EMISSIONS MODEL FOR THE AUSTRALIAN AIR QUALITY FORECASTING SYSTEM

Yuk L. Ng, Sean Walsh and Neil Wong
Environment Protection Authority,
GPO Box 4395QQ, Melbourne, VIC 3000, Australia

Presented at the 15th International Clean Air & Environment Conference. Sydney, Australia, 26-30 November 2000

Summary

The Australian Air Quality Forecasting System produces high-resolution, meteorological and air quality forecasts for the major urban areas of Australia, and is being initially tested in Melbourne and then demonstrated in Sydney during the 2000 Olympics. The emissions model acts as an input to the air quality forecasting model.

The emissions model consists of several submodels dealing with different sources of emissions. Five submodels: point sources, area sources, biogenic sources, motor vehicles, prescribed burning and wildfires will be discussed in this paper. Emissions from motor vehicles are estimated based on vehicle kilometres travelled; however, emissions on some major roads in Sydney are estimated by a power consumption based vehicle emission model.

The emissions model estimates emissions depending on the season (or month), time of day and whether it is a weekday, Saturday or Sunday. The effect of temperature on the emissions from wood burning (part of the area source module) and on motor vehicles, and the effects of temperature and solar radiation on biogenic emissions are considered in the model.

Keywords: emissions model, emissions inventory, forecasting, day-specific emissions, power-based model

1. Introduction

The Australian Air Quality Forecasting System (AAQFS) is being developed with funding from the Air Pollution in Major Cities Program. The short term goal of the project is to develop, validate and trial an accurate, next day (36 hours) numerical air quality forecasting system for a three-month demonstration period in Sydney, which includes the 2000 Olympics. Currently forecasts are produced in both Melbourne and Sydney. After the Olympics, the AAQFS will be available for forecasting health- and visibility-related air quality metrics in the other major population centres of Australia. Principal project partners are the Bureau of Meteorology, CSIRO, Environment Protection Authority of Victoria and Environment Protection Authority of New South Wales.

The project has a number of specific goals: to provide the ability to generate 36 hour air quality forecasts twice per day; provide forecasts for a range of air pollutants; provide forecasts at a resolution sufficient to consider suburban variations in air quality; and to provide the ability to generate simultaneous forecasts for different emission scenarios such as minimal motor vehicle usage scenario.

The AAQFS consists of five major components: a numerical weather prediction system (LAPS), an emissions inventory module (EIM), a chemical transport module (CTM) for air quality modelling, an evaluation module, and a data archiving and dissemination module. The development of the AAQFS is proceeding in two phases: 1) the construction and operation of a pilot system using components that were available at the time of study inception; and 2) the development of a demonstration system, through the enhancement of components in the pilot system, and where necessary, through the construction of new modules. The principal difference between the pilot and demonstration systems is that significant components of the emission modelling and chemical transport modelling are conducted online, i.e. modules are called directly by LAPS, in the demonstration system. This contrasts with the pilot system, where a meteorological forecast is first completed, stored and post processed prior to the execution of the chemical transport model.

LAPS has been described by Hess et al. (1999) and CTM by Cope et al. (in press). This paper presents an overview of the EIM developed for the demonstration system, emphasising the design and formulations of the model.

2. Overview of the Emissions Model

2.1. General Overview

Traditional emission models usually produce gridded, hourly, speciated emissions on data files, which are then read into an air quality model. These data files are

produced for some specific days which are pre-determined by modellers.

The challenge of the EIM is to estimate emissions on a daily basis that allows for weekday/weekend, monthly or seasonal, and meteorological dependencies. Also the emissions must be generated for a 36 hours period, rather than 24 hours as in a traditional emission model. Special events or scenarios, such as minimal motor vehicle usage, need to be considered in the model.

Another challenge of the model is to incorporate the emissions data obtained from a power-based vehicle emissions model, which has been developed by CSIRO, in the EIM. These emissions are road-specific, which are quite different from the traditional forms of emissions that are based on points or grid cells.

