



# A semi-empirical model for predicting the effect of changes in traffic flow patterns on carbon monoxide concentrations

Kim N. Dirks<sup>a,\*</sup>, Murray D. Johns<sup>b,1</sup>, John E. Hay<sup>c</sup>, Andrew P. Sturman<sup>d</sup>

<sup>a</sup> Department of Physiology, University of Auckland, Private Bag 92019, Auckland, New Zealand

<sup>b</sup> Department of Physics, University of Auckland, Auckland, New Zealand

<sup>c</sup> School of Environmental and Marine Sciences, University of Auckland, Auckland, New Zealand

<sup>d</sup> Department of Geography, University of Canterbury, Private Bag 4800, Christchurch, New Zealand

Received 9 October 2002; received in revised form 11 February 2003; accepted 17 February 2003

## Abstract

A simple semi-empirical model for predicting the effect of changes in traffic flow patterns on carbon monoxide concentrations is presented. The traffic component of the model requires average vehicle emission rate estimates for a range of driving conditions, as well as traffic flow data for the site of interest. The dispersion component of the model is based on a modified empirically optimised box model requiring only wind speed and direction information. The model is evaluated at a suburban site in Hamilton, New Zealand. Despite the simplicity of the model, produces reliable concentration predictions when tested on days with significantly different traffic flow patterns from those days with which the optimum model parameters were evaluated.

© 2003 Elsevier Science Ltd. All rights reserved.

**Keywords:** Carbon monoxide; Urban air quality; Traffic modelling; Vehicle emissions; Empirical modelling

## 1. Introduction

Predicting the effect of changes in traffic flow patterns on air pollution levels requires an urban air pollution model. Many of the existing commercial models are too complex to be operated routinely given the simplicity of the available meteorological and traffic data collected in New Zealand monitoring programmes. As a practical alternative, a site-specifically optimised model based on routinely available traffic flow information and meteorological data is presented. The traffic component of the model requires information from laboratory-based vehicle emission testing as well as traffic flow rates measured with pneumatic counters. Using an extension of simple traffic flow theory and empirical modelling,

estimates of road emission rate ( $\text{g km}^{-1} \text{s}^{-1}$ ) are made for vehicle densities ranging from zero (completely free-flowing) to the road jam density (road completely blocked due to congestion). The dispersion component of the model is based on a modified empirically optimised box model requiring only wind speed and direction information as input. Both the height of the box and the background concentrations are estimated empirically (see Dirks et al. (2002) for a complete description of the meteorological component of the model). In the present paper, the traffic component of the model is developed and evaluated using data collected at a suburban site in Hamilton, New Zealand.

The inclusion of traffic and emissions information in the current model allows the user to make predictions about the effect of changes in both emissions and meteorology on concentrations near roads. For example, it is possible to predict the effect on concentration as a result of a 10% increase in traffic flow for a particular wind speed at a particular time of day. Both versions of

\*Corresponding author. Tel.: +64-9-373-7599; fax: +64-9-3737-499.

E-mail address: k.dirks@auckland.ac.nz (K.N. Dirks).

<sup>1</sup> Deceased.

the model have been developed and evaluated for carbon monoxide but could be readily adapted for other major vehicle pollutants.

## 2. Traffic model description

### 2.1. New Zealand vehicle emissions testing

The purpose of the traffic component of the model is to provide estimates of the road emission rate (RER) ( $\text{g km}^{-1} \text{s}^{-1}$ ) for a range of traffic flow rates observed at the site of interest based on vehicle emissions rate information from a New Zealand emissions testing program and traffic flow data collected using pneumatic counters.

A vehicle emission testing programme was recently carried out in New Zealand (Raine et al., 1997). A vehicle equipped with kinematic monitoring devices was driven along 'typical' roads in an attempt to obtain drive cycles for various road types and under various states of congestion. Average vehicle emission rates were obtained from 23 vehicles, each operated through 12 different drive cycles. The vehicles tested consisted of nine carburetted vehicles, two carburetted with catalyst, seven fuel injected and five fuel injected with catalyst. These selected vehicles were approximately representative of the proportions typical of the New Zealand petrol passenger fleet (Raine et al., 1997). At this stage, no similar information is available for trucks. The average vehicle emission rates (AVER) for these 23 vehicles operated through a suburban road drive cycle under a constant speed of  $50 \text{ km h}^{-1}$ , and under free-flow, interrupted and congested conditions, were 9, 16, 19 and  $23 \text{ g km}^{-1} \text{veh}^{-1}$ , respectively, with average drive cycle speeds of 50, 38, 23 and  $18 \text{ km h}^{-1}$ , respectively. These are comparable with the results of the passenger vehicle emissions estimated by Mukherjee and Viswanathan (2001) for Singapore, and the emissions estimated for light-duty vehicles in Milan by Cernuschi et al. (1995). Note that, as expected, the average vehicle emission rate increased when the driving conditions went from a state of free-flow to congested. Similar data were obtained for other road types.

