRAWL and COMPACT afternoon (12:00 – 18:00) average surface temperature fields between at 1 km resolution.

5.2. Air quality modelling

5.2.1. BASE simulations

Here the air quality results for the annual simulation of BASE are presented. The air quality model configuration and its application are those described in §3.2. For BASE the simulation used emissions data for 2005 (there are no emission estimates for 2006, since the national inventory is updated with a 2-year periodicity). Data from the Northern Region's air quality monitoring network [76] for 2006 was used for the validation of BASE simulations. [45] recommends a group of statistical parameters for air quality models evaluation; from the proposed group, three parameters were selected for a quantitative error analysis: the correlation coefficient (r), the root mean square error (RMSE) and BIAS:

$$r = \frac{\sum_{i=1}^n (C_{obsi} - \bar{C}_{obs})(C_{modi} - \bar{C}_{mod})}{\sqrt{\sum_{i=1}^n (C_{obsi} - \bar{C}_{obs})^2 \sum_{i=1}^n (C_{modi} - \bar{C}_{mod})^2}} \quad (5)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (C_{obsi} - C_{modi})^2} \quad (6)$$

$$BIAS = \frac{1}{n} \sum_{i=1}^n (C_{obsi} - C_{modi}) \quad (7)$$

where: n is the total number of sample pairs, C_{obsi} is the observed value at time i and C_{modi} is the respective simulated concentration. These three parameters offer complementary information: the correlation factor (r) translates the linear relation between concentrations, reflecting a better or worst reproduction of physical and chemical atmospheric processes; RMSE and BIAS give an indication of the deviation between observed and simulated concentrations, either in absolute (RMSE) or in systematic terms (BIAS), allowing the inference of the magnitude and trend of the errors, respectively. For both the ideal value is zero.

Table 5 shows the statistical results for ozone and PM10, averaged over the air quality monitoring sites, already mentioned in §2.3 for the 1km resolution simulation. For ozone statistical parameters are given considering the entire year (from January to December) and considering only the summer months (April to September). These statistical parameters are within the range of those obtained with this and other air quality modelling systems [62, 77].

Air quality monitoring station	PM10			O ₃		
	r	BIAS ($\mu\text{g.m}^{-3}$)	RMSE ($\mu\text{g.m}^{-3}$)	r	BIAS ($\mu\text{g.m}^{-3}$)	RMSE ($\mu\text{g.m}^{-3}$)
Espinho	0.41	-5.2	26.9	n.a	n.a	n.a
Baguim	n.a	n.a	n.a	0.66	-27.2	35.8
V.N.Telha	0.44	1.1	23.6	0.62	-20.1	31.8
Vermoim	0.63	1.1	23.2	0.62	-25.1	34.9
Custoias	n.a	n.a	n.a	0.64	-19.5	32.5
L.Balio	0.65	-16.9	17.9	0.65	-26.6	36.8
Matosinhos	0.58	-10.2	32.7	0.66	-32.2	41.1
Perafita	0.43	1.8	14.4	0.62	-16.4	30.6
Antas	0.56	-18.8	49.1	0.62	-24.7	36.4
S.Hora	0.49	-12.9	34.4	n.a	n.a.	n.a
Boavista	0.44	-6.3	24.7	0.62	-15.9	18.8
Ermesinde	0.61	-10.2	25	0.64	-21.8	36.4
AVERAGE	0.53	-7.7	27.2	0.64	-22.9	33.5

Table 5. CAMx statistical results obtained for O₃ and PM10.

In addition to the statistical analysis of the model performance, another possible and interesting exercise is the comparison of observed and simulated BASE concentrations in terms of the legislated values for O₃ and PM10. In this scope, Figure 23a presents the number of exceedances to the PM10 daily limit value ($50 \mu\text{g.m}^{-3}$, not to be exceed more than 35 days along the year, indicated by the red line) observed and BASE simulated; Figure 23b shows the number of annual exceedances to the ozone information threshold ($180 \mu\text{g.m}^{-3}$) observed and BASE simulated.

Figure 23. Observed and BASE a) number of exceedances to PM10 daily limit value, and b) number of exceedances to O₃ information threshold

Regarding the number of daily average PM10 exceedances the model, although the higher over-prediction at Antas, and Leça do Balio, and the under-prediction at Vermoim and Ermesinde, correctly identifies that all the air quality monitoring sites are not in compliance with the legislation. Model results point to exceedances to the ozone information threshold in Baguim, Matosinhos and Boavista, while these have not been observed; for the remaining air quality sites, the model presents a good agreement with observations.

5.2.2. Scenario simulations

For SPRAWL and COMPACT, simulations are performed with land use and emissions data produced according to the procedures previously described. Meteorological inputs are given by the respective MM5 annual simulation. Results from the two scenarios are analysed against the BASE simulation and against each other in order to identify the main differences between them.