The EIM provides forecasts of emissions for a range of air pollutants including carbon monoxide (CO), oxides of nitrogen (NOx), particulates (PM_{10}), sulphur dioxide (SO_2), volatile organic compounds (VOC), ammonia, benzene, 1,3-butadiene and formaldehyde. Particulates are speciated into discrete compounds and size fractions, and VOC is speciated into individual Carbon Bond IV species (Gery et al. 1989). The EIM accepts data for any grid size, cell size and coordinate system although latitudes and longitudes are used for the AAQFS.

The model is designed in such a way that it uses the minimal amount of time and disk space to run. In order to minimise the time to run the model, static data, i.e. data which do not have temporal dependency, such as spatial data, are preprocessed and put on the system. To minimise the use of disk space, the size of data sets are kept to the minimum. For example, instead of storing a large data set of area source gridded emissions, these emissions are generated in the model by distributing the annual emissions by spatial data, such as population.

The emissions model consists of eight submodels: point source model, area source model, motor vehicle model, biogenic model, prescribed burning and wildfires model, sea-salt model, windblown dust model and meteorological data model. Only the first five models are considered in details in this paper, the latter three models require tight integration with LAPS and are being developed by CSIRO. The meteorological data model extracts data from LAPS for emissions estimation and will be described briefly in this paper.

Each of the first five models is a subroutine that can be called from the CTM. Each subroutine supplies spatially disaggregated, hourly, speciated emissions to the CTM for a given grid domain and forecasting time period.

2.2 Point Source Model

Figure 1 shows the data flow diagram for the point source model, which illustrates the data sets required for the model and how they are used to generate the hourly emissions and, in turn, speciated hourly emissions for individual point sources.

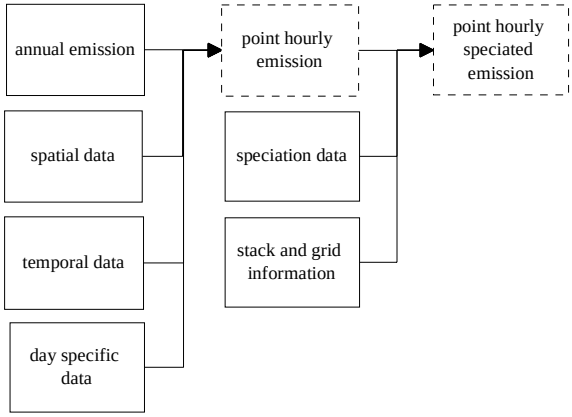


Figure 1 Data flow diagram for point source model

Individual point sources are selected for a given domain based on the information in the spatial data set. The annual emissions are then disaggregated into hourly emissions by applying temporal factors derived from the temporal data set according to the following equation:

$$E_h = A \times M \times D \times H_h / W \quad (1)$$

where E_h is hourly emission for hour h (kg/hr),
A is annual emission (kg/yr),
M is monthly temporal factor,
W is weekly temporal factor,
D is daily temporal factor, and
H_h is hourly temporal factor for hour h.

The day-specific data contains information on public holidays and special events. For a public holiday, a daily temporal factor for Sunday is used. For an event, an event factor is used instead of the daily temporal factor.

The hourly emissions are speciated using the information in the speciation data set (see Section 2.8) before read into the CTM.

2.3 Area Source Model

Figure 2 shows the data flow diagram for the area source model.

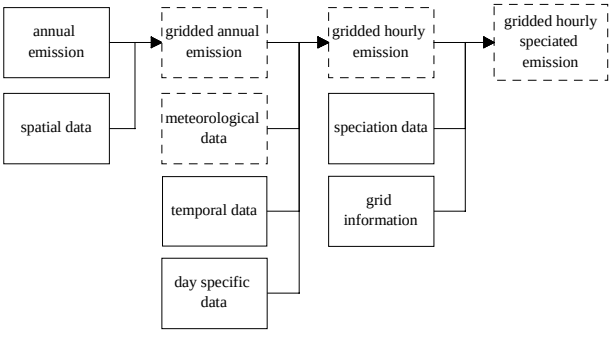


Figure 2 Data flow diagram for area source model

Area source emissions estimates are allocated to grid cells through the application of spatial surrogates, such as population. Each area source (s') which has been

assigned to a spatial surrogate (s) can be allocated to grid cells (c) through the application of the following equation:

$$G_{c,s'} = A_{s'} \times R_{c,s} \quad (2a)$$

where $G_{c,s'}$ is gridded annual emission for an area source s' and grid cell c (kg/yr),
$A_{s'}$ is annual emission for the area source s' over the whole state (kg/yr),
$R_{c,s}$ is gridded surrogate ratio for spatial surrogate s and grid cell c, and

$$\sum_{c} R_{c,s} = 1, \text{ for all spatial surrogates s} \quad (2b)$$

where the sum is over the whole state.