### 2.2. Site description and traffic data

In order to estimate emission rates for a particular road, vehicle flow rates for the site of interest are also required. Hourly average vehicle count rates for 1 week were available from pneumatic counters. Manual measurements of traffic data at the site revealed that the queue in the branch of the intersection on which the monitoring took place generally cleared completely every cycle, even during peak traffic conditions. The

road therefore did not generally reach congested traffic conditions.

### 2.3. Basic traffic flow modelling

Given that a low traffic flow rate can be due to a lack of vehicles on the road or because of heavy congestion, the relationship between vehicle density  $D$  ( $\text{veh km}^{-1}$ ) and traffic flow rate first needed to be determined. This was achieved through standard traffic flow modelling, as now described.

If it is assumed that vehicles travelling along a road are evenly spaced and travelling at the same speed  $V$  ( $\text{km h}^{-1}$ ) at a flow rate of  $T$  ( $\text{veh h}^{-1}$ ), then

$$D = \frac{T}{V}. \quad (1)$$

Greenshields (1943), in one of the earliest studies of traffic flow, found that the relationship between the vehicle density and the vehicle speed was well represented by

$$V = V_0 \left( 1 - \frac{D}{D_j} \right). \quad (2)$$

In this equation,  $D_j$  ( $\text{veh km}^{-1}$ ) is the jam density, or the density at which the road is completely blocked due to congestion, and  $V_0$  ( $\text{km h}^{-1}$ ) is the maximum free-flow speed. A summary of the results of the Greenshields study can be found in Salter (1989).

Substituting Eq. (1) into Eq. (2) gives the quadratic relationship

$$T = DV_0 \left( 1 - \frac{D}{D_j} \right). \quad (3)$$

The slope of any line joining the origin to the quadratic function of traffic flow versus density is the average vehicle speed for a particular density (see Fig. 1).

Observations of traffic flow at the site suggest that a jam density of  $120 \pm 20 \text{ veh km}^{-1}$  is appropriate. This was estimated by counting the number of vehicles along the stretch of road leading up to the traffic lights while the vehicles were queued. The maximum free-flow speed ( $V_0$ ) is assumed to be  $50 \pm 5 \text{ km h}^{-1}$ , the speed limit of the road. Knowing the average vehicle speeds for each of the New Zealand derived drive cycles, it was possible to determine the expected traffic flow rate and vehicle density associated with each of the three drive cycles. These are also shown in Fig. 1. The density associated with the maximum traffic flow rate ( $D_{\text{maxflow}}$ ) is  $60 \text{ veh km}^{-1}$ , half the jam density.

The vehicle density may be calculated for any flow rate by solving Eq. (3) for  $D$ . This gives

$$D = \frac{D_j}{2} \left( 1 \pm \sqrt{1 - \frac{4T}{V_0 D_j}} \right). \quad (4)$$

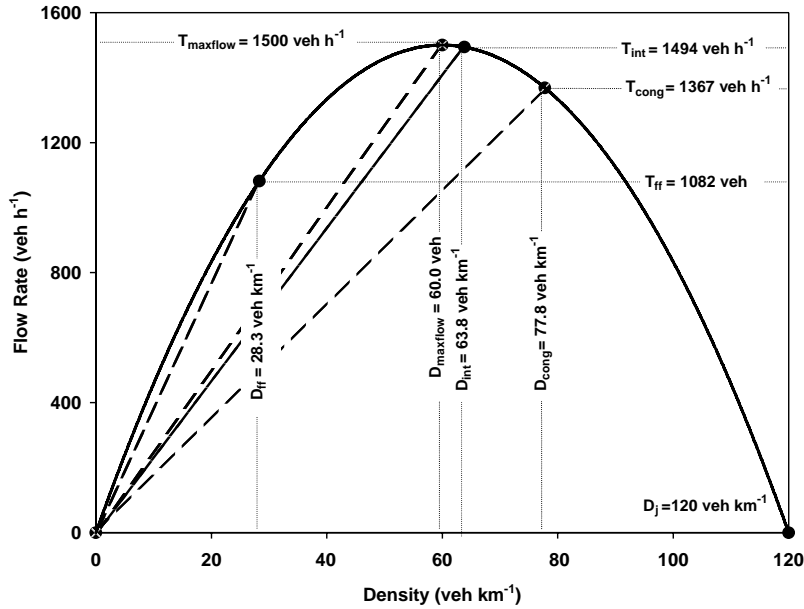


Fig. 1. Theoretical relationship between vehicle flow rate and density for a road with a speed limit of  $50 \text{ km h}^{-1}$  and a jam density ( $D_j$ ) of  $120 \text{ veh km}^{-1}$ . The slopes of the dotted lines represent the average vehicle speeds for various states of congestion. The subscripts ff, int and cong represent free-flow, interrupted and congested, respectively. The subscript maxflow represents state of maximum traffic flow rate.