Figure 24 presents the spatial distribution of PM10 annual average concentrations calculated for BASE, SPRAWL and COMPACT, highlighting the areas for which the legislated annual limit value ($40 \mu\text{g.m}^{-3}$) is exceeded. BASE and COMPACT present a larger area of high PM10 annual averages ($> 40 \mu\text{g.m}^{-3}$) over Porto municipality and its immediate surroundings, in comparison to SPRAWL. This is because the SPRAWL scenario implies a further decrease in Porto's population, and therefore emissions, and a consequent increase in neighbouring municipalities. The result is a decrease of emissions in Porto and therefore in pollutants concentrations. Nevertheless, considering the entire simulation domain, SPRAWL shows the highest PM10 annual concentrations ($> 70 \mu\text{g.m}^{-3}$), and larger areas above the annual limit value in Gondomar and Vila Nova de Gaia. The comparison between COMPACT and BASE suggests that the higher concentrations take place in exactly the same areas, with COMPACT revealing slightly higher concentrations ($> 65 \mu\text{g.m}^{-3}$). This is due to the population concentration in already urbanized areas, with the consequent increase of emissions.

To better analyse the differences between the scenarios, the spatial distribution of the concentration differences are presented in Figure 25. Air quality monitoring stations are also represented for further analysis. Differences between annual averages from SPRAWL and BASE range from -15 to $+24 \mu\text{g.m}^{-3}$, with negative values mainly over Porto, as a result of the

Figure 24. PM10 annual average for a) BASE, b) SPRAWL and c) COMPACT (the orange lines surround the areas for which the legislated annual limit value is exceeded).

decrease in emissions from traffic in this municipality. Higher positive differences are found over certain parts of the municipalities in the first metropolitan ring corresponding to areas of urban expansion. Differences between COMPACT and BASE range from -5 to $+8 \mu\text{g.m}^{-3}$, with higher positive differences over Matosinhos, in areas previously urbanized but with a greater population density in COMPACT. However, for the most part of the simulation domain differences are small.

Figure 25. PM10 annual average differences between a) SPRAWL and BASE, and b) COMPACT and BASE.

Figure 26 presents the results for PM10 annual averages for BASE, SPRAWL and COMPACT for each air quality monitoring site located in the simulation domain.

For the majority of the air quality sites, SPRAWL presents the highest annual average of the three simulations. The results for Baguim, located in Gondomar are not representative of the municipality, with areas of increased PM10 concentrations, not captured by the air quality monitoring site. Also, sites which in BASE did not exceed the legislated annual average, such as Boavista and Leça do Balio, now exceed the limit with SPRAWL and COMPACT. Other sites which were already in non-compliance show a deterioration of their situation (such as Matosinhos and Senhora da Hora). In Antas, Baguim, and Ermesinde both scenarios improve the PM10 levels.

Figure 26. PM10 annual average for BASE, SPRAWL and COMPACT (the red line indicates the legislated annual limit value, $40\mu\text{g.m}^{-3}$), at the air quality monitoring sites.

Besides the obtained concentrations for each scenario it is also important to assess the number of individuals affected by high PM10 concentrations, since the population distribution across the study area is quite different for BASE, SPRAWL and COMPACT. Therefore, the maps of annual average concentrations (Figure 24) were crossed with population data per grid cell, to calculate the number of individuals affected by PM10 concentrations above the annual limit value. The results in terms of percentage of population (and not absolute since BASE has a lower population) are shown in Figure 27.

Figure 27. Population affected by PM10 concentrations above the annual limit value in BASE, SPRAWL and COMPACT.

COMPACT presents the greatest share of population affected by PM10 concentrations above $40 \mu\text{g.m}^{-3}$ (17%, corresponding to 370 000 inhabitants), while SPRAWL has the lowest number (12.5%, around 270 000 inhabitants). For the three considered concentration ranges, SPRAWL has the lowest share of people affected, while BASE and COMPACT show similar concentrations, although generally lower for BASE. Notwithstanding the existence of higher PM10 concentrations in SPRAWL, results indicate that the dispersion of the population along the study region withdraws people from the areas of higher concentrations. In turn, the COMPACT scenario places a greater part of the region’s population in areas of highest PM10 levels.

The combination of increased temperatures (for SPRAWL) and different emissions (for both scenarios) produces the ozone concentration pattern changes displayed in Figure 28. The spatial distribution of the ozone summer (April to September) average concentration differences between BASE, SPRAWL and COMPACT are shown. Air quality monitoring stations location is also depicted for further analysis.

