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# Air quality and MOLAND: Description of a methodology to determine emissions output and affected populations

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## Abstract

In recent years, awareness of air quality issues in urban areas has increased significantly. The negative consequences for human health as a result of poor air quality have resulted in numerous laws being enacted both in Ireland and around the world, in an attempt to limit exposure. Within the urban environment, motor vehicles are one of the most significant contributors to pollution. As a result, constant monitoring takes place but little work is done on predicting likely changes in air quality, for better or worse, as a result of changes in landuse or transport. The MOLAND model can provide the basis for an emissions estimation methodology to predict changes in vehicular emissions, and consequently air quality, both now and in the future, enabling policy makers and planners to examine the air quality implications of their decisions.

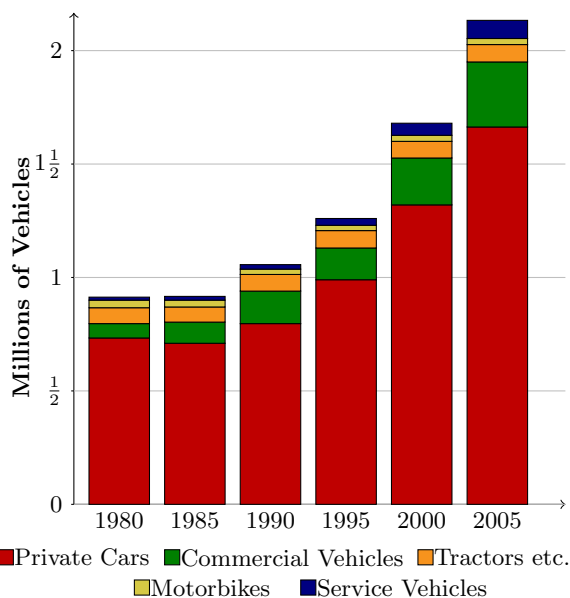
**Keywords:** *Air quality, transport, emissions, MOLAND*

## 1 Introduction

Most people will be aware that a large number of sources contribute to the degradation of air quality in the urban environment. These sources include power generation stations burning fossil fuels close to urban centres, construction work within the city, commercial or residential heating or power systems based on a combustion process, or vehicular combustion systems in automotive applications. It is believed that such mobile sources are one of the most important contributors to poor air quality in any city (Reynolds and Broderick, 2002).

In recent years, the rapid expansion of the urban environment has led to a significant increase in the spatial distribution of population (Williams et al., 2007). However, this increased dispersion has not been reflected in the recent development of public transport infrastructure, meaning that many people have to use personal modes of transport for work and social activities. Thus, there is a significant reliance in Ireland on private road transport. Indeed, between 1980 and 2005, the Irish private passenger car fleet has doubled, growing from 734,371 in 1980 to 1,666,157 by 2005 (Figure 1). In the same period

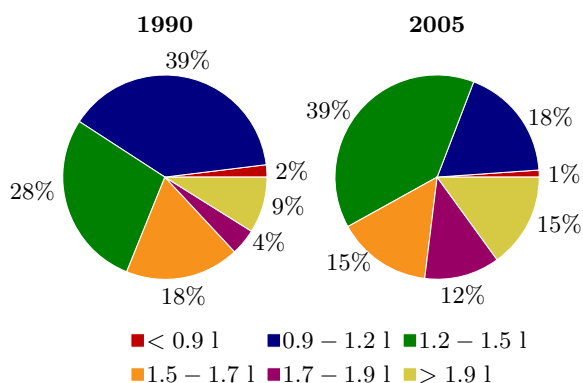
we have seen a quadrupling of the commercial fleet in Ireland, from 65,052 to 286,548, with the largest increases in Dublin and the surrounding counties (VRU, 2001, 2006). During part of the same period, the size of engines used in vehicles has increased, as is demonstrated in Figure 2 below (Howley et al., 2006).



**Figure 1** – Expansion of the vehicle fleet in Ireland, 1980 – 2005. Taken from VRU (2001, 2006).

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Since these vehicles all employ the internal combustion engine as the mode of providing motive power, combustion products and by-products contribute significantly to concentrations of harmful chemical species in the atmosphere and to greenhouse gas (GHG) emissions within the city. The physical layout of the city has the added problem of the canyon effects and microclimates caused by the physical makeup of streets, leading to relatively high pollutant species concentrations in these areas (Berkowicz et al., 2006).



**Figure 2** – Change in passenger car engine size, 1990 – 2005. Taken from Howley et al. (2006).

With ever more stringent emissions regulation legislation (EEC, 1970, 1991, 1993; EC, 1994, 1996, 1998) and a heightened interest in reducing greenhouse gas emissions under the Kyoto Protocol (EPA, 2008), reductions in emissions are being sought. However, the increase in vehicle numbers leads to significant levels of congestion, increased journey times and consequently, increased emissions.

In order to quantify and examine this problem, this paper will describe a possible methodology for the application of the MOLAND model to the Greater Dublin Area (GDA) in an attempt to predict future trends in vehicle numbers and emissions from the fleet and, hence, to describe the likely populations affected by pollution. In this way, the system should provide planners and policy makers with a decision support tool, which would allow them to examine the likely changes in air quality caused by developmental and infrastructural changes, such as the development of the road or rail networks, new housing or further development of mixed use buildings.

## 2 Air Quality Monitoring and Modelling

In order to understand why such a model would be useful, it is important to understand the current state of air quality monitoring and modelling

in Ireland.

At a national level, the Environmental Protection Agency (EPA) is responsible for the dissemination of current and past trends in atmospheric pollutant concentrations. One significant problem with the current system is the lack of spatial representation by the monitoring sites (O’Leary, 2007). Currently, only six such monitoring sites exist in Dublin, for example. Background levels of pollution are measured in the Phoenix Park. Urban levels are measured in Rathmines, Marion and Ballyfermot, as well as on Winetavern Street and Coleraine Street.

The concentrations described by this type of data include the effects of pollutant species dispersion from their original source, which may include power generation plants, industrial, commercial and domestic heating systems and emissions from vehicles, to the sink at which it is measured. Thus, it is difficult to derive accurate values for local exposure away from these monitoring sites (Fuentes, 2002; Matejicek et al., 2006). It is also impossible to distinguish between background concentrations, concentrations from stationary sources or emissions caused by vehicular traffic.

In light of these difficulties, it is necessary to develop a robust method of determining vehicular emissions and their subsequent dispersion. Neither is a trivial task. However, since little spatial data exists for emissions levels, it is useful to examine the root of such emissions and thus improve our understanding of the underlying principals of pollutant formation and dispersion. In so doing, it is possible to develop a data set that describes the location of pollutant sources, particularly mobile sources, (which is covered in this paper), which would feed into a suitable dispersion model. The combined system would be a tool that would help planners to examine shifts in emissions and air quality as a result of their proposals and, hence, determine affected populations at a local spatial scale.

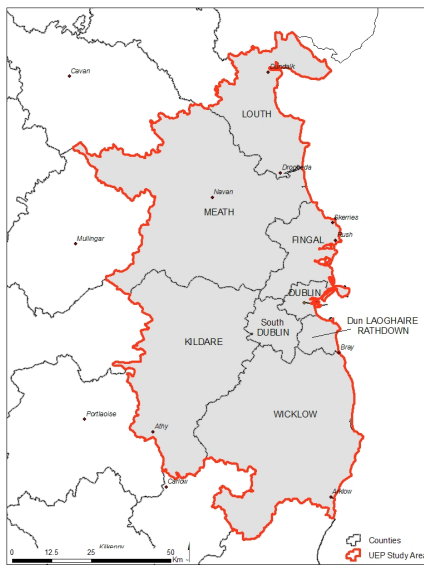
The methodology proposed in this paper will use MOLAND output data, in the form of population projections and landuse maps, and attempt to describe current emissions and their likely changes as a result of changes in these parameters, with a view to better informing a dispersion model.

## 3 A brief description of the MOLAND model

The MOLAND model is a landuse dynamics model developed by the Research Institute for Knowledge Systems (RIKS b.v.) in the Netherlands for the

Joint Research Centre (DG JRC) of the European Union (Engelen et al., 2004). The system has been applied to a variety of case studies to examine the likely changes in land use over long periods of time (Brennan and Twumasi, 2008).

In the Irish case, the Urban Environment Project (UEP) is examining the Greater Dublin Area, which comprises the counties of Louth, Meath, Kildare and Wicklow and the four local authority areas of Dublin (Fingal, Dublin City, South Dublin and Dún Laoghaire-Rathdown).



**Figure 3** – Map of area covered by MOLAND simulation

The model itself is based on cellular automata (CA), which in this case describes a cell of 200 m by 200 m. The cell is assigned a specific landuse, either as a function that can change over time, or as a feature, which remains static<sup>1</sup>. The change is based on a series of mathematical rules and various input maps that describe the accessibility, the suitability and the zoning status of each cell. Along side these, a series of inertial rules govern the likelihood of a cell changing from one cell type to another. A stochastic perturbation factor is also included in the calculation scheme to allow for more realistic patterns of development. The cell type, in broad terms, is categorised according to its use, be it residential, industrial, commercial, agricultural or semi-natural. A more detailed description of the

<sup>1</sup> This static nature refers only to the fact that such cells do not change of their own accord, as a result of transition rules. Rather, they are forced to change due to the development of other cell types, such as residential, industrial or commercial classes

rules is given in Twumasi (2008) and Engelen et al. (2004).

Using this landuse change system, the model is able to predict possible changes in the structure of the landuse and also assigns population and socio-economic changes to the system. Thus, changes in population and in the number of jobs, as predicted by the model, based on landuse changes and urban development, are output along with the relevant landuse map for a time step of one year. These data can then be augmented by ancillary data sets and used to describe the likely changes in vehicle numbers and, consequently, fleet composition. It should also be possible to spatially locate these emissions and determine what populations are affected. This last step is not as straight forward as the others, as will be demonstrated by the following sections, but can be achieved with careful use of MOLAND and ancillary maps.

#### 4 A methodology for using MOLAND to predict air quality

As has been stated previously, motor vehicles are one of the most significant contributors to local pollution levels within urban environments. In recent years, ever more stringent emissions limits have seen reductions in tailpipe emissions<sup>2</sup>. However, many of the benefits of these reductions have been eroded by the increased number of vehicles on Irish roads.

Any model that aims to predict emissions from vehicles must take into account changes in vehicle numbers, vehicle technology and vehicle usage. The following sections will describe the link between certain ancillary data sets and MOLAND outputs in order to achieve a robust methodology for the determination of future emissions from vehicles.

##### 4.1 Trends in vehicle numbers

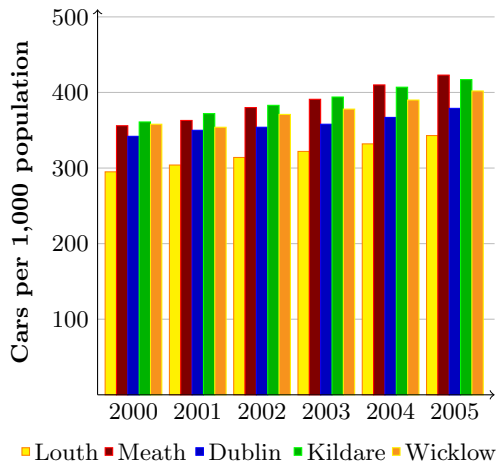
The number of vehicles on roads in any country is closely linked with both population and wealth. Figure 4 shows the increase in the number of cars per thousand population in Ireland over the past six years. These values are comparable to European values (Howley et al., 2006). It should be noted that the figures used here are for the absolute population, not simply the adult population, since it must be compatible with the MOLAND output values.

A simple regression model can be used to predict the likely changes in vehicle numbers into the future, based on current trends. It is likely that a

<sup>2</sup> Emissions from the tailpipe of a vehicle have been passed through a catalytic converter to further reduce the concentrations of harmful species.

model using a linear regression curve would over estimate the total number of vehicles and so a logarithmic or exponential curve should be used. It is also most unlikely that more than half the population will be in a position to drive a vehicle – hence a value of more than about 550 cars per thousand population is most unlikely, although not necessarily impossible. Also, a more advanced model would need to take account of changes in Gross Domestic Product (GDP) or Gross National Product (GNP).

With a description of the total number of private cars, including a likely future projection, it is possible to determine the total vehicle fleet by scaling the predicted population from MOLAND by the cars per thousand population figure. This can be done at both a regional or county level, although certain counties have shown significantly higher growth in vehicle numbers than others in recent years, as shown in Figure 4. This leads to slightly skewed results, such as vehicle ownership heading towards 700 cars per thousand population. So, educated interpretation of the results is required.



**Figure 4** – County car ownership per thousand population. Based on MOLAND simulations and VRU data.

At this point, one has a description of the total number of vehicles in the regional or county fleet over the entire modelling period. This absolute value can be disaggregated into groups of vehicles based on engine size, fuel type and vehicle age. The standard engine size bands are  $< 1.4$  l,  $1.4 - 2.0$  l and  $> 2.0$  l for petrol engines, and  $< 2.0$  l and  $> 2.0$  l for diesel engines. For both fuel types, the current EURO Standards are given by Pre-EURO Engines and EURO 1 to EURO 4 Engines. Table 1 describes the current passenger car split for Ireland in 2006. Similar data sets can be extracted from Vehicle Registration Unit data for the counties in question and hence the region.

Thus, at this point in the exercise, one should have a

description of the total vehicle fleet and a description of the relative contributions based on engine size, fuel type and vehicle age, which may be described by a set of matrices:

$$M(v_p) = \begin{pmatrix} v_{11} & \cdots & v_{1n} \\ \vdots & \ddots & \vdots \\ v_{m1} & \cdots & v_{mn} \end{pmatrix}_p \quad (1)$$

$$M(v_d) = \begin{pmatrix} v_{11} & \cdots & v_{1n} \\ \vdots & \ddots & \vdots \\ v_{m1} & \cdots & v_{mn} \end{pmatrix}_d \quad (2)$$

where  $p$  and  $d$  represent petrol and diesel vehicles respectively,  $v$  is the number of vehicles in each category, described in terms of engine size,  $n$ , and emissions standard,  $m$ .

#### 4.2 Emissions Determination

The determination of emissions is not a trivial task, particularly when trying to predict emissions levels in the future. Recent legislative limits have seen significant reductions in permitted emissions values, as described in the European Directives, but many argue that there is little room for further emissions reduction from conventional vehicles through engine adjustments (EEA, 2008) and after treatment is quickly reaching saturation. This, coupled with a reduced supply of petrol and diesel does point to the fact that conventional vehicles may not be used in the future. In this particular work, we will assume that conventional vehicles do retain their dominance in the fleet, although this is not at all certain.

Emissions can be determined in a number of ways, either by direct measurement of emissions or by application of emissions factors<sup>3</sup> based on empirical expressions derived from real-world tests. The most useful data sets for this work would come in the form of the COPERT (Computer Programme to estimate Emissions from Road Transport) or the TRL (Transport Research Laboratory) emissions factors. Both these inventories describe emissions in terms of grams per kilometre travelled ( $\text{g km}^{-1}$ ) and are functions of vehicle speed, such that for the TRL factors:

$$EF_{i,m,n} = k + a\dot{x} + b\dot{x}^2 + c\dot{x}^3 + \frac{d}{\dot{x}} + \frac{e}{\dot{x}^2} + \frac{d}{\dot{x}^3} \quad (3)$$

where  $a$ ,  $b$ ,  $c$ ,  $d$ ,  $e$ ,  $f$  and  $k$  are coefficients specific to a given engine size,  $m$ , and technology level,  $n$ ,  $\dot{x}$

<sup>3</sup> A value to describe pollutant emissions as a function of distance travelled. Certain factors take the vehicle velocity at the time of testing into account and so change as a function of vehicle speed



**Table 1** – Fleet composition in Ireland in 2006 based on standard bands. The total vehicle fleet is 1,661,482. Values in brackets indicate the percentage of the total fleet in each category. Taken from VRU data.

Emission Standard	Petrol Engines			Diesel Engines	
	<1.4 l	1.4–2.0 l	>2.0l	<2.0 l	>2.0 l
Pre-Euro	44,390 (2.67%)	22,685 (1.37%)	2,428 (0.15%)	8,395 (0.51%)	1,863 (0.11%)
EURO 1	143,078 (8.61%)	62,516 (3.76%)	4,701 (0.28%)	31,064 (1.87%)	5,512 (0.33%)
EURO 2	382,574 (23.03%)	148,044 (8.91%)	10,874 (0.65%)	58,309 (3.51%)	8,505 (0.51%)
EURO 3	343,218 (20.66%)	233,981 (14.08%)	16,901 (1.02%)	107,965 (6.50%)	24,469 (1.47%)

is the average vehicle speed in kilometres per hour ( $\text{km h}^{-1}$ ) and  $EF_{i,m,n}$  is the emissions value, in grams per kilometre travelled ( $\text{g km}^{-1}$ ) for a given species  $i$ , of age  $m$  and engine size,  $n$ . Emissions calculations exist for each of carbon dioxide ( $\text{CO}_2$ ), carbon monoxide (CO), particulate matter (PM), oxides of nitrogen ( $\text{NO}_x$ ) and unburned hydrocarbons (UHC).

A similar equation exists for the COPERT model and takes the form<sup>4</sup>:

$$EF_{i,m,n} = \left( \frac{\alpha + \gamma\dot{x} + \epsilon\dot{x}^2 + \zeta\dot{x}^{-1}}{1 + \beta\dot{x} + \delta\dot{x}^2} \right) (1 - RF) \quad (4)$$

Here,  $EF_{i,m,n}$  and  $\dot{x}$  have the same meanings and units as above and  $\alpha, \beta, \gamma, \delta, \epsilon, \zeta$  and  $RF$  are coefficients specific to a given engine size,  $m$ , and technology level,  $n$ .

Using either methodology, it is possible to construct a further set of matrices to represent emissions at a given speed, which would take the form:

$$M(e_p) = \begin{pmatrix} e_{11} & \dots & e_{1n} \\ \vdots & \ddots & \vdots \\ e_{m1} & \dots & e_{mn} \end{pmatrix}_p \quad (5)$$

$$M(e_d) = \begin{pmatrix} e_{11} & \dots & e_{1n} \\ \vdots & \ddots & \vdots \\ e_{m1} & \dots & e_{mn} \end{pmatrix}_d \quad (6)$$

where  $e$  represents the emissions factor ( $\text{g km}^{-1}$ ) of a given species, and all other symbols have the same meaning as previously.

Some further analysis is necessary if emissions are to be predicted into the future. Currently five EURO emissions standards exist, as described above. However, work is already being carried out in preparing EURO 6 and beyond. Thus, trend analysis of recent standards is required to develop a model to predict likely emissions standards in the future. This

<sup>4</sup>The particular equation is suitable for use with EURO 3, spark ignition engines. Similar, but not identical, equations exist for other categories of vehicles. A full listing of these equations is given in the COPERT software.

trending must be coupled with an understanding of realistic changes to the standards. It is foolish to propose a 50% reduction in  $\text{CO}_2$  emissions by 2015, based on current conventional vehicle trends, for example.

It is necessary to have an accurate value for total distance travelled for each vehicle category in each county, for a proper description of the aggregated emissions.

$$M(e_p) = \begin{pmatrix} x_{11} & \dots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \dots & x_{mn} \end{pmatrix}_p \quad (7)$$

$$M(e_d) = \begin{pmatrix} x_{11} & \dots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \dots & x_{mn} \end{pmatrix}_d \quad (8)$$

where  $x$  is the distance travelled per year (km) and all other symbols have the same meaning as previously.

These data could be extracted from various sources such as the NCT (National Car Test) data set and from the new POWCAR (Place of Work Census Anonymised Records) data set. This, again, is not a trivial task since both data sets are very large and their use is relatively restricted for security reasons. These data sets, or their previous analogues, have been instrumental in calibrating transport models, such as the one employed by the DTO (Dublin Transportation Office).

Since it is likely that vehicles from different engine size and technology level categorisations will travel different total distances, it is important to have a method of predicting the likely changes in distances travelled. It may be possible to extract this data from the MOLAND model. Within the model, a series of indicators exist, one being the distance indicator. This parameter can be used to describe the change in distance between the centroids of clusters of cells of a given land use. It would seem reasonable to suppose that people live in residential areas but work in commercial or industrial area, thus creating an origin and destination matrix, of sorts.



Determining the distances between them, both now and in the future, should describe the change in distance travelled. However, the current system as incorporated into MOLAND can only describe the shortest straight line distance and does not describe flow through the transport network and so is only suited to showing increases in travel distances over time, provided a base year distance exists. No account is taken of the real network and so congestion cannot be adequately modelled.

### 4.3 Aggregated Emissions

It is possible to multiply each of the matrices discussed above to determine the relative contribution of each category of vehicle in each county.

$$E_{tot,i} = M(v) \cdot M(e) \cdot M(x) \quad (9)$$

where  $E_{tot,i}$  represents the total mass of emission species  $i$  (g), and  $M(v)$ ,  $M(e)$  and  $M(x)$  are the matrices as discussed previously. From the point of view of informing policy makers, it is now possible to show which vehicle categories contribute most significantly to emissions output and hence poor air quality. It is also possible to test policy decisions by switching certain vehicle classes ‘off’ (by replacing their vehicle number by zero in the appropriate matrix and reassigning the number of vehicles to other categories) and examining the effects on aggregated pollutant levels.

## 5 Limitations of MOLAND in modelling air quality

While this is a very useful piece of data, it unfortunately does not answer all the required questions, namely, where do peak emissions occur, how are they dispersed and who is affected.