The two solutions correspond to the congested and free-flow traffic conditions. Traffic information at the suburban site revealed that traffic flow rates remained well below  $T_{\text{maxflow}}$ , even during times of peak congestion. Therefore, for this site, only the negative solution

$$D = \frac{D_j}{2} \left( 1 - \sqrt{1 - \frac{4T}{V_0 D_j}} \right) \quad (5)$$

applies (solutions associated with vehicle densities of less than  $60 \text{ veh km}^{-1}$ ). The maximum vehicle density observed at the site is  $25 \text{ veh km}^{-1}$ . This is approximately equal to the free-flow rate and well below the density associated with a maximum flow rate.

#### 2.4. Road emission rates

The next step was to determine empirically the relationship between the vehicle density and the average vehicle emission rate. From the four drive cycles, a function was required which related the vehicle emission rate to all vehicle densities ranging from 0 to  $120 \text{ veh km}^{-1}$ . The constraints of the function were that the emission rate for near-zero flow had to approach  $9 \text{ g km}^{-1} \text{ veh}^{-1}$  (the VER for near-zero flow) and the VER was required to tend to infinity as the density approached the jam density. The function

$$\text{VER} = \frac{(aD^2 + bD + c)D}{(D_j - D)} + \text{VER}_0 \quad (6)$$

was found to be of a form representative of the data, where  $a$ ,  $b$  and  $c$  are constants and  $\text{VER}_0$  is the near-zero flow average vehicle emission rate. Based on the values found in the New Zealand emissions testing programme, for suburban New Zealand roads, the constants  $a$ ,  $b$ ,  $c$  and  $\text{VER}_0$  were found to be 0.006, 0.943, 44.6 and 9.0, respectively.

The emission rate for the road as a whole,  $Q_1$  ( $\text{g km}^{-1} \text{ s}^{-1}$ ), is given by

$$Q_1 = \frac{\text{VER} \times T}{3600} \quad (7)$$

Substituting Eq. (6) for VER and Eq. (3) for  $T$ , Eq. (7) becomes

$$Q_1 = \frac{V_0 D}{3600 D_j} [(aD^2 - bD + c)D + \text{VER}_0(D_j - D)] \quad (8)$$

with  $a$ ,  $b$ ,  $c$  and  $\text{VER}_0$  as given above.  $D$  can be found from the flow rate using Eq. (5) and VER from Eq. (6).

Note that the road emission rate (as is the vehicle density) is a multi-valued function of the traffic flow rate (the same traffic flow rate corresponds to two vehicle densities and therefore two emission rates) (Fig. 2). The traffic flow rates observed at the suburban site remained well below  $T_{\text{max}}$  and therefore were associated with the lower of the two emission rates possible for the given traffic flow rate. From these results, and using the traffic flow rate throughout the day, it is possible to estimate the road emission rate for both weekend days and weekdays for the site of interest.

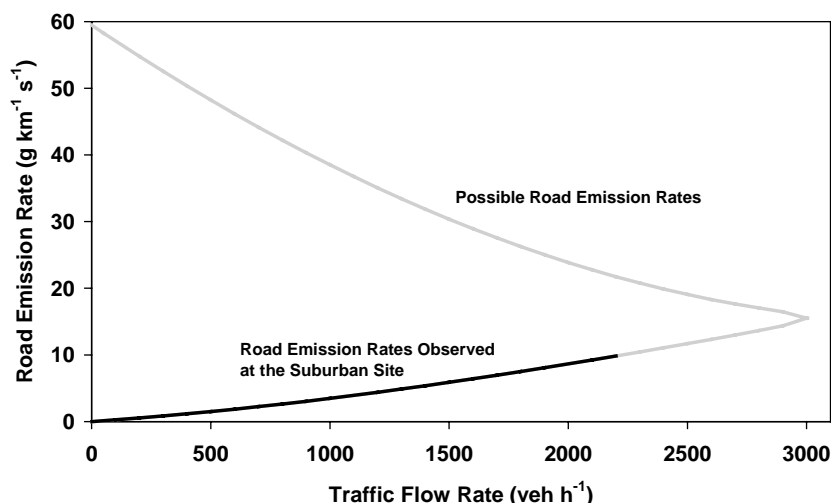


Fig. 2. The effect of traffic flow rate on road emission rate,  $Q_1$ . Note that  $Q_1$  is a multi-valued function of traffic flow rate.