Figure 28. Ozone summer average differences between a) SPRAWL and BASE, and b) COMPACT and BASE.

The immediate analysis of the maps reveals that differences between the scenarios and BASE are much smaller than those obtained for PM₁₀. Differences between SPRAWL and BASE range from -6 to +4 $\mu\text{g.m}^{-3}$, with negative values mostly found over Matosinhos, Maia and Gondomar (centre), in areas where the population expanded and emissions increased. In fact, comparing this map with the one for PM₁₀ (Figure 25), negative differences for ozone are found in the areas of positive PM₁₀ differences. Still regarding SPRAWL, ozone increases occur over Porto and part of Gondomar (N and S) in areas downwind the largest emission increase, such as Matosinhos, Maia and the centre of Gondomar municipality, as a result of air pollutants transport and consequent ozone formation. This is consistent with the prevailing NW wind direction in the region. Differences between COMPACT and BASE range from -1.5 to +2 $\mu\text{g.m}^{-3}$. Negative differences take place in Porto municipality as an outcome of the population densification in that area and the corresponding emissions increase, which lead to the local consumption of ozone. For both scenarios the largest part of the simulation domain presents very small positive differences, less than 1 $\mu\text{g.m}^{-3}$, meaning that average concentrations are slightly higher in comparison to BASE.

Under the combined effects of increased urbanization and increased emissions, ozone decreases are not completely unexpected and have been found in previous research works [42, 44]. This is probably due to the higher ozone removal by titration caused by higher anthropogenic emissions in an already emissions-dense region. Also, as investigated in [78], the non-linear response of ozone concentrations to changes in precursor emissions was found to increase with tonnage and emission density of the source region; this seems to be the case in the study region. According to the modelling study conducted by [79], the

synergy among precursor's emission source categories may sometimes suppress O_3 , acting as negative source contributions. These authors concluded that the full potential of each source category in O_3 formation (the pure contribution) is not achieved when emissions from the other source categories are accounted for.

Figure 29 presents the number of exceedances to the hourly ozone information threshold ($180 \mu\text{g.m}^{-3}$), obtained for BASE, SPRAWL and COMPACT. SPRAWL presents the lowest number of exceedances, except in Espinho where the three simulations produced similar results. COMPACT is the worst scenario, with more exceedances than BASE for Boavista, Vila Nova da Telha, Senhora da Hora and Perafita.

Figure 29. Number of exceedances to the ozone information threshold for BASE, SPRAWL and COMPACT.

The comparison of these results with the concentration patterns presented in Figure 27, reveals that there are no air quality sites in the areas of concentration increases, mainly for SPRAWL. However, if the same analysis is carried out for Gondomar in an area where no monitoring stations exist and for which higher positive differences are observed in the map of Figure 38, results are quite different: SPRAWL yields more exceedances (8) to the ozone information threshold in comparison with BASE (5) and COMPACT (6).

Regarding the number of persons affected by high ozone concentrations, the combination of the annual average concentrations maps with population data per grid cell, allows the determination of the number of individuals affected by ozone summer average concentrations above $70 \mu\text{g.m}^{-3}$. This value was chosen because it is the concentration above which differences between the three situations are more substantial. The results are presented in Figure 30.

Once more, differences between scenarios and BASE are smaller than those observed for PM_{10} . COMPACT presents the highest share of inhabitants affected by ozone summer average concentrations above $70 \mu\text{g.m}^{-3}$ (48.5%, corresponding to roughly 1 million people). However, looking at other concentration ranges the situation is different, since above $75 \mu\text{g.m}^{-3}$ BASE is the worst situation, with 21% of the population.

Figure 30. Population affected by ozone summer average concentrations above 70, 75 and 80 µg.m⁻³ in BASE, COMPACT and SPRAWL.

6. Main findings

The main aim of this study was to explore the relationship between the structure of the urban area and its air quality. Several research studies had demonstrated already that compact cities with mixed land uses are energetically more efficient and are responsible for lower emissions of atmospheric pollutants in comparison with sprawling cities. But a fundamental question remained unanswered: do compact cities promote a better air quality when compared to sprawling cities? And, given the ever-growing concentration of population in urban areas, do compact cities promote a healthier atmospheric environment? Given the signs provided by the energy and emissions aspects, the answers may seem obvious and straight forward but, as it was demonstrated along this study, they are not.

To answer these questions a strategy was drawn. The strategy, or approach, relied on the use of advanced atmospheric modelling tools for the evaluation of different urban development scenarios.

Aiming to assure a correct and complete analysis, a step-by-step methodology was defined and applied. First, it was necessary to characterize the current state of knowledge on the subject, including the genesis and growth of the problem, the tools available to tackle it, and gain insight from the studies previously conducted by several researchers on the field.

The selected working area is located in Portugal’s Northern region, covering the Porto urban region, which is composed of a regional conglomerate of cities with a total population of over two million. Maps of land use and population parameters and an emission inventory were established for the situation as it is today (BASE). Moreover, two distinct future urban development scenarios - COMPACT and SPRAWL - were created, based on population and land use changes. The population of the study region was increased, to reflect a 20-years period, and differently distributed among municipalities according to each scenario. The land use patterns of the area were modified following a scenario of urban sprawl (SPRAWL) and maintained through the concentration of people in already existent urban areas

(COMPACT). New emissions were estimated for each scenario, taking into account population growth and land use changes.

The modelling system was then applied for SPRAWL and COMPACT, and also BASE, for a full-year simulation. The analysis of the meteorological results revealed that, owing to the land use changes in SPRAWL, the average temperature increased by 0.4°C. However local increases reaching 3°C were also detected; and some were even estimated in areas where land use changes were not implemented.

Regarding air quality, SPRAWL presented the highest PM₁₀ concentrations, with an aggravation of the annual average values especially over areas of urban expansion and increasing emissions. Also, in the sites corresponding to the current monitoring stations, an increase in the number of exceedances to the daily limit value was found. For COMPACT slightly higher PM₁₀ concentrations than BASE were estimated, due to the population increase in already urbanized areas, and consequent increase of emissions in those same areas.

For ozone, while the largest part of the domain had small concentration increases for both scenarios, smaller concentrations are found in areas where the population expanded and emissions increased, as a result of ozone titration by NO in the polluted atmosphere. Instead higher ozone levels are estimated for areas downwind the greatest emission increases, as a result of air pollutants transport and consequent ozone formation. Differences between scenarios and BASE were smaller than those found for PM₁₀.

Finally, the population affected by higher PM₁₀ and O₃ concentrations was determined for each scenario and for BASE. The analysis revealed that although the existence of higher PM₁₀ concentrations in SPRAWL, the increase of the population density in COMPACT places a greater part of the inhabitants in areas of highest PM₁₀ levels. This means that individually each inhabitant is exposed to lower PM₁₀ concentrations in COMPACT, however, looking at the population as a whole, in terms of public health, the situation is inverted and SPRAWL presents a lower number of people affected by the highest concentrations. For ozone, results are not so clear, with BASE and COMPACT sharing the highest number of individuals affected, and SPRAWL clearly presenting the lowest number of total inhabitants affected by higher concentrations.

In conclusion, it seems clear that changes in land use patterns in urban areas lead to changes in meteorology, emissions, air quality, and population exposure. The signal of the change is evident: sprawling urban areas, when compared to contained urban development, are responsible by higher temperatures, higher emissions of pollutants to the atmosphere and higher atmospheric pollutants concentrations. However, compact urban developments imply a higher number of individuals exposed to the higher concentrations.

According to the review of the literature on the present subject, this was the first time a long term study was performed to analyse the impacts of urban growth, and consequent land use

changes, on air quality, through the development of alternative urban development scenarios and the application of an air quality modelling system. Also, the methodology can be applied to any city or urban area for which the required data is available. However, the methodology presented here can be improved. Future work shall focus on the use of land use models for the simulation of land use changes, and traffic modelling to simulate the effect of land use changes on traffic volumes and their spatial distribution.

Along the next decade, it is expected that changes in the land use will take place. More likely, as revealed by the current trends, urban sprawl, the destruction of agricultural lands, and forestation and deforestation are expected to alter the landscape. These patterns will, in turn, lead to changes in population, energy consumption, traffic and anthropogenic and biogenic emissions. The results of this work suggest that changing land use patterns should be taken into consideration when using models to evaluate changes in quality levels (in particular ozone and PM₁₀) stemming from various emissions reduction scenarios in urban areas.

Also, it is important to note that, such as technology alone has not been able to tackle the air quality problems, more compact urban development patterns alone will not be sufficient to fully address urban air quality problems. Technological advances in emissions control have proven to be highly effective in reducing emissions over the last decades, and emerging technologies, such as hybrid or electric vehicles and alternative fuels, are expected to continue these reductions. The importance of land use-oriented approaches to air quality management lies in the potential for these strategies to limit the dramatic growth in traffic, which has greatly diluted the benefits of technological improvements so far, and also in addressing the local meteorological drivers of air pollution, such as temperature.

In the years to come, cities will continue to be the main centres of economic activity, innovation and culture. Therefore, managing the urban environment and the quality of life of its inhabitants goes well beyond the concern for the well-being of the urban population, affecting instead the well-being of humanity as a whole. This work presents an achievable approach to urban sustainable development supporting the objective of the UN Conference Rio+20.

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