For wood combustion, emissions depend on daily temperature (Ng & Minchin., forthcoming) and the following equation is used to find the adjustment factor:

$$f = -0.1539 \times t + 3.0205, \; f > 0 \quad (3a)$$

where f is the wood burning emission adjustment factor, and
t is the average daily temperature over the modelling grid (°C).

The temperature t needs to be extracted from the LAPS. If the adjustment factor calculated by the above equation is negative, the adjustment factor is set to 0.

The wood burning emission is then obtained by:

$$G' = G \times f \quad (3b)$$

where G' is the adjusted wood burning emission (kg/yr), and
G is the unadjusted wood burning emission (kg/yr).

After the wood burning emissions are adjusted, the emissions of each area source are temporally allocated by applying temporal factors derived from the temporal data set according to the following equation:

$$E_h = G \times M \times D \times H_h / W \quad (4)$$

where E_h is the hourly emission for hour h (kg/hr),
G is the gridded annual emission (kg/yr),
M is monthly temporal factor,
W is weekly temporal factor,
D is daily temporal factor, and
H_h is hourly temporal factor for hour h.

The day-specific data contains information on public holidays and special events. For a public holiday, a daily temporal factor for Sunday is used. For an event, an event factor is used instead of the daily temporal factor.

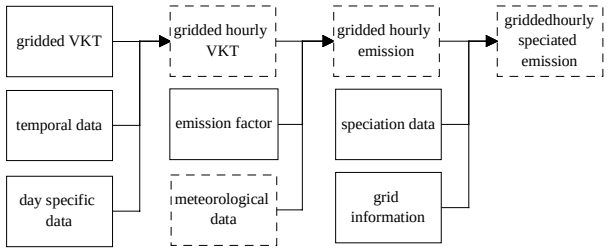
The hourly emissions are speciated using the information in the speciation data set (see Section 2.8) before being passed to the CTM.

2.4. Motor Vehicle Model

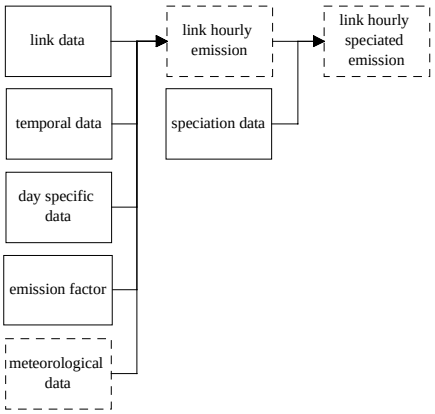
There are two submodels for the motor vehicle model: 1) main model and 2) power-based model. To distinguish it from the power-based model developed by CSIRO, the power-based model developed for the EIM will be referred to as 'EIM power-based model'. The CSIRO power-based model does not estimate emissions on a day-by-day basis and is not part of the AAQFS but its results are used as input to the EIM.

The main model estimates gridded, hourly, speciated emissions for domains where the power-based model is not used. If the power-based model is used, the main model provides the background gridded, hourly, speciated emission for the domain. The background emissions are total motor vehicle emissions minus those estimated for the power-based model. The EIM power-based model estimates hourly, speciated emissions for each road link where the power-based model is applied.

Figure 3 shows the data flow diagrams for the two models.



(a)



(b)

Figure 3 Data flow diagrams for motor vehicle (a) main model and (b) power-based model.

2.4.1 Main model

Prior to computing the motor vehicle emissions estimates, the gridded, hourly vehicle kilometres travelled (VKT) are calculated and the VKT adjusted to the specific modelling day:

$$G_{c,r,h} = V_{c,r} \times M \times D \times H_h \quad (5)$$

where $G_{c,r,h}$ is VKT for grid cell c, road type r and hour h (km/hr),
$V_{c,r}$ is daily VKT for grid cell c and road type r (km/day),
M is month-specific VKT adjustment factor,
D is the day-specific VKT adjustment factor, and
H_h is the hour-specific VKT fractional profile factor for hour h.

The temporal factors M, D and H_h are supplied through the temporal data set. The day-specific data contains information on public holidays and special events. For a public holiday, the day-specific adjustment factor for Sunday is used. For an event, such as minimal motor vehicle usage, an event factor is used instead of the day-specific adjustment factor.

The model computes day-specific, gridded, hourly motor vehicle emissions estimates of VOC, CO, NOx, PM_{10} and SO_2 according to the following equation:

$$E_{m,t,p} = \sum_r F_{m,t,p,r} \times G_r \quad (6)$$

where E is gridded, hourly emission (kg/hr),
F is fleet composite emission factor (kg/km),
G is gridded, hourly VKT (km/hr),
m is index for process type (evaporative or exhaust),
t is index for technology type (gasoline, diesel, or liquefied petroleum gas),
p is index for pollutant; and
r is road type index.

The emission factors of VOC, CO and NOx depend on temperature, and these emission factors are obtained from a data set which contains emission factors for a range of temperature. The temperature on the day in a specific hour is obtained from the meteorological data model (see Section 2.7). The emission factor closest to this temperature is then chosen for estimating the emission. Note that the emission factor is fleet composite emission factor, ie it has been weighted according to fleet VKT composition.

Evaporative emission factor for petrol fuelled vehicles is adjusted by an adjustment factor for Reid Vapour Pressure (RVP), which may differ for different periods in a year:

$$F'_r = F_r \times R \quad (7)$$

where F'_r is adjusted evaporative emission factor (kg/km),
F_r is unadjusted evaporative emission factor (kg/km),
R is RVP adjustment factor for a particular period, and
r is road type index.

Emissions for toxics (benzene, 1,3-butadiene and formaldehyde) are estimated from VOC using speciation fractions.

$$E_{m,t,p} = E_{m,t,voc} \times S_{m,t,p} \quad (7)$$

where E is gridded, hourly emission (kg/hr),
S is mass fraction of a species in VOC,
m is index for process type,
t is index for technology type, and
p is index for pollutant (benzene, 1,3-butadiene or formaldehyde).

2.4.2 Power-based model

The power-based model as developed by CSIRO (Williams et al. 1994) estimates exhaust emissions for CO, NOx and hydrocarbons (HC). These emissions are provided for each hour and road link for an average weekday, Saturday and Sunday in a data file for the EIM power-based model. It is assumed that VOC is equivalent to HC and no conversion factor is used.

The power-based model does not estimate evaporative emission and emissions of other pollutants (PM_{10}, SO_2 and toxics) on roads, so these emissions are estimated by the EIM power-based model using data from the main model.

Evaporative emission and emissions of PM_{10} and SO_2 on a road link are estimated by the following equation:

$$L_{m,t,p} = F_{m,t,p} \times V \quad (8)$$

where L is hourly emission on a road link (kg/hr),
F is fleet composite emission factor (kg/km),
V is hourly VKT on the road (km/hr),
m is index for process type,
t is index for technology type, and
p is index for pollutant.

For evaporative emission, the emission factor varies with temperature and hence is different for each grid cell. The emission factor is also adjusted for RVP as in the main model.

Emissions on a road link are adjusted to the specific modelling day according to the following equation:

$$L'_{m,t,p} = L_{m,t,p} \times M \times D \quad (9)$$

where L' is adjusted hourly emission on a road link (kg/hr),
L is unadjusted hourly emission on a road link (kg/hr),
M is month-specific VKT adjustment factor,
D is event factor if a particular event happens on the day;
m is index for process type,
t is index for technology type, and
p is the index for pollutant (CO, NOx, VOC, PM_{10} or SO_2).

Emissions for toxics (benzene, 1,3-butadiene and formaldehyde) are estimated from VOC using speciation fractions.

$$L'_{m,t,p} = L'_{m,t,voc} \times S_{m,t,p} \quad (10)$$

where L' is the hourly emission on a road link (kg/hr),
S is the mass fraction of a species in VOC;
m is the index for process type;
t is the index for technology type, and
p is the index for pollutant (benzene, 1,3-butadiene or formaldehyde).

Emissions are estimated for the EIM power-based model only for some major roads in the metropolitan area. Emissions from other roads are still needed to be included in the model. These 'background' motor vehicle emissions are calculated by gridding and subtracting the emissions estimated for the EIM power-based model from the total gridded emissions.

$$B_{m,t,p} = E_{m,t,p} - L_{m,t,p} \quad (11)$$

where B is background gridded, hourly emission (kg/hr),
E is the total gridded, hourly emission (kg/hr),
L is the gridded, hourly emission estimated from the EIM power-based model (kg/hr),
m is the index for process type,
t is the index for technology type, and
p is the index for pollutant.

The link data set contains information for the grid cell location of each road link, which is used to grid the link emissions estimated for the EIM power-based model.

2.5 Biogenic Model

Figure 4 shows the data flow diagram for the biogenic model.

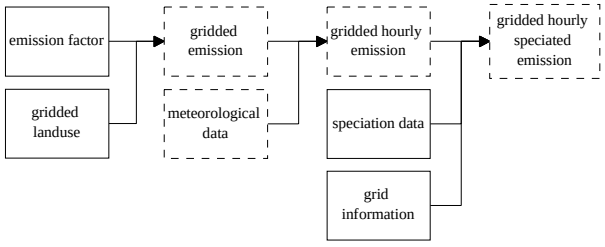


Figure 4 Data flow diagram for biogenic model

The model estimates gridded biogenic emission estimates at a standard condition (30°C and 1000 μE/m²/hr) from the emission fluxes in the emission factor data set and gridded land use data. There are emission fluxes for low, medium and high foliage cover density, which are used for winter, spring or autumn, and summer respectively. The following equation is used to obtain the gridded, standardised biogenic emissions estimates:

$$G_{p,c} = \sum F_{p,u} \times L_{u,c} \quad (12)$$

where $G_{p,c}$ is gridded biogenic emission of pollutant p in grid cell c (μg/hr),
$F_{p,u}$ is emissions flux of pollutant p for land use type u (μg/ha/hr), and
$L_{u,c}$ is area of land use type u in grid cell c (ha).

The gridded, standardised biogenic emissions are temporally allocated and adjusted using the meteorological data (solar radiation and temperature) supplied from the meteorological data model (see Section 2.7). The following equation is used:

$$E_{p,c,h} = G_{p,c} \times H_{p,c,h} \quad (13)$$

where $E_{p,c,h}$ is gridded, hourly biogenic emission of pollutant p in grid cell c at hour h (μg/hr),
$G_{p,c}$ is gridded, standardised biogenic emission of pollutant p in grid cell c (μg/hr), and
$H_{p,c,h}$ is biogenic adjustment factor for pollutant p in grid cell c at hour h.

The adjustment factors are based on formulations developed by CSIRO. Emissions are estimated for NOx and VOC.

2.6 Prescribed Burning and Wildfires Model

Figure 5 shows the data flow diagram for the prescribed burning and wildfires model.

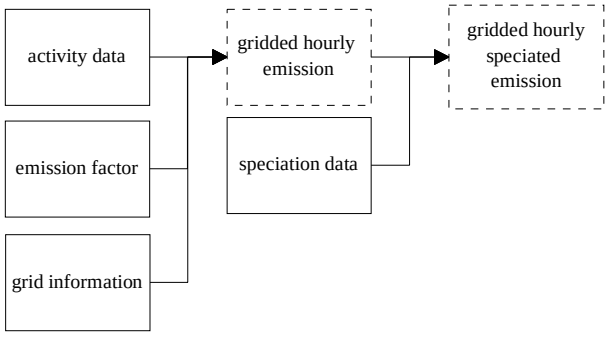


Figure 5 Data flow diagram for prescribed burning and wildfires model

The activity data file contains location and time of fires, fire size and fuel load of the area. The emission factor file contains the emission factors for prescribed burning and wildfires for different pollutants. Because the day and location of these sources vary throughout the year, the model need to find the grid cell location of the fires and select fires occurring on the specific modelling day,

The gridded, hourly emissions are obtained by the following equation:

$$E_{p,c,h} = A_c \times L_c \times F_p / 24 \quad (14)$$

where $E_{p,c,h}$ is emission of pollutant p from prescribed burning or wildfire in grid cell c at hour h (kg/hr),
A_c is fire size in grid cell c (ha),
L_c is fuel load in grid cell c (t/ha), and
F_p is emission factor for pollutant p (kg/t).

Because the duration of a fire cannot be forecasted, it is assumed that the fire spreads evenly over a 24 hour period.

2.7 Meteorological Data Model

This model extracts meteorological data used in the motor vehicle and biogenic models from LAPS. The data extracted are 1) gridded, hourly solar radiation in µE, and 2) gridded, hourly temperature in °C.

2.8 Speciation

The point, gridded or link, hourly emissions estimated by each model are speciated for NOx, PM_{10}, SO_2 and VOC. NOx is speciated into NO and NO_2, PM_{10} into discrete compounds (elemental carbon, organic carbon, sulphate and other particles) with eight size fractions, and VOC into individual Carbon Bond IV species. SO_2 is speciated into SO_2 and eight size fractions of sulphate particle. The following equation is used for the speciation:

$$C = E \times S / M \quad (15)$$

where C is point, gridded or link, hourly, speciated emission (mol/hr),
E is point, gridded or link, hourly emission of the pollutants (g/hr),
S is speciation fraction,
M is molecular weight (g/mol, 1 for VOC and particle species).

3. Conclusion

The AAQFS is evolving from the pilot stage to the demonstration stage. The EIM has been designed to forecast day-specific emissions which vary for weekday/weekend, month/season, and by meteorological conditions. This significantly improves the accuracy of emission estimates provided to the CTM. The power-based model is incorporated in the EIM which generates road-specific vehicle emission fluxes for the purpose of near-road impact modelling.

The EIM can provide forecast for special events or scenarios. The latter may correspond to a minimal motor vehicle usage scenario and will be used to indicate the reduction in population exposure that could result from a concerted public response to a forecast of poor air quality for the next day. In summary, the EIM acts an important channel for inputting scenarios of different policy options to the air quality model, and hence in bridging policy and science.

Acknowledgments

The authors would like to thank the Bureau of Meteorology and CSIRO for granting EPA's access to the NEC-SX supercomputer for development of the emissions model.

References

Birth T.L. and Geron C.D. 1995, *User's Guide to the Personal Computer Version of the Biogenic Emissions Inventory System (PC-BEIS), Version 2.0*, Computer Sciences Corporation and USEPA, Research Triangle Park, North Carolina, USA.

Cope M., Hess D., Lee S., Azzi M., Carras J., Wong N. and Young M., in press, 'Development of the Australian Air Quality Forecasting System', *Proceedings of the International Conference of Urban Climatology, Sydney, 1999*.

Galbally I.E. and Weeks I.A. 1992, *Natural Emissions of Hydrocarbons, Nitrogen Oxides, Carbon Monoxide and Sulfur Gases in the Kooragang Island Region of Newcastle, NSW*, CSIRO Division of Atmospheric Research, Aspendale, Victoria., Australia.

Gery M.W., Whitten G.Z., Killus J.P. and Dodge M.C. 1989. 'A photochemical kinetics mechanism for urban and regional scale computer modeling', *J. Geophys. Res*., **94**:12925-56.

Hess G.D., Cope M.E., Lee S. and Tory K. 1999, 'LAPS and the Australian Air Quality Forecasting System', in Parallel Computing in Meteorology and Oceanography, BMRC Research Report No. 75, Jasper J.D. and Meighen P.J. (eds), Bureau of Meteorolgy, Australia.

Ng Y.L. and Minchin M., forthcoming, 'Spatial and temporal allocation of emissions from wood combustion', *Proceedings of the 15th International Clean Air and Environment Conference, Sydney, 2000*, Clean Air Society of Australia & New Zealand, Eastwood, NSW, Australia.

Williams D.J., Shenouda D.A. and Carras J.N. 1994, 'Modelling air toxic emissions from motor vehicles', *Proceedings of the Air Toxics Conference, Sydney, 1994*, Clean Air Society of Australia & New Zealand and CSIRO, NSW, Australia.