### 3. Dispersion model description

The dispersion component of the semi-empirical model is based on the box model approach where the road emission rate  $Q_1$  ( $\text{mg m}^{-1} \text{s}^{-1}$ ) is assumed to be constant along a road and the pollutants are mixed uniformly within a box of height  $\Delta z$  (m). The horizontal wind speed,  $u$  ( $\text{m s}^{-1}$ ), which is assumed to be uniform within the layer and running at an angle  $\theta$  to the road, removes the pollutants through advection. At the same time, pollutants are introduced into the box through advection of the background concentration. If the background concentration is given by  $C_1$  ( $\text{mg m}^{-3}$ ), and the concentration leeward of the road  $C$  ( $\text{mg m}^{-3}$ ) is assumed to be in steady state, then

$$C = \frac{Q_1}{u \Delta z \sin \theta} + C_1. \quad (9)$$

Dirks et al. (2002) showed that for this suburban site, provided leeward and windward conditions are treated separately, concentration may be taken to be independent of wind direction. With this and with the inclusion of a wind speed offset,  $u_0$  ( $\text{m s}^{-1}$ ), to avoid severe over-predictions in very light wind speed conditions as suggested by Chock (1978), Eq. (9) becomes

$$C = \frac{Q_1}{\Delta z(u + u_0)} + C_1 \quad (10)$$

for leeward conditions (wind conditions such that the monitor is leeward of the road). The emissions term for leeward conditions ( $Q_1$ ) incorporates both emissions from the road adjacent to the monitor and emissions from other roads in the vicinity. For windward condi-

tions, the model becomes

$$C = \frac{Q_w}{\Delta z(u + u_0)} + C_w, \quad (11)$$

where  $Q_w$  is the emission component from other roads in the vicinity and  $C_w$  is the background concentration for windward conditions. The optimum value for  $u_0$  was determined empirically through the minimization of the model root-mean-squared (RMS) error.

For a site without emissions or traffic information, it is possible to sort the data by time of day and perform linear regressions of  $C$  ( $\text{mg m}^{-3}$ ) on  $(u + u_0)^{-1}$  for leeward conditions. In this case, the regression coefficient becomes  $Q_1 \Delta z^{-1}$  with  $C_1$  representing the background concentration. One set of regression parameters is obtained for each 10-min period throughout the day. A model of this form is the one presented in Dirks et al. (2002). If we include the road emissions information and perform a linear regression of  $C$  on  $Q_1(u + u_0)^{-1}$ , the regression coefficient becomes  $\Delta z^{-1}$ . The advantage of the inclusion of traffic and emissions information into the model is that the optimum parameters allow predictions to be made for days for which traffic flows patterns are significantly different from those with which the model parameters were optimised, allowing the user to investigate 'what-if' scenarios associated with changes in traffic flow patterns. As with the semi-empirical model for urban  $\text{PM}_{10}$  concentrations presented by Kukkonen et al. (2001), new parameters are needed if the model is to be used for a different site.

The data set consists of two sets of 60 days of weekday data and 27 days of weekend data for a suburban site in Hamilton, New Zealand. The monitoring station collects 10-min averaged continuous wind speed, wind

direction data as well as carbon monoxide concentrations, giving a total of 144 observations per day. The site is flat and surrounded with suburban-type housing and vegetation.

#### 4. Results

To evaluate the model with the emission data included, the fictitious point method was used whereby each day was systematically removed from the data set, predictions were made for that day and then compared with the observed concentrations. This procedure was then repeated for all days in the data set. The model was evaluated by optimising the model parameters based on weekday data and using these parameters to predict for weekends and vice versa. Data were also sorted by season to take into account the seasonal variations in the meteorology. Fig. 3 shows an example of model predictions for 1 week of data. Predictions were made for leeward wind conditions only. The correlation coefficient, RMS error, and mean absolute error for the summer season were 0.7, 0.21, and  $0.15 \text{ mgm}^{-3}$ , respectively, while the equivalent results for the autumn season were 0.7, 0.65, and  $0.43 \text{ mgm}^{-3}$ , respectively, when using weekend data to predict for weekdays. The fraction of two,  $f_2$  (the fraction of data for which the ratio of the predicted to observed concentrations fall within 0.5 and 2), are 0.78 and 0.73 for the summer and autumