

FINAL REPORT

VANCOUVER OXIDANT STUDY

DEVELOPMENT OF EMISSIONS DATA BASE

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EXECUTIVE SUMMARY

The Canadian national ambient air quality objectives specify that the maximum acceptable one hour average concentration of ozone is $160 \mu\text{g m}^{-3}$ (82 ppb). This level is frequently exceeded in Vancouver. In fact, the maximum tolerable concentration ($300 \mu\text{g m}^{-3}$ or 151 ppb) has also been exceeded several times each year since at least 1978.

Development of an ozone control strategy for Vancouver will require the use of a computer model of transport, dispersion and photochemical transformation, in conjunction with an inventory of emissions of oxides of nitrogen (NO_x) and volatile organic compounds (VOC) for the region. This report reviews existing models which have been used in this way, and provides a plan for the construction of an appropriate emission inventory.

The models reviewed were EKMA/OZIPP, a photochemical box model, and three Eulerian models (LIRAQ, UAM and the model developed by Seinfeld and coworkers for application to Los Angeles.). On the basis of this review it has recommended that an Eulerian model based on the formulation of McRae, Goodin and Seinfeld (1982) be developed for Vancouver. This approach is to be preferred over acquiring the model code from the developers, because it ensures familiarity with the operation of the model.

Development of this model will probably take one to two years. It is therefore, recommended that initial control strategy development be based on the EKMA/OZIPP procedure, with an upgraded chemical mechanism incorporated in the OZIPP model.

The format of the emission inventory for Vancouver is largely dictated by the input requirements of the model. The recommended format is:

Domain: Bounded by the U.S. border in the south, the watershed boundary in the north, the water's edge in the west and to include Chilliwack, B.C. in the east. Consideration should be given to extending the eastern boundary to Hope, B.C. if this is required to contain the full travel of air parcels moving under the influence of land breeze/sea breeze circulation.

Grid Size: 5 by 5 kilometers on the UTM grid.

Temporal Resolution: 1 hour.

Chemical Species: NO, NO₂, and at least 6 VOC classes (ethylene, other alkenes, alkanes,

aromatics, formaldehyde and other aldehydes). The emission inventory currently under development in Ontario considers 10 VOC classes. If review of this work (when available) indicates that reliable speciation factors are available for 10 classes, ten should also be used for Vancouver to accommodate possible future model developments.

Source Types:

Point, line and area sources to be included.

This inventory will be suitable for use with the recommended Eulerian model, and also with the simpler modelling approaches recommended for interim use.

For compiling point source emissions GVRD files, and the experience and expertise of the GVRD inspectors will form an important resource. Data from source testing will be incorporated where possible.

Area and line source emissions will normally be calculated as the product of an emission factor and an activity rate. Wherever possible, emission factors appropriate to Canadian conditions will be

used. Sources of the required emission factors and activity rates have been identified for each of the source sectors involved, including vegetative emissions. Typical examples of activity rates are amount of fuel consumed per unit time for combustion related sources, and vehicle miles travelled per unit time for motor vehicles.

Spatial and temporal resolution of the activity rates will also be required, and will be obtained from local sources (e.g. traffic count data), supplemented by published values. Chemical speciation of the VOC emissions will be based largely on information obtained from the literature.

The combination of the computer model and emission inventory described in this report will provide the tool required to develop cost effective control of oxidant levels in Vancouver. The model will be suitable for use in other affected areas in Canada and elsewhere.

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1. INTRODUCTION

The Canadian national ambient air quality objectives specify that the maximum acceptable one hour average concentration of ozone is $160 \mu\text{g m}^{-3}$ (82 ppb). This level is frequently exceeded in Vancouver. In fact, the maximum tolerable concentration ($300 \mu\text{g m}^{-3}$ or 151 ppb) has also been exceeded several times each year since 1978 (CSC, 1982).

A study of air quality in the area, with particular reference to ozone (CSC, 1982) indicated that these high ozone concentrations arise from photochemical transformation of locally emitted precursors. Control of ozone in Vancouver therefore requires control of local emissions, particularly emissions of volatile organic compounds (VOC).

Oxidant control strategies will be based, in large measure, on application of a computer model of transport, dispersion and photochemical transformation, in conjunction with an accurate emission inventory for the region. The study described in this report was designed to identify a suitable model and to provide a detailed plan for the construction of an emission inventory for oxides of nitrogen (NO_x) and VOC for Vancouver.

Specifically, the terms of reference were:

- Review current ozone control strategies with respect to the photochemical model used, and the format of the emission data base.
- Recommend a model or models to be used in Vancouver.
- Describe the data required for the implementation of the model(s).
- Provide a detailed plan for the construction of an emission inventory for oxides of nitrogen (NO_x) and volatile organic compounds (VOC) for the Vancouver region.
- Provide a time and cost estimate for the construction of the emission inventory.

The organization of this report is as follows. Chapter 2 contains a brief overview of ozone formation in the atmosphere. Existing and proposed oxidant control strategies are discussed in Chapter 3, with particular reference to photochemical models and their associated emission inventories. The detailed design plan for the Vancouver emission inventory is given in Chapter 4, while Chapter 5 discusses the issues to be addressed in implementing a photochemical

model for Vancouver. Chapter 6 presents detailed cost and time estimates for the actual construction of the Vancouver emission inventory, and the conclusions and recommendations of the study are summarized in Chapter 7.

2. OVERVIEW OF ATMOSPHERIC CHEMISTRY

Detailed mechanisms of atmospheric photochemistry, including the reactions of organic species, have been published by a number of authors (e.g., Demerjian et al., 1974; Derwent and Hov, 1980; Falls and Seinfeld, 1978; Lloyd, 1978; Graedel et al., 1976). Stated briefly, the production of atmospheric ozone is as given below:

Ozone formation is generally initiated by the photolysis of NO_2 , followed by reaction of the resulting oxygen atom with an oxygen molecule.



The reverse reaction also occurs.,



and a stationary state is often reached where the net rates of the forward and reverse reactions are equal.

$$\text{i.e. } k_1 [\text{NO}_2] = k_2 [\text{NO}] [\text{O}_3]$$

$$\therefore [O_3] = \frac{k_1[NO_2]}{k_2[NO]} \quad (a)$$

(Reaction 2 is very rapid and is assumed to occur essentially instantaneously).

The implication of equation (a) is that enhanced conversion of NO to NO₂ will produce an enhancement of ozone production.

The importance of organic species in the atmosphere arises because they are readily converted to reactive species (notably peroxy radicals, RO₂) which bring about the conversion of NO to NO₂.



The initial step in the conversion of VOC usually involves cleavage of the organic molecule to produce a free radical. This may occur as a result of photolysis, or following attack by OH, O or O₃.



Rapid reaction of the free radical then takes place, often involving oxygen molecules and producing peroxy radicals.



Other reactions lead to the formation of hydroxyl (OH) and hydroperoxy (HO₂) radicals.

The importance of organic species in ozone production is underscored by combining reactions 1, 2, 4 and 6.



This indicates that the net effect of the free radical (plus light) is to bring about the conversion of oxygen to ozone. Note in particular that the oxides of nitrogen are not consumed in this process, which can thus continue as long as hydrocarbons are present. However, a certain amount of NO_x is required before the process can begin.

All organic compounds are not equally effective in producing the reactive species important in the reactions discussed above. Ideal-

ly each compound should be considered separately, but this approach is not feasible, since upwards of 400 organic species have been identified in the atmosphere (Graedel, 1978). It is, therefore, general practice to group organic species into classes, within each of which the reactivities are approximately equal. There is wide variation of the number of classes used, as will be seen in the discussion of models in Section 3.1. Typically, subdivision ranges from four classes for many models (e.g. Demerjian and Schere, 1979a; Penner, 1984) to ten for a large model currently under development for the Province of Ontario (Wong, 1984), and as many as thirty-five in one example (Derwent and Hov, 1980).

It should be stressed that this is a very brief review of the relevant chemistry, omitting a number of the finer details, e.g. the fate of the various reaction products. Many of these are themselves reactive species, thus enhancing the effects discussed above.

3. REVIEW OF CONTROL STRATEGIES

With very few exceptions, descriptions of oxidant control strategies originate from the United States. Central to all of these strategies is the use of some sort of mathematical model to relate pollutant emissions to ambient air quality. However, the models cover a very wide spectrum in terms of their complexity and the degree of realism with which they reflect atmospheric transport, dispersion and transformation. This in turn has resulted in a wide range of degrees of complexity in the required emission inventories.

Models in modern use in oxidant control strategy development (current and proposed) and the associated emissions data base formats are discussed separately below.

3.1 Models

The earliest reported examples of oxidant control in the U.S. made use of rollback type models in estimating the emission reductions required to achieve the desired air quality standard. These assume a linear relationship between the rate of pollutant emission (non-methane hydrocarbons in the case of ozone) and the peak atmospheric concentrations of the species of interest.

This procedure takes no account of the complexities of atmospheric chemistry, as outlined briefly in Chapter 2, and will therefore not be considered further. Four possible modelling procedures will therefore be reviewed here:

- Empirical Kinetic Modelling Approach (EKMA)
- Box Models
- Lagrangian (trajectory) models
- Eulerian models.

Note that this review includes only those models which have actually been applied in ozone control strategy, or are proposed for this use. Models falling under the four different headings are discussed in more detail below.

3.1.1 EKMA

The empirical kinetic modelling approach is described separately because it is currently the most widely used modelling technique employed in oxidant control. It is, however, not a separate type, being in fact a simple trajectory model, which has been used in a number of slightly different forms. The so-called city-specific EKMA, or Level III Analysis (U.S. EPA, 1981), is the most widely applicable, and is the version which will be discussed here.

The EKMA procedure properly consists of two parts. The first part involves the application of a computer model (OZIPP - the ozone isopleth plotting package) to relate the mid-afternoon peak ozone concentration to measured concentrations (6 a.m. to 9 a.m. average) of NO_x and non-methane hydrocarbons (NMHC).

OZIPP follows the chemical reactions in a column of air which originates at the urban core at 8 a.m. Initial concentrations within this column are the measured 8 a.m. (or 6 a.m. to 9 a.m. average) concentrations, and provision is thus made for consideration of ozone and other species transported from other areas. The column of air is assumed to follow a straight line trajectory at constant velocity to the point at which the peak ozone concentration is observed. Along this trajectory NO_x and NMHC are emitted into the column, and dilution occurs as the mixing height rises. The emissions are input on an hourly basis, and are scaled relative to the "initial" emission rate. This quantity is calculated in terms of the rate of emission per unit surface area into the column of air at 8 a.m. which gives the observed 8 a.m. concentration of that species.

Organic compounds are considered to consist of 25 % propylene plus 75 % n-butane, with addition of a further 5 % of acetaldehyde.

The output from OZIPP is a set of ozone isopleths relating the peak ozone concentration to the 8 a.m. NO_x and NMHC concentrations.

These isopleths are then used in the second part of the procedure to calculate the reduction required to achieve the desired ozone level.

EKMA is simple to apply, and its data requirements are modest. However, it has been subject to considerable criticism of late. In particular, the chemistry package in OZIPP has been felt to be too highly simplified to represent reality at all adequately (e.g. Jones et al., 1983; Hov and Derwent, 1981; Carter et al., 1982).

Other possible problem areas include the assumption of a straight line trajectory followed at uniform velocity, and the implicit assumption that atmospheric NO_x and NMHC concentrations are directly proportional to emission rates. This assumption is made in the scaling of emission rates, and also when the required reduction in 8 a.m. concentration is translated into a reduction in emissions. The current scientific direction therefore appears to be to the use of more complex models.

3.1.2 Box Models

In one respect box models are actually less complex than EKMA, in that the photochemistry is allowed to take place within a stationary parcel (or box) of air located over the entire urban area. Pollutant transport and dispersion are thus greatly simplified, and it is assumed that emitted pollutants are instantaneously and uniformly mixed

throughout the volume. This simplification makes it possible to include a detailed photochemical mechanism in the model, without placing great demands on available resources.

An example of a box model which has been used in the assessment of air pollution abatement strategies is described by Derwent and Hov (1980) and Hov and Derwent (1981). This model was applied to the airshed of London, England, and included an unusually detailed chemical mechanism. The reactions of 39 precursor species were considered (NO , NO_2 , CO , SO_2 and 35 organic compounds), and a further 145 inorganic and organic intermediates were involved.

Other processes affecting pollutant concentrations which are normally treated in box models are:

- dilution as the mixed layer depth increases
- simultaneous entrainment of species originally above the mixed layer
- advection of pollutants into and out of the box
- dry deposition (wet deposition is usually not treated, since box models are designed for assessment of short-term effects driven by solar radiation).

Box models are, like EKMA, simple to apply and also have relatively modest input data requirements. They have been proposed for use

in preliminary screening of air quality problems and control strategies. However, because they treat the airshed as being entirely homogeneous, they are unlikely to prove adequate in areas which have complexities and/or non-uniformities of terrain, wind field or emissions.

3.1.3 Lagrangian Models

Lagrangian models consider pollutant dispersion and transformation relative to a coordinate system transported with the air parcel. The use of Lagrangian models in air quality studies has been described in the literature (e.g. Lurman et al., 1982). However, they have apparently not been used in the development of oxidant control strategies. This is understandable, since, although the Lagrangian formulation is ideally suited to the evaluation of effects downwind of a single source, its application to an urban airshed requires a run for each source (or group of sources), with superposition of the resulting concentration fields. Alternatively a receptor based approach may be used, with back trajectories, necessitating a run for each receptor or group of receptors.

Under certain circumstances, e.g. if control of the emissions of a restricted source region is required, use of a Lagrangian model will offer advantages. This possibility should be borne in mind for Vancouver.

3.1.4 Eulerian Models

Eulerian models consider the transport, dispersion and transformation of pollutants within a fixed coordinate system. Although more demanding of resources than Lagrangian models on a run for run basis, they provide air quality simulation for an entire airshed in a single run. As noted above, the same result would typically require many runs of a Lagrangian model. Modern usage therefore appears to represent a continuing trend towards the use of Eulerian models in oxidant control strategy development. Three such models have been identified as being used, or proposed for use, in oxidant control strategies. These three models are described separately below.

3.1.4.1 LIRAQ

The Livermore Regional Air Quality Model (LIRAQ) was described by MacCracken et al., (1978). Designed for use in the San Francisco Bay area, LIRAQ uses a grid which may have dimensions of 1, 2 or 5 km, and treats a single layer in the vertical. In practice, two versions of LIRAQ were described. LIRAQ-1 considered only essentially inert species, such as CO, and employed a relatively sophisticated diffusion scheme. Maximum model domain size, limited by the memory size of the computer, was 45 by 50 grid squares.

LIRAQ-2 was able to treat the photochemical reactions of 19 chemical species, but required simplification of the transport/dispersion and restriction of the model domain (to 20 by 20 grid squares). The chemical mechanism included reactions of three classes of organic compounds (alkenes, alkanes and aldehydes). In addition to these three species, emission data were required for NO, NO₂ and CO.

LIRAQ-2 has since been upgraded to incorporate the reactions of aromatic compounds. Attempts to verify LIRAQ for St. Louis data (Shreffler and Schere, 1982) were unsuccessful, because of problems associated with implementing it on a computer other than its normal host. Good correspondence between LIRAQ predictions and measured data was subsequently reported by Penner et al., (1983) for both San Francisco and St. Louis.

LIRAQ was then used to determine the extent to which organic compound emissions must be controlled to bring the Bay area into compliance with the requirements of the Clean Air Act (Hunsacker et al., 1984). The indication is that these emissions must be reduced by 378 tons per day (or approximately 35%). Further development work on LIRAQ is under way (Penner, 1984). This includes the addition of a second vertical layer, and extension of the modelling domain. These improvements will allow the simulation of multi-day events.

3.1.4.2 UAM

The Urban Airshed Model is included in the North East Corridor Regional Modelling Program (NECRMP). Initial plans called for application of UAM to all five major urban areas in the North East Corridor (Washington, D.C., Baltimore, Philadelphia, New York City and Boston). Modelling of the Philadelphia airshed has commenced (Cole, 1981); resource limitations may, however, restrict further urban modelling work in this program.

Apart from its use in NECRMP, UAM has also been applied to a number of other urban airsheds in the U.S. and also in Great Britain and the Netherlands (SAI, 1984). It has, like other large models, undergone continuous refinement and evolution over its lifetime (Tesche, 1981).

The model domain of the current version covers 30 by 30 grid squares, each normally two miles on a side. There are up to 7 layers in the vertical. The chemical mechanism used in UAM is the carbon bond mechanism (CBM) described by Whitten et al., (1980). Five classes of reactive organic compounds are normally considered - olefins, paraffins, carbonyls, aromatics and ethylene.

UAM has been subjected to a number of sensitivity tests and validations (Tesche, 1981; Seigneur et al., 1981). Its capabilities

have been recognized in that it has been selected for the urban modelling component of NECRMP. However, it remains the property of its developers, System Applications, Inc. of San Rafael, California. For this reason it is difficult to obtain details of its formulation, and it is unlikely that it will be released for use by outside agencies.

3.1.4.3 McRae and Seinfeld

An Eulerian model for urban scale application has been described by McRae et al., (1982) and McRae and Seinfeld (1983). It is our understanding that this model has been developed for use in ozone control strategy development for the California South Coast Air Basin, and it possesses a number of features which mean that it currently represents the state of the art in urban scale photochemical modelling.

The modelling domain is subdivided into 5 by 5 km grid squares, and also includes vertical resolution. The test runs described by McRae and Seinfeld (1983) were for a domain of approximately 50 by 26 grid squares (the domain was not rectangular) with five vertical layers. The model is able to simulate multi-day events, particularly with regard to the storage of ozone (and other species) above the nocturnal inversion, with downward mixing the following day. Care was taken to ensure that the model domain was large enough to contain the respective out and return flows of the land breeze and subsequent sea breeze.

The chemical mechanism considers the reactions of, among other species, NO , NO_2 and four VOC classes (alkanes, olefins, aromatics and oxygenated compounds).

Further examples of the care which has been taken in the formulation of the model are:

- 1) the solar intensity is adjusted for variation with altitude, corresponding to increased absorption and scattering as the altitude decreases.
- 2) Point source emissions are treated separately, according to whether or not they penetrate into elevated (stable) layers. The plumes from point sources are allowed to retain their identity, and spread downwind following a Gaussian prescription. The alternative method, used in most models to date, is to assume that point source emissions are added to the grid cell which corresponds to the position of final plume rise. This approach is computationally simpler, but can cause serious errors in the calculation of chemical reaction rates, since the desired cell average reaction rate is properly derived from the cell average of the product of concentrations at all points in the cell. This can be very different from the product of the cell average of concentrations, which is given by the second procedure described above.

To date, the performance of this model has been tested against measured data for the California South Coast Air Basin corresponding to the 26th and 27th of June 1974 (McRae and Seinfeld, 1983). Very good agreement was demonstrated.

3.2 Emission Inventories

This review of emission inventories will generally concentrate on those which have been used in conjunction with the models described in Section 3.1. A more comprehensive review of recent emission inventory work has been given by CSC (1983).

3.2.1 Emission Inventory for use with EKMA

The emission inventory requirements for EKMA are described by the US EPA (1981). Since EKMA makes use of a trajectory formulation, emission data are only required for that area covered by the trajectory. However, the trajectory path will vary from day to day, which means that in practice the entire study area must be inventoried.

The recommended inventory procedure for EKMA (US EPA, 1981) involves assembling total emissions of reactive VOC and NO_x on a county wide basis. These emissions are adjusted seasonally and then assumed to occur uniformly in each hour within the season, i.e. the emissions for the season are divided by 2190 hours per season.

If finer resolution (spatial or temporal) is available, EKMA can make use of these data. However, it is not recommended that a gridded inventory be specifically developed for use with EKMA (US EPA, 1981). Also, because of the averaging assumptions implicit in the OZIPP/EKMA formulation, a spatial resolution finer than 10 x 10 km should not be used.

It should be noted that county scale emission data for the United States are contained in the National Emission Data System (NEDS) maintained by the US EPA. Also the Canadian National Emissions Inventory System (NEIS) maintained by the Environmental Protection Service contains source sector emission data based on census divisions. This spatial resolution is compatible with the scale requirements of the EKMA/OZIPP model.

3.2.2 Emission Inventories for Box Models

For photochemical box models no spatial resolution of the emission data is required. It will be necessary, though, for the emission inventory area to correspond to that of the model. The temporal and chemical resolution will be as required by the model.

Thus, for the box model described by Derwent and Hov (1980), emissions were required for a domain extending 32 x 50 km over London. A resolution of 1 hour was required, and emissions data were required

for NO, NO₂, SO₂, CO and thirty-six volatile organic compounds. This level of chemical speciation is very much more detailed than has been required for any other emission inventory described in the literature.

3.2.3 Emission Inventories for UAM

Two emissions inventories have recently been described, which were specifically designed for use with the Urban Airshed Model. These inventories were constructed for Tulsa, Oklahoma (Engineering - Science, 1980) and Philadelphia (Engineering - Science, 1982), and included data for NO, NO₂, SO₂, TSP and 5 reactive VOC classes.

Tulsa was covered in a 2 x 2 km grid, requiring 1550 grid squares in total. For Philadelphia, 502 grid squares were used, each 5 x 5 km. For both cities, area source emissions were generally calculated as the product of an activity rate and an emission factor (US EPA, 1977).

For a few source sectors, direct spatial apportionment was possible (e.g. in the case of aircraft emissions) but for the majority of sectors, spatial apportionment was made on the basis of surrogate parameters. (e.g. population, dwelling units, total employment or commercial employment.)

For point sources stack data (location, height and internal diameter and stack gas temperature and exit velocity) were stored together with the emission data. These emission data were obtained from existing inventories wherever possible, with supplementation by questionnaire and site visit as required.

For both point and area sources VOC and NO_x split factor files and temporal split factor files were developed. The former files, contain chemical speciation data for each source sector or process, as follows:

For VOC emissions

- paraffins
- olefins
- aromatics
- carbonyls
- ethylene
- non-reactive species

For NO_x emissions, the split is between NO and NO₂. In general these data were obtained from the VOC Species Data Manual (US EPA, 1980), and were supplemented where necessary with data from the Regional Air Pollution Study (RAPS) in St. Louis (Rockwell, 1978) and the North East Corridor Regional Modelling Study (NECRMP) (US EPA, 1980).

The preferred method for obtaining the temporal profile of emissions for each source sector, was by direct contact with individuals working in the appropriate area. Where this was not possible, data developed for RAPS were also used (US EPA, 1975; 1976) together with other data from the US EPA (1978). The final temporal resolution is by hour of day for a typical weekday during the ozone season (June, July and August).

3.2.4 San Francisco Emission Inventory

Perardi et al. (1979) have described an emission inventory for the San Francisco Bay area. This is resolved on a 1 x 1 km grid for a 20,000 square kilometer area, and has a 1 hour temporal resolution through a typical summer day. These features were designed for compatibility with the model LIRAQ (McCracken et al., 1978).

Considerable emphasis was placed on accurate estimation of automotive emissions, with attention to trip type, vehicle class and age, hot or cold start, etc. These emissions were calculated by means of a link type traffic model, which included approximately 14,000 links and 440 zones. The output from the link model was combined with an emissions model to obtain the time-resolved emissions per link. Evaporative emissions from the hot vehicle at the end of the trip, known as hot soak emissions, were also included.

Spatial apportionment for other area sources was based on surrogate variables as in the case of the Tulsa and Philadelphia emission inventories. Temporal resolution was carried out by engineers of the source inventory group.

Major point sources were defined as those emitting more than 25 tons of a pollutant per year. Emissions data and temporal resolution were generally obtained from regulatory agency files and operating schedules.

Negative VOC emissions were also inventoried on the 1 x 1 km grid for San Francisco (Hunsaker and Moreland, 1982). The required emission factors were obtained by a Delphi survey of experts working in the field, and were combined with land use data derived from satellite (LANDSAT) photographs.

Neither of the reports of the San Francisco emission inventory (Perardi et al., 1979; Hunsaker and Moreland, 1982) discusses the chemical speciation of the emissions data. It must be presumed that this speciation is incorporated into the model as a pre-processor.

3.2.5 Los Angeles Emission Inventory

Several emission inventories have been described for the Los Angeles area (e.g. Lloyd et al., 1979). McRae and Seinfeld (1983) give

some details of the emission inventory used in conjunction with the model of McRae et al. (1982).

As required by the model, the emissions from 130 source categories were spatially distributed on the 5 x 5 km grid. Temporal resolution was provided to a scale of one hour, and VOC emissions were broken down to six classes (formaldehyde, other aldehydes, ethylene, other olefins, aromatics and aldehydes). Although apparently not used by McRae and Seinfeld (1983) in their modelling work, an inventory of vegetative VOC emissions is also available for the area (Winer et al., 1982). Emission factors were determined by an enclosure technique and land use apportionment was derived from high altitude photographs. Of particular interest is the procedure described by McRae and Seinfeld (1983) for estimating the errors in the emission data. For volatile organics, the error estimates incorporate a weighting of the uncertainty by the chemical reactivity of the species in question. Thus large uncertainties in methane emissions (for example) are unimportant because this species is essentially unreactive.

3.2.6 Ontario Emission Inventory

Although this inventory is not connected with one of the models described in Section 3.1, it is of interest because it is the most advanced emission inventory currently in Canada.

It has been constructed piece-wise. Existing data for all SO₂ and point source emissions were felt to be of good quality, so construction of the NO_x area source inventory was initiated in late 1982. Work on an inventory of VOC emissions commenced in late 1983 and is apparently now approaching completion.

The Ontario emission inventory features a variable grid spacing - 5 x 5 km in the most heavily populated or industrialised areas (e.g. Toronto, Sarnia-Windsor), 10 x 10 km for less populated areas, progressing to 50 x 50 and 100 x 100 km for remote areas. Temporal resolution is such that seasonal, day of week and hourly data are available. Ten classes of organic compounds are considered as required for the model of the transport and deposition of acidic pollutants (TADAP) currently under development jointly for Ontario, AES and West Germany. It is to be presumed that this inventory will also be required for the North East Corridor Regional Modelling Program (Cole, 1983), since south eastern Ontario falls into the modelling domain of that program.

3.2.7 Summary

A relatively small number of detailed emission inventories have been discussed here. These represent a small fraction of the

effort currently being devoted to emission inventory development, since it is now recognized that an accurate knowledge of emissions is essential in the assessment and control of air pollution problems.

It is clear from the discussion of emission inventories given above that there is considerable uniformity in their format and the methods used in their construction. This fact has been noted previously in a review of a larger number of inventories (CSC, 1983).

Model and emission inventory characteristics are summarized in Table 1.

Table 1

Summary of Models and Emission Inventories

Model	Type	City	Resolution		
			Spatial	Temporal	VOC speciation
EKMA	Trajectory	Many	-	1 hour	3 classes
Box	Box	London plus others	None	1 hour	up to 35 classes
UAM	Eulerian	Philadelphia plus others	2 km, Several layers	1 hour	5 classes
LIRAQ	Eulerian	San Francisco	1 km, 1 layer	1 hour	4 classes
McRae and Seinfeld	Eulerian	Los Angeles	5 km, 5 layers	1 hour	4 classes

3.3 Recommendations

3.3.1 Choice of Model for Vancouver

On technical grounds, the model described by McRae et al., (1982) has clear superiority over the other models reviewed here. This statement can be made even though full details of the UAM formulation could not be readily obtained.

LIRAQ is technically inferior in its limited vertical resolution. It has been shown to perform well in the San Francisco Bay area, but significant problems were encountered when an attempt was made to implement it elsewhere (Shreffler and Schere, 1982). These problems are attributable to difficulties encountered when implementing LIRAQ on a different computer system, and having it run by personnel not familiar with its formulation. LIRAQ makes use of special features of its normal host computer.

It is felt that simpler formulations (e.g. EKMA and box models) will not meet the long-term requirements for modelling of air quality in the Vancouver region. They may, however, provide valuable information in the short-term (see below).

It is therefore recommended that an Eulerian model be developed for the Vancouver area, based on the formulation of McRae et al., (1982). This approach is to be preferred over merely acquiring the model code from its developers (assuming that it would be made available), since experience has shown that a thorough understanding of the workings of such a model is essential if usable and meaningful results are to be obtained. Such an understanding is best obtained through actual construction of the model. The potential pitfalls of the alternative, or "black box", approach are exemplified by the experience of Shreffler and Schere (1982) with LIRAQ.

Construction of the Eulerian model will probably take in excess of a year. It is therefore recommended that an initial approach to oxidant control strategy development be based on a simpler modelling approach, such as EKMA or a photochemical box model. There appears to be very little difference between the two in terms of their respective resource requirements and applicability to the Vancouver situation.

Box models have been found to perform best in stagnant or near stagnant conditions (Shreffler and Schere, 1982) as are normally associated with ozone episodes in Vancouver. However, some difficulties might occur because of the complexities of the terrain in Vancouver. Concord Scientific Corporation has constructed a photochemical box model, which has been found to perform well in initial tests on the Toronto airshed (unpublished material).

EKMA/OZIPP is obtainable from the US EPA and a copy is held by EPS in Ottawa, though it has not yet been implemented (Dann, 1984). It is recommended that EKMA not be used unless the chemical mechanism is upgraded.

3.3.2 Emission Inventory Format

In contrast to the wide variations found in photochemical modelling formulations, there is a considerable degree of uniformity in the approaches and formats used in the current generation of emission inventories. This has also been noted in a previous review, which considered a larger number of emission inventories (CSC, 1983).

It is recommended that the emission inventory for the Vancouver area has the following characteristics:

Domain: Bounded by the U.S. border in the south, the watershed boundary in the north, the water's edge in the west and to include Chilliwack B.C. in the east. Consideration should be given to extending the eastern boundary to Hope, B.C., if this is required to contain the full travel of air parcels moving under the influence of land breeze/sea breeze circulation.

Grid Size: 5 by 5 kilometers on the UTM grid.

Temporal Resolution: 1 hour.

Chemical Species: NO, NO₂, and at least 6 VOC classes (ethylene, other alkenes, alkanes, aromatics, formaldehyde and other aldehydes). The emission inventory currently under development in Ontario considers 10 VOC classes. If review of this work (when available) indicates that reliable speciation factors are available for 10 classes, ten should also be used for Vancouver to accommodate possible future model developments.

Source Types: Point, line and area sources to be included.

This inventory will be suitable for use with the recommended Eulerian model, and also with the simpler modelling approaches recommended for interim use. The detailed plan for the construction of this inventory is given in the next chapter.

4. EMISSION INVENTORY PLAN

This chapter discusses in detail a plan for the construction of an emission inventory for NO_x and VOC for Vancouver. The following will be covered in separate sections.

- (i) Definition of point, line and area sources.
- (ii) Identification of the source sectors to be considered.
- (iii) Sources of speciation data for VOC emissions.
- (iv) Methods for determining the NO_x and/or VOC emissions and their temporal variation for each source sector, for each grid square.
- (v) Methods to be used in assessing the accuracy of the derived emission rates.
- (vi) Miscellaneous issues related to the construction and maintenance of the emission inventory.

In accordance with the recommendations of Chapter 3, the emission inventory plan assumes the use of a 5 x 5 km grid. A substantial portion of the study area is covered by the 1:25,000 series of the Canadian National Topographic Map System which will be used for spatial allocation of emissions. Maps from the 1:50,000 series will provide adequate resolution for the remainder of the study area. Since these maps normally only identify major streets, local street maps will probably also be required for accurate location of point sources.

4.1 Definition of Point, Line and Area Sources

It is proposed that the emission inventory for Vancouver consider line sources (i.e. major highways) in addition to point and area sources. Although few models in current use actually distinguish line sources from area sources, this approach allows future model refinements to be accommodated. It is a relatively simple matter to consolidate line source emissions into the appropriate grid square for use with current models. The reverse process, i.e. generation of line source data, requires considerably more effort.

The following definitions are proposed:

Point source: An individual source emitting at least 50 kg per day (averaged over one year) of the pollutant in question.

Line source: A highway which carries an average (over one year) of at least 24,000 vehicles per day (total of both directions).

Area sources: All other sources shall be included as area sources.

These definitions are compatible with those proposed for use in the Ontario emission inventory (CSC, 1983). Note that for point sources the 50 kg per day of pollutant is total NO_x or total VOC as appropriate. This definition is also compatible with that used in the emission inventories for Tulsa and Philadelphia (Engineering-Science, 1980; 1982) which specified a minimum of 25 tons per year.

City streets are specifically excluded from the definition of line sources, since the stop-go nature of city traffic will tend to introduce considerable non-uniformities of emissions along the street. The number of vehicles per day is averaged over a year to avoid the possible problem of highways which may meet the criterion for only a part of the time, eg. summer or weekends.

4.2 Source Sectors

4.2.1 Point Sources

No attempt will be made here to provide a definitive identification of all point sources to be included in the Vancouver emission inventory. The prime data source for identification of point sources will be the GVRD permit files and the personal knowledge, experience and expertise of the GVRD inspectors. Some examples of typical point sources are thermal power plants, oil refineries and municipal incinerators.

4.2.2 Area Sources

A basic list of source sectors which fall into the category of area sources is given below:

- Application of surface coatings
- Bakeries
- Crude oil production
- Diesel and gasoline marketing
- Diesel powered engines
- Dry cleaning
- Forest fires
- Fuel combustion-stationary sources
- Gasoline-powered motor vehicles
- General solvent use
- Landfill sites
- Natural gas production
- Non-highway use of gasoline
- Off-highway mobile sources
- Plastics fabrication
- Slash burning
- Solid waste incineration
- Structural fires
- Tire wear
- Natural sources

This list is used in the National Emission Inventory System (NEIS), and is similar to the lists used in most current emission inventories. It should be noted that the final data base will contain a finer resolution of some source sectors. For example, gasoline powered motor vehicles will be subdivided to automobiles, light duty trucks, medium duty vehicles, heavy duty vehicles, motorcycles and snowmobiles, while off-highway mobile sources comprise aircraft, railroads and marine sources.

Natural sources to be considered include:

Vegetation

Wetlands, swamps, bogs

Insects

Animals

Natural gas leakage

The natural sources emit essentially no NO_x , and, of the sources identified above, vegetation is the most important because of the emission of photochemically reactive species such as isoprene and the terpenes. The other sectors emit essentially only methane which is usually considered to be non-reactive.

The lists given above should not be regarded as closed since it is possible that data collected during the construction of the inven-

tory will result in the identification of additional sectors. A possible example follows from the suggestion (Rowlands, 1983) that, with the ban on chlorofluorocarbons, aerosol spray use in California now constitutes a significant source of organic compounds.

4.3 Sources of Speciation Data

As will be discussed in detail in Section 4.4, emissions are initially calculated in terms of mass NO_x or VOC emitted per unit time. For purposes of photochemical modelling the NO_x data must be partitioned into NO and NO_2 , while the VOC emissions must be allocated to the appropriate number of chemical classes. As was recommended in Section 3.3, six VOC classes will be used.

The split between NO and NO_2 generally lies in the range 75%/25% to 99%/1%, with the higher proportion of NO being associated with hotter, more efficient combustion (Engineering-Science, 1980). The prime source of data on the split between NO and NO_2 will be the compilation by Milligan (1979). These data were used in the preparation of emission inventories for Tulsa (Engineering-Science, 1980) and Philadelphia (Engineering - Science, 1982). They were also used in the emission inventories prepared for NECRMP (GCA, 1979). Apart from this compilation, very few data are available on the breakdown between NO and NO_2 . Exceptions are the information presented by Fanick and Dietzmann (1980) on natural gas compressor station engines, and

measurements made on automobile emissions (e.g. Lenner et al., 1983).

For the speciation of VOC emissions the prime data source will be the Volatile Organic Compound Species Data Manual (U.S. EPA, 1980). This is the second edition of the compilation used in the Tulsa and Philadelphia emission inventories (Engineering - Science, 1980, 1982), and has been used in the NECRMP inventories (GCA, 1979). A number of other sources will also be consulted for VOC speciation data, eg. Lahre (1979); Lamason and Lahre (1980); U.S. EPA (1978, 1979); Rockwell (1978) and SRI (1977).

The VOC emission inventory currently under construction for the province of Ontario includes breakdown to ten VOC classes (Wong, 1984). The methods used in this work will also be reviewed when the report becomes available.

4.4 Methods of Compilation of Emission Data

For all sources, annual emissions of NO_x and VOC are required, together with the temporal patterns of these emissions. The temporal resolution will be by season, by day of week and by hour of day. It is recommended that the emission data be generated independently of the National Emission Inventory System (NEIS). Subsequently comparison with

NEIS will then provide a check on data quality. Details of the procedures for obtaining the required information are given below.

4.4.1 Point Sources

The preferred approach for obtaining point source data is to make use of GVRD files, and the experience and expertise of the GVRD inspectors. Data gathered in this way will be supplemented as necessary by questionnaire and plant visit. Wherever possible, it is recommended that these activities also involve GVRD inspectors because of their knowledge of the local situation and their established contacts with industry.

For point sources outside the GVRD boundaries, information will be sought from the British Columbia Ministry of the Environment permit files, with supplementation as described above.

Note that data have already been published for some point sources within the study area. For example, source tests have been carried out for the Burrard Thermal Generating Plant (B.C. Hydro, 1980) while emissions data for oil refineries have been published by the Petroleum Association for the Conservation of the Environment (PACE, 1980).

For point sources, the following additional information, required for modelling purposes, will also be stored:

- Location
- Stack height and diameter
- Stack gas temperature and exit velocity.

Apart from its use in conjunction with a mathematical model, an emission inventory represents a valuable bank of information for other purposes, such as identifying all sources of a particular pollutant. It is possible, therefore, that further information should be stored, depending on the requirements of the regulatory agencies who will make use of the data base. A possible example of additional data which might be stored is whether or not pollution control equipment is installed, and what level of control is used.

4.4.2 Area Sources

All of the source sectors discussed below are emitters of volatile organic compounds; not all are sources of NO_x . This will be noted on a sector by sector basis. Apart from the details of emission rate determination and temporal profiling, an indication is given for each source sector of its approximate relative contribution to total emissions. This has been calculated for Vancouver, based on NEIS data for 1978, and is of value in identifying the most important source sectors.

The individual source sectors are considered below in the order in which they appear on the NEIS list as given in Section 4.2.2. For each source sector the annual emissions are normally calculated as the products of an activity rate (e.g. vehicle miles travelled per year, fuel consumption, etc.) and an emission factor. Since emission factors tend to have a geographic dependence, because, for example, of regional variations in fuel composition, temperature dependence of emissions, etc., data source is the compilation by EPS (1981). In all cases these will be reviewed in conjunction with the factors contained in the US compilation known as AP-42 (US EPA, 1977 and supplements). In a few cases emission factors are also available from the literature. In general these factors are based on more extensive data than those quoted in the compilations given above, and will therefore be preferred. Examples of such emission factors are those quoted for gas fired domestic heating by Muhlbaier (1981), for forest fires (Yamate et al., 1975) and for vegetable oil processing (Battistoni and Fava, 1984).

i) Application of Surface Coatings

This sector is responsible for VOC emissions only and the emission factors are expressed in terms of mass of VOC emitted per ton of coating applied. They are broken down for paint, varnish and shellac, lacquer, enamel and primer. Also included in this sector is cutback asphalt application.

Some industries involved in surface coating operations include aircraft companies, container manufacturers, furniture and appliance manufacturers, automobile refinishers and plastic product manufacturers. In addition there is domestic and construction use of surface coatings.

Individual industrial users can be located accurately and allocated to grid squares accordingly. Information on total usage of the various coatings can be obtained from individual manufacturers (listed in Statistics Canada publication 46-210, abbreviated as SC 46-210), directly from all identified users or through a survey of randomly selected industrial users of each type of coating.

For domestic and construction use of surface coatings, emission factors are also available on a per capita basis (Lamason and Lahre, 1980). Use of these factors will also permit the spatial apportionment of emissions.

Temporal resolution of emissions will require survey of a sample of industrial coating users, house painters and homeowners. Guidelines are also available from Lahre (1979)

This sector contributes approximately 8% of total Vancouver VOC emissions.

ii) Bakeries

This sector is responsible only for VOC emissions and the emission factors are expressed in terms of mass VOC (mainly ethanol) emitted per ton of dough processed for both the sponge-dough and the straight-dough processes. The sponge-dough process emissions are approximately 10 times larger per ton of dough than for the straight-dough process.

Available information from Statistics Canada on bakeries includes a breakdown of the number of establishments per municipality/county, with the number of employees and the value of goods manufactured (SC 32-203 and SC 31-209). It will be necessary to locate individual bakeries in order to apportion the emissions in space. Depending on the number of bakeries within the inventory boundaries, temporal variations and breakdown by type of process can either be assessed by interviews with all bakeries or estimated from interviews with a sample of the bakeries. Additional to the above, large grocery stores may have in-store bakeries not listed specifically in the Statistics Canada publication and will require identification. This information should be available from general offices of the larger supermarket chains.

This sector contributes approximately 0.5% of Vancouver VOC emissions.

iii) Crude Oil Production

There are no operating oil wells within the study area, though drilling is currently being carried out (information supplied at Vancouver Oxidant Committee meeting, March 1, 1984).

iv) Diesel and Gasoline Marketing

Evaporative losses of VOC occur at the following points in the marketing chain:

- a) Depot storage
- b) Transport to retailers (including handling)
- c) Storage by retailers
- d) Filling of vehicle fuel tanks at service stations

Emissions relating to these operations have been the subject of studies funded by the Petroleum Association for the Conservation of the Canadian Environment (PACE). The final report covering service station operations has recently been released (Nichols, 1983). Compilation of the remaining emissions is currently under way.

For calculation of emission rates, data are required on fuel volumes handled in the stages given above. Net sales of gasoline, broken down by month, are available from Statistics Canada Catalogue No. SC 53-218. The diurnal pattern of sales has been determined for other locations (e.g., Smith and Biller, 1975). This information will serve as a basis for Vancouver, but should be checked by surveying a representative sample of filling stations (i.e., including those in residential and commercial areas, and those on highways).

Spatial allocation of depots can be carried out individually since they are relatively limited in number. This should also be possible for individual service stations. There are approximately 600 service stations in Vancouver (data from PACE draft report), which will be allocated individually from their street addresses. Throughput of individual service stations may be available from oil company records. If confidentiality requirements restrict the release of such information, it will have to be estimated on the basis of storage capacity and/or local population.

This sector contributed more than 14% of the total VOC emissions for Vancouver in 1978, and therefore merits careful attention.

v) Diesel Powered Engines

Included in this source sector are the following sub-categories, all of which emit both NO_x and VOC:

- a) Diesel powered road vehicles
- b) Construction equipment
- c) Agricultural equipment
- d) Railroads
- e) Marine
- f) Industrial engines

Railroad and marine sources will be considered separately below. For road vehicles the emission factors for NO_x and VOC are given as mass of pollutant emitted per mile travelled. The subsequent calculation of emissions is as for gasoline powered vehicles (see below).

For construction and agricultural equipment of different types, the NO_x and VOC emission factors are expressed as grams per hour, grams per kilowatt hour or kilograms per thousand litres on the basis of running time, power output or fuel consumed respectively. Annual equipment usage has also been broken down into averaged annual operating times (US EPA, 1977) and can be used in conjunction with an equipment

count to determine average yearly emissions. Diurnal and seasonal variation can be estimated from a survey of specific operators.

Spatial apportionment of the emissions of this sector can be derived from GVRD Agricultural Land Reserve Maps and from the Provincial Agricultural Land Commission. Construction equipment emissions can be spatially allocated using information from Canada Mortgage and Housing giving type of unit and from the GVRD General Monitoring System (GEMONI). Construction site information for roads and industrial/commercial facilities can be obtained from the Provincial Ministry of Highways and Transportation, and from the Planning Department of the GVRD.

Spatial apportionment and temporal profiling for small industrial engines will require an extensive manual search program. B.C. Hydro operates standby generators that will be included in this category. Frequency of operation and emission data are available from B.C. Hydro Authorities. For other stationary diesel engines, inventories may be worked up from engine and equipment sales and diesel fuel sales and may include power generation equipment, refrigeration units, fork lift trucks, pumps, portable well drilling equipment, etc.

For Vancouver in 1978 this sector contributed 27% of total NO_x emissions, and 3% of total VOC emissions.

vi) Dry Cleaning

Emission factors for dry cleaning relate emission of VOCs to the mass of laundry processed for each solvent used (i.e. synthetic or petroleum based). No NO_x is emitted, and this sector contributes 1 % of Vancouver VOC emissions.

Spatial resolution will be based on addresses obtained from the Dry Cleaners and Launderers Institute with cross checking by a search of the Yellow Pages. A survey of a sample of dry cleaners as to the quantity of laundry processed and the type of solvent used, will aid in estimating the emissions from this sector. Seasonal variation as well as diurnal variation in emission may be evident. Information regarding temporal variation will also come from a survey of individual dry cleaning establishments. It is likely that there are relatively few dry cleaning operations in the emission inventory area and individual attention to each facility will not cause excessive problems. A survey of coin operated laundry facilities should be conducted to determine the number of these facilities with dry cleaning machines. Seasonal and diurnal variation in these areas will be difficult to assess but could be estimated from interviewing coin-operated laundry owners. The emissions from this source will be small in comparison with the commercial units and uncertainties will not cause significant errors.

vii) Forest Fires

Forest fires contribute both NO_x and VOC emissions. The emission factors are expressed in terms of mass of pollutant per ton of fuel burned. Required data are therefore area burned and fuel loading for that area. Knowledge of the type of vegetation burned is also required, since this also affects the emission factor.

Forest fire frequency and severity has a marked seasonal dependence, which is available from GVRD and B.C. Ministry of Forests data. Within the season, forest fires have been assumed to occur randomly, 24 hours a day, 7 days a week (GCA, 1979). The validity of this hypothesis should be checked against historical data.

Forest fire contributions to total emissions are not quoted by NEIS for Vancouver. For Canada as a whole, the contribution is 7% to NO_x and 31% to VOC (EPS, 1981).

viii) Fuel Combustion Stationary Sources

This sector is subdivided into three categories: industrial, commercial and residential. It generally accounts for space heating requirements, though small scale process heating in the industrial category is also included.

For all categories, emission factors for both NO_x and VOC are given in terms of the type and quantity of fuel consumed. The emission inventory for this sector can be worked up from fuel sales data obtained both from Statistics Canada (SC 57-208) and from fuel suppliers.

Residential heating in the study area is mainly by natural gas (SC 64-202), for which upgraded emission factors are available (Muhlbaier, 1981).

Residential wood burning will be included in this category but will be more difficult to assess because of the difficulty of quantifying fuel sales. It is therefore likely that a home-owner survey will be required to retrieve information on wood burning. Spatial allocation of residential fuel combustion emissions may be carried out on the basis of population data. Temporal variation will be estimated by using degree-day data from the Atmospheric Environment Service (Taylor, 1981). Commercial and industrial emission estimates will be based on fuel consumption data gathered from individual suppliers and as tabulated by Statistics Canada (SC 57-208). A cross-check utilizing fuel sale data will be conducted to ensure that duplications and omissions have not occurred. Spatial apportionment will be based on land use data obtained from the GVRD. Temporal variations are available from the US EPA guidelines (Lahre, 1979), which will be checked for compatibility with climatic conditions in Vancouver.

This sector contributes 16 % of Vancouver NO_x emissions and approximately 0.5 % of VOC emissions.

ix) Gasoline Powered Vehicles

Since the inventory area contains of a major urban centre, this sector will be the largest single contributor to emissions of both NO_x and VOC. The activity rate parameter for this sector is vehicle miles travelled per unit time, and the emission factors are expressed as mass of pollutant emitted per vehicle mile travelled for a number of vehicle classes.

Detailed descriptions of the methods used in estimating emissions for this sector are reported in the literature (e.g. Perardi et al., 1979; Bailey, 1982). Briefly, it is possible to follow a largely computer based procedure or a largely manual procedure.

The computerised procedure combines the output of a sociologically based model of traffic flow with the predictions of a model such as MOBILE 1 or MOBILE 2, which calculates the composite emission factors over the driving cycle. The traffic model used in Vancouver, however, is only designed to predict peak morning traffic flows, and is not adaptable for emission calculations (GVRD, 1984).

It will therefore be necessary to follow the largely manual procedure, which is more laborious, but which generally provides better resolution. In this case actual traffic count data are used in conjunction with composite emission factors developed by the Mobile Sources Division of the Air Pollution Control Directorate of EPS. Traffic count data are available from GVRD for many streets and highways with traffic densities ranging from 4,000 to over 70,000 vehicles per day. Emissions for travel on minor streets will be calculated from fuel consumption data. Careful reconciliation will be required to avoid omitting emissions or counting them twice. For highways outside the GVRD traffic count data will be obtained from the B.C. Ministry of Transportation.

The methods described above will also be applicable to the determination of emissions by diesel powered road vehicles. Note that highway segments carrying more than 24,000 vehicles per day will be treated as line sources, which will be identified by their end points.

Gasoline powered vehicles contribute 42% to Vancouver NO_x emissions and 47% to VOC.

(x) General Solvent Use

This sector, which contributes VOC emissions only, covers evaporative losses of solvents not included under dry cleaning, surface coating, or diesel and gasoline marketing. The emission factors are expressed in terms of mass VOC emitted per unit mass solvent used. This

source sector will be difficult to quantify because it covers a wide variety of individual sources.

It will be necessary to create a list of solvent users which can be derived from a variety of sources:

- a) Ministry of Labour officials and GVRD inspectors.
- b) Fire safety inspectors from insurance companies and the Fire Marshall's Office.
- c) Solvent manufacturers and retailers.
- d) Scrutiny of yellow pages and survey of potential users.
- e) Some information is available from SC 31-209.

The above information is required both for estimation of the amount of solvent used and for spatial apportionment of the emissions. Only solvent retailers and users themselves will be able to estimate quantities used and any seasonal or diurnal variations in this source sector.

Areas of extensive solvent use include:

- a) Graphic arts (printing companies)
- b) Solvent degreasing (removing grease from metal parts)
- c) Wind shield washer fluid

- d) Polishes and waxes
- e) Space deodorants
- f) Aerosols
- g) Some laundry detergents and treatments.

Emission factors for some of the above activities are given on a per capita basis, which will simplify the inventory calculations and manipulation for the sectors involved.

Solvent usage contributes approximately 4% to Vancouver VOC emissions.

(xi) Landfill Sites

The emission factor is expressed as mass of VOC emitted per unit time per unit area of landfill. Data on landfill area will be sought from local authorities, while the temporal variation of the emission rate will be derived from ambient temperature data.

Uncertainties are high for this sector, but the emissions are essentially only of methane. This is treated as unreactive in photochemical models, so that the uncertainties are not of great consequence. Also, the estimated contribution of this sector to Vancouver VOC emissions is small (less than 1%).

(xii) Natural Gas Processing

There are no natural gas wells within the study area, so the only emissions attributable to this sector will be from leaks in the distribution system. Since the material leaked is methane, which is essentially unreactive, it will not be necessary to consider these emissions in detail.

(xiii) Non-highway Use of Gasoline

This sector, which is responsible for NO_x and VOC emissions, encompasses a wide range of equipment. Gasoline powered internal combustion engines include the following categories:

- a) Agricultural equipment
- b) Construction equipment
- c) Small engined (2 and 4 stroke) equipment
(e.g. lawnmowers, chainsaws, snowblowers, etc.)

Emissions from agricultural and construction equipment will be treated as has been discussed for the diesel-powered engine sector.

Small engine emissions are mainly related to household use, particularly in lawnmowers, and may thus be spatially apportioned on the basis of dwelling-type. Statistics Canada publication SC 64-202 "House-

hold Facilities and Equipment" will be used together with sales information from engine and equipment manufacturers and retailers to estimate the population of this engine type.

The emission factor for these small engines relates the mass of pollutant emitted to the amount of fuel used. Some guidance as to fuel usage is given by EPS (1981), and procedures for adjusting emissions for climatic effects and the presence of multiple dwelling units are given by Engineering - Science (1982).

The contribution to this sector to Vancouver emissions is approximately 3 % in the case of NO_x and 4 % for VOC.

(xiv) Off-highway Mobile Sources

This sector includes railway, marine and aircraft emissions, which will be considered separately below.

a) Railway

VOC and NO_x emission factors for railways are related to the quantity of fuel consumed. Fuel usage is documented in the literature (Statistics Canada Publications SC 45-208, SC 52-207, SC 52-209) and may be augmented by interview with railway companies (e.g. CP).

Spatial and temporal allocation of emissions can be accomplished by use of traffic information contained in SC 52-210, detailed land use maps and by incorporating details from operating schedules.

Railways contribute approximately 7% to annual NO_x emissions in Vancouver and 1% to VOC.

b) Aircraft

The emission factors for aircraft are expressed as mass VOC/ NO_x emitted per landing/take-off cycle, for each class of aircraft (determined by type and number of engines, size of aircraft, etc.).

It follows that the information required to determine emissions in this sector are:

- a) Landing/take-off frequency for each of the airports
- b) Class of aircraft involved
- c) Typical schedules giving diurnal, weekly and weekend variations

An emission inventory for the Vancouver International Airport was prepared for 1975 (Wituschek, 1984) and will serve as a basis for the present work. There are several other airports within the inventory area, including

- a) Boundary Bay
- b) Vancouver Harbour Seaplane Base
- c) Abbotsford International.
- d) Pitt Meadows
- e) Langley
- f) Chilliwack

For each of these the emissions will also be calculated as described above.

Sources of the required information for emission calculation and temporal resolution will be the authorities at the Airports, and the Provincial and Federal Transport Ministries.

The emissions will essentially be located at the airport, with a partial allocation to approach and take-off paths as described by Engineering-Science (1980, 1982). Aircraft emissions contribute 1.5% to NO_x emissions and less than 0.5% to VOC emissions in Vancouver.

c) Marine

This sector includes NO_x and VOC emissions of craft ranging from outboard motor driven pleasure craft to ocean going vessels. For the latter, emission factors are given in AP-42 (US EPA, 1977) related

to fuel consumption for a number of fuel types, vessel classes and operating modes. An emission calculation for the Houston Ship Canal (Yu, 1982) illustrates the use of these factors.

However, marine emissions contribute relatively little to the total for Vancouver (0.6% to NO_x and 0.3% to VOC), so that a detailed analysis is not justified. Instead, composite emission factors developed by EPS (1981) will be used, giving mass of pollutant emitted per call in port for a number of fuel types. The required data on shipping traffic are given by Statistics Canada (SC 54-209, SC 54-210). Temporal resolution of the emissions will be based on data gathered from the harbour authorities. By far the largest fraction of emissions from vessels is attributable to operations while berthed (running of engines for power generation, etc.) Spatial apportionment of emissions will therefore be by berth, neglecting emissions associated with the relatively short duration activities of entering and leaving port.

For small craft the emission factors are given as mass of pollutant emitted per brake horsepower hour. The population is obtainable from Statistics Canada Publication SC 64-202, while spatial apportionment will require a survey of users, clubs and harbour authorities. Guidelines for temporal resolution of emissions are given by Lahre (1979).

(xv) Plastics Fabrication

This sector, which is responsible only for VOC emissions, relates to fabrication of articles from plastic, generally in the form of sheet or pellets. To quantify emission rates and to allocate emissions spatially it will be necessary to obtain specific facility data.

Identification of fabricators is available from SC 31-209 with additional information from SC 47-006, SC 47-007 and SC 46-222, and will include, for example, toy manufactures, kitchen utensil manufacturers, garbage bag manufacturers, etc.

Temporal variations may be estimated from interviews with a sample of the fabricators in the sector.

This sector contributes less than 2% to Vancouver VOC emissions.

(xvi) Slash burning

This sector accounts for both NO_x and VOC emissions. It will be treated in essentially the same way as forest fires (number vii). In fact the emission factors used for forest fires were mainly obtained under slash burning conditions (US EPA, 1977).

NEIS does not list slash burning emissions for Vancouver. For Canada as a whole this sector contributes 0.5% of NO_x emissions and 0.7% of VOC emissions (EPS,1981).

(xvii) Solid Waste Incineration

Municipal incinerators will fall into the category of point sources. Under consideration here are the small scale operations associated with (for example) shopping plazas, apartment blocks, etc. Both VOC and NO_x are emitted, but the contribution to total emissions is small (less than 0.05% for both pollutants).

Nevertheless, these operations are regulated and data are available from GVRD (Mennell, 1984).

Potentially more significant are the emissions from wigwam burners used for waste disposal in the forestry industry. For Canada as a whole this source contributes 0.1% of NO_x emissions and 1% of VOC emissions. These operations are also carried out under permit, and may, in some cases, actually amount to point sources.

Temporal profiles for incineration have been given by Lahre (1979).

(xviii) Structural Fires

Although this is a combustion source, emissions of NO_x are considered to be negligible (EPS, 1981). The emission factor relates the mass of VOC to the type of building burned, i.e. to its size and the construction materials.

Individual fire departments will be contacted for statistical data on which to base spatial apportionment and temporal profiling of these emissions.

Structural fires contribute approximately 0.4% to Vancouver VOC emissions.

(xix) Tire Wear

This is a very small source, emitting VOC only (contributing 0.05%). However, the emission factors are expressed as mass emitted per vehicle mile travelled per tire. The emissions are therefore readily calculated at the same time as other vehicle related emissions.

(xx) Natural Sources

Apart from forest fires, natural sources of NO_x may be considered to be negligible. There are, however, significant natural sources of VOCs, whose contribution should be considered in constructing an emission inventory. Over Canada as a whole, natural VOC emissions are believed to exceed anthropogenic emissions by a substantial margin. Oxidant control strategies currently in preparation for the San Francisco area have included vegetative VOC emissions in the emission inventory (Hunsaker et al., 1984; Penner, 1984).

Natural sources of VOC include:

- a) Wetlands, swamps and bogs
- b) Insects
- c) Animals
- d) Natural gas percolation
- e) Vegetation

The first four of these source types emit essentially only methane. Since this is considered to be unreactive in urban and regional scale oxidant formation, it is proposed that their emissions not be included in the Vancouver inventory.

It has been known for some time that reactive hydrocarbons, notably isoprene and the monoterpenes, are emitted by vegetation (e.g.

Rasmussen and Went, 1965; Graedel, 1978). However, it is by no means clear whether or not they do actually contribute to ozone formation. The difficulty arises because there are two reaction paths open to these species:

- i) Reaction with the hydroxyl radical leads to the formation of free radical species which participate in the production of ozone (see Chapter 2).
- ii) Reaction with ozone leads to formation of particulate matter with consumption of ozone. This contrasts with the case of many anthropogenically emitted VOC, for which reaction with ozone also leads to free radical formation with net ozone production.

The relative balance between the two pathways determines whether vegetative hydrocarbons cause net production or consumption of ozone. The current view at the US EPA is that vegetative VOC emissions are not important in ozone production (eg. Bufalini, 1980; Altshuller, 1983). However, recent work (Killus and Whitten, 1984) indicates that, at least in the case of isoprene, the rate of reaction with ozone is slow relative to that with OH, so that isoprene is important in ozone formation. The same is probably not true of the monoterpenes. In support of the importance of vegetative VOC emissions is the finding that incorporation of vegetative VOC emissions in the San Francisco area

leads to a significant increase in predicted ozone levels (Penner, 1984).

Emission factors are available which relate the mass of VOC emitted to the equivalent dry mass of vegetation. For calculation of emissions the following data are therefore required:

- i) For each grid square, the areal coverage of each vegetation species.
- ii) A factor relating the dry vegetation mass to the ground area covered (the biomass factor).
- iii) The emission factors for the species of concern, and their temporal variation.

The GVRD maintains an extensive land use data base which will be of assistance in determining areal coverage of vegetation. The data base does not, however, give adequate resolution by vegetation type to provide all the information required, since it is mainly designed for listing commercial use of land. The B.C. Ministry of Forests maintains a forest inventory for crown managed lands (Quenet, 1984) while data on agricultural land use are obtainable from the B.C. Ministry of Agriculture (Thompson, 1984). However, because of the lack of suitable data for the GVRD it may prove most cost effective to make use of

satellite photographs to refine and consolidate the land use inventories.

The methodology of vegetation type apportionment from satellite data is well established (Jain, 1983). Satellite imagery has been used in emission inventory preparation in Virginia (Salop et al., 1983) and San Francisco (Hunsaker and Moreland, 1982). For the Vancouver emission inventory one satellite image may be sufficient, depending on the area inventoried.

Success rates of 95% for vegetation identification from satellite photographs were achieved by Salop et al., (1983). It will be necessary to check that comparable success is achieved for Vancouver. This can be done by cross comparison with land use data from GVRD and the B.C. Ministry of Agriculture, and by on-site survey.

Average biomass factors have been tabulated by a number of workers (eg. Zimmerman, 1979; Winer et al. 1982). These will be used for Vancouver, accepting that some uncertainties will be introduced by using factors developed for other areas. Direct determination of biomass factors is labour intensive, and is not justified in view of the uncertainties known to exist in reported vegetative emission factors.

These are a consequence of the difficulties involved in making measurements on what are individually very small sources. Vegetative

emission factors were reviewed in 1983 (CSC, 1983). Since then work has continued on the measurement of vegetative emissions (APCA, 1984), but uncertainties remain relatively large, and there are still no measurements which relate to plants growing out of doors under Canadian conditions. The seasonal and diurnal variation of emissions is also not well quantified (CSC, 1983).

With these considerations in mind it is nevertheless proposed that literature values be used for vegetative emission factors. These will be taken from Zimmermann (1979), Winer et al., (1982), Westberg (1983), Arnts et al. (1978, 1982) and APCA (1984). If future photochemical modelling indicates that vegetative VOC emissions are significant in causing ozone production in the Vancouver area, it will be necessary to upgrade the biomass and emission factors. The spatial apportionment derived from satellite imagery will be suitable for use with upgraded factors, provided that there are no major changes in land use patterns.

4.5 Errors

There are two aspects to be considered with regard to errors in the emission inventory. Firstly, good quality control is required to minimize the errors. Secondly, the probable errors should be quantified as far as possible.

Quality control procedures should generally be as follows:

- i) For each grid square the largest emitter (source sector) should receive the most careful attention. For populated areas this will normally be the mobile (automobile) sources.
- ii) As a corollary to the above, the most densely emitting areas should receive the most careful treatment.
- iii) Wherever possible cross checking should be carried out. For example, AP-42 (US EPA, 1977) also gives information on solid waste incineration emissions on a per capita basis. The emissions calculated in this way can be used as a check on emissions calculated from the amount of refuse burned. Per capita emission factors are also given by Lamason and Lahre (1980). As a final check the inventory should be compared with the NEIS data, and any differences reconciled.
- iv) Standard quality assurance procedures for database construction should be followed to reduce to a minimum the occurrence of keypunch errors, etc.

Estimation of the error bars on the final emission rate requires a knowledge of the error in each of the factors involved in the calculation of the emission rate. Typically these are an emission

factor and an activity rate, and estimates of the errors are provided by Working Group 3B of the U.S. - Canada Memorandum of Intent (MOI) on Transboundary Air Pollution (MOI, 1982). Error estimates will also be required for the temporal and speciation patterns.

A standard analysis of the propagation of errors (Kline and McClintock, 1952) was followed in the MOI report (MOI, 1982). However for VOC emissions the procedure described by McRae and Seinfeld (1983) appears to be more useful. They included a weighting by the reactivity of the emitted species.

Calculation of the probable errors in the individual source emissions permits identification of those areas in which further refinements will provide the maximum benefit.

4.6 Other Issues

The calculation of emissions is the major activity in the preparation of an emission inventory, but a number of other issues must also be addressed. These are discussed briefly below.

4.6.1 Database format

The Vancouver emission inventory will be set up on a grid covering approximately 300 squares each 5 x 5 km, and will contain a

considerable amount of data. The usefulness of the data base will depend critically on the ease of access of these data, and thus on its format. The detailed design of this format is beyond the scope of this report, but it is suggested that there be separate point and area source files. Associated with the area source file will be separate files for NO_x and VOC speciation and for temporal resolution (both listed by source sector). This arrangement will permit updating of a part of the set (e.g. speciation factors) without adjustment of the entire inventory.

4.6.2 Maintenance

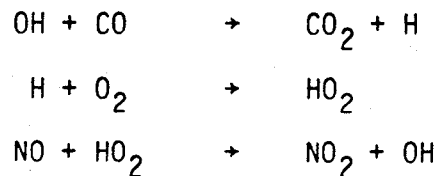
Construction of a gridded emission inventory is a considerable undertaking. For example, the inventory for Washington, D.C. (Bailey, 1982) required six manyears for its preparation. It is essential that this investment be protected by maintaining the inventory. A decision will therefore be required as to who will be responsible for storing and updating the inventory. In the latter context current experience is that a simple procedure works best, e.g. with one person working continuously on updating (Sellars, 1982; Mennell, 1984).

4.6.3 Other Pollutants

For the source sectors included in the Vancouver emission inventory it will be relatively simple to incorporate the emissions of

other pollutants. The activity rates and temporal profiles will have been collected and stored for the calculation of NO_x and VOC emissions. All that will be required will be the appropriate emission factor(s).

It is recommended that this actually be done for the case of carbon monoxide. Carbon monoxide emissions are required for input to most photochemical reactions because of its participation in an important chain reaction causing the oxidation of NO to NO_2 :



In spite of this reaction chain, the concentration of CO is essentially unaffected by chemical reaction, because it is present in the atmosphere in such large amounts. It is therefore valuable in modeling because it provides an internal check on the adequacy of the treatments of transport, dispersion and deposition.

Another species which can be included is SO_2 . Particulate matter cannot readily be included since a number of sources are involved which do not contribute to NO_x or VOC emissions.

4.6.4 Confidentiality

It is possible that some of the activity rate data collected for emission calculations will be regarded as confidential by the plant

owners concerned. Thus, in the U.S. National Emission Data System, certain data are not released to outside users (Barkhau, 1983). Clearly the data are required for the development of meaningful ozone control strategies, and appropriate procedures will therefore have to be developed for the maintenance of data confidentiality (where and if required).

4.7 Summary

A plan has been given for the construction of an inventory of emissions of NO_x and VOC for Vancouver. In most cases the emission will be calculated as the product of an activity rate and an emission factor. Procedures have been given for allocating the emissions to a 5 x 5 km grid, and for deriving the required temporal and chemical resolution. This has been done for each of the source sectors believed to be important in Vancouver. A brief summary is contained in Table 2.

Although every effort has been made to provide as detailed a design plan as possible, the actual construction of the inventory will require considerable scientific experience and expertise because of the many data gaps and uncertainties which remain. It will be particularly important to assess the impact that these uncertainties will have on the predictions of air quality models.

Table 2
Summary of Inventory Procedures for Area Sources

Sector	Activity Rate	Spatial Apportionment	Species Emitted
Application of Surface Coatings	Mass of paint	Direct location of major users Land use data for building type apportionment	VOC
Bakeries	Mass of dough	Direct location of bakeries	VOC
Crude Oil Production	N/A		
Diesel and Gasoline Marketing	Fuel throughput	Direct location of all points in marketing chain	VOC
Diesel Powered Engines	Fuel consumption Power output Running time	CMHC and land use data for construction and agriculture	VOC, NO _x
Dry Cleaning	Mass of laundry	Direct location of plants	VOC
Forest Fires	Fuel consumed	Ministry of Agriculture and GVRD historical records	VOC, NO _x
Fuel Combustion Stationary Sources	Fuel consumed	Population, commercial land use data.	VOC, NO _x
Gasoline Powered Vehicles	Vehicle miles travelled	Traffic counts	VOC, NO _x
General Solvent Use	Mass of solvent used	Direct location of users, employment data	VOC
Landfill Sites	Area	Direct Location	VOC
Natural Gas Production	N/A		
Non-highway Use of Gasoline	Fuel consumption, Power output, Running time	As for diesel powered engines	VOC, NO _x
Railways	Fuel consumption	Direct location of tracks	VOC, NO _x
Marine	Calls in port	Direct location of berths	VOC, NO _x
Aircraft	Landing/take-off cycles	Direct location of airport	VOC, NO _x
Plastics Fabrication	Mass processed	Direct location of processors	VOC
Slash Burning	Area burned	GVRD and Ministry of Agriculture data	VOC, NO _x
Solid Waste Incineration	Mass burned	GVRD permits	VOC, NO _x
Structural Fires	Number of buildings burned	Fire Department data	VOC
Tire Wear	Distance travelled per tire	Traffic counts	VOC
Vegetative Emissions	Areas covered	Satellite photographs	VOC

5. MODEL IMPLEMENTATION

The availability of good quality emission data is probably the single most important factor required for the successful implementation of a photochemical model. However, there are a number of other requirements which must also be addressed. These are outlined briefly below. It is beyond the scope of this study to provide a detailed model implementation plan.

5.1 Model Availability

Two options exist for obtaining a suitable model.

- Acquire a working code from the developer
- Develop a computer code, either from scratch, or based on an existing mathematical formulation.

At first sight the first option appears to offer the lower cost route. However, experience has confirmed the large advantages in overall cost effectiveness of the second route. The recommendation was therefore made in Section 3.3 that a model be developed for Vancouver, based on the formulation of McRae et al. (1982). It is worth restating briefly some of the advantages to be gained from following this course.

- i) A complete understanding of the workings of the model is obtained. The problems to be faced in implementing somebody else's program should not be underestimated, and are exemplified by the problems experienced by Shreffler and Schere (1982) in attempting to run LIRAQ. This type of understanding is essential if future model refinements are to be successfully incorporated.

- ii) All existing models of the type required were developed in the United States. The required experience, knowledge and expertise is to be found in Canada, however, and the opportunity now exists to develop a Canadian capability in this area. This is particularly important because ozone problems occur in a number of other Canadian urban centres (e.g. Toronto, Montreal, and Quebec City), and there will thus be a continuing need for such a modelling capability.

5.2 Meteorological Data

Model input data are required corresponding to the following meteorological (and closely related) parameters.

- a) Topography.
- b) Surface roughness.

- c) Wind field.
- d) Mixing height.
- e) Solar insolation.
- f) Relative humidity.
- g) Temperature.

Of these, topography and surface roughness will remain fixed from run to run, and thus need only be determined once. The topographical information is readily available; surface roughness must be estimated for each grid square using, for example, the tabulation given by McRae et al.,(1982). Surface roughness is dependent on the type of ground cover, and ranges from approximately 10^{-5} m for ice to 10 m for the central business district of a city.

Relative humidity and temperature are readily available (at ground level at least). Routine vertical profiles of temperature can only be obtained from pilot balloon ascents at Vancouver International Airport.

The calculation of solar zenith angle and the associated photolysis rate constants is described in the literature (Schere and Demerjian, 1977; MacCracken et al., 1978). The effect of clouds has been discussed (Zafonte et al., 1977; Stedman et al., 1977) as has the effect of altitude (Demerjian et al., 1980).

The most important meteorological factor in the model is the wind field, which is three dimensional for the model recommended here. For application in Los Angeles the wind field was derived by interpolation between ground and upper level observations (McRae and Seinfeld, 1983). The suitability of the Vancouver observational network for this purpose requires careful investigation.

The mixed layer depth is not constant throughout the Vancouver area, mainly because of topographic effects. The variability of the mixed layer depth has been studied (Steyn, 1980) but it is likely that more information will be required for model implementation.

Also related to meteorological factors is the actual size and extent of the model domain. As discussed by McRae and Seinfeld (1983), it is important that the model domain be large enough to contain the full excursion of a parcel of air moving under the influence of land and sea breezes. When a parcel leaves the domain its identity is lost and it is not treated correctly if it subsequently returns. The sea breeze phenomenon in Vancouver is, and has been, the subject of considerable study (see, for example, the summary in CSC, 1982).

5.3 Other Data Needs

Additional data requirements for model implementation are for initial and boundary conditions and for verification data. Both catego-

ries consist of air quality data. In addition, to routine monitoring data already collected for Vancouver, the following will be required, and can be collected in short term intensive studies.

- Speciated VOC data, both within and at the boundaries of the study area.
- Ozone data at the boundaries of the study area and aloft.

The importance of the initial conditions is reduced in a model which is capable of simulating air quality over two or more days. Note also that boundary conditions will have to be specified even if simple models are used (e.g. EKMA or a box model).

6. COSTING OF CONSTRUCTING THE EMISSION INVENTORY

The total cost of constructing the Vancouver emission inventory, as described in this report, is estimated to be approximately \$185,000.

7. CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

The main conclusions of this study are:

- a) There is an increasing trend towards the use of Eulerian models in the development of urban scale oxidant control strategies.
- b) On technical grounds the Eulerian model described by McRae et al. (1982) is superior to other models currently available.
- c) Data exist to permit the construction of an appropriate emission inventory for NO_x and VOC for Vancouver.
- d) The source sector providing the largest relative contribution to emissions will be gasoline powered vehicles.
- e) The source sectors whose emissions will be subject to the largest uncertainties will be general solvent use, diesel powered vehicles and natural sources.

7.2 Recommendations

The following are the major recommendations arising from this study.

- a) An emission inventory should be constructed for the Vancouver area, covering the region bounded by the watershed boundary in the north, the U.S. border in the south and the water's edge in the west and extending to at least Chilliwack in the east. Consideration should be given to extending the eastern boundary to Hope. The inventory should have the following characteristics:
 - i) Spatial resolution to 5 x 5 km.
 - ii) Temporal resolution to 1 hour.
 - iii) Chemical species to be included are NO, NO₂ and at least 6 VOC classes.
 - iv) Point line and area sources are to be included.
 - v) Although they are subject to relatively large uncertainties, natural sources should be included.

- b) The emission inventory should be extended to include also the emissions of CO, since this species participates in atmospheric reactions, but is also useful as an approximately

conservative internal tracer for testing model treatment of transport, dispersion and deposition.

- c) An Eulerian model should be developed for Vancouver, based on the formulation of McRae et al., (1982). This approach is strongly recommended over the alternative of attempting to acquire a working code.

- d) Since development of such a model will take a substantial amount of time, an interim modelling effort should be initiated, based on the use of a photochemical box model or EKMA. If EKMA is used, the chemical mechanism must be upgraded.

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