The system proposed thus far does not describe the spatial distribution of the pollution. Instead, it describes the total output of pollution from the region or subregion. Since all of the distance lines, as described above, are straight, there is little opportunity to assign emissions to routes in a meaningful way. It would also not be particularly useful to assign emissions to just one landuse class, say residential, since the emissions are formed in moving from home to work, school or recreation and back again. Perhaps it would be more useful to split the emissions, assuming that the trip to work is the same as the trip back home, between both residential and employment classes.

It may also be more useful to assign emissions based on density of development. Within MOLAND, with regard to the residential landuse classes, there are

four categories based on density, ranging from continuous dense urban fabric to discontinuous sparse urban fabric. However, these densities refer to the density of the built surface and not to the population. While there is obviously a density value within the system, this is not readily accessible. Without this value, it is difficult to assign population numbers and hence vehicle numbers, and emissions, to any residential land class. The same is true of the economic sectors, such as commercial and industrial. Currently there is no value for job density within the system that can be accessed easily. Thus, assigning destination data to these areas is also difficult. So, even with just the associated density values, total emissions could be disaggregated, according to origin and destination at least, between residential (home) land classes and commercial or industrial (work) classes.

In order to circumvent these issues, it would be necessary to use ancillary data sets, such as outputs from transport models, such as SATURN, as employed by the DTO. The difficulty with this is the need to run multiple models in isolation, whereas in reality, transport usage is influenced by, and influences, landuse, and vice versa. Thus, such a system would require that the new total vehicle number and the vehicle split data be determined for each year, fed into SATURN, the origin destination matrix be determined for each year based on the landuse and population figures, and the model be run. This would have to be done manually for each modelled year based on the population figures and the landuse map from the previous year. While such a situation is workable, it does necessitate many extra processing steps and would be exceptionally time consuming. Such a model would, of course, allow for better spatial representation of the vehicle movements, since a full network is required and modelled but the extra effort quickly erodes its usefulness. Overlaying of this map on the MOLAND landuse maps should allow for assessment of who is affected.

## 6 Methods of improving MOLAND as a system to estimate emissions

In recent months, much work has been carried out by RIKS and the JRC on the development of an integrated transport model for use in MOLAND ([van Delden et al., 2008](#)).

The transport model takes a number of inputs, many of which are very similar to the inputs required by SATURN. These inputs include a description of the transport zones within the modelling area, a map of the transport network and a series

of matrices to describe inter-zonal movements.

These matrices describe the total number of trips required, the length of the trips and the time taken for the trip. Thus average speed can be extracted from the system. A cost matrix, to account for tolls or delays, can also be applied. The model is also able to account for the differences in trip type, according to the time of day – clearly, the vast majority of morning trips will be associated with travelling to work and school, whereas evening trips will most likely be social or personal in nature. Account is also taken of the degree of urbanisation of an area, to account for congestion associated with various land classes.

While this does not necessary expand the functionality of MOLAND beyond that of SATURN, the most significant advantage is that the transport model links directly with the landuse change model. Thus, changes in the origin and destination matrices and the distance matrices, as a result of urban development or redevelopment, are automatically included in the next simulation year, reducing the need for loose coupling of multiple models.

This integrated model would also provide a solid link between the transport network and the landuse map, making it significantly easier to assign emissions to specific locations, and hence gauge the level of exposure and the number of people affected.

Clearly, such a model can provide a significant amount of data about the movement of vehicles within the network and the changes in flows as a result of development. The fact still remains, however, that the actual determination of vehicle fleet composition and emissions output will have to take place outside the MOLAND model. The subsequent use of Geographic Information Systems (GIS) for the purpose of describing emissions dispersion is also required.

## 7 Conclusions

In its current form, MOLAND does provide a relatively sound basis for the estimation of emissions from road vehicles. However, the wide variety of required ancillary data sets makes it somewhat cumbersome. These data sets do require a certain degree of manipulation to make them suitable for use in such an application.

With the inclusion of the MOLAND Transport Model, significant improvements in terms of landuse influences and spatial representation can be made. It is imperative, from the point of view of

a functioning air quality model, compatible with MOLAND that the transport model be used. The inclusion of the Transport Model does come at a cost, however. There is a significant overhead in terms of preparing the required data sets for inclusion in the model. It may be possible to work with other organisations, such as the DTO, who have a firm understanding of such models, in an attempt to further develop the viable use of the Transport Model.

In the interim, further work will be done using the current system in an attempt to further develop the methodology and examine the application of various MOLAND scenarios to the emissions inventory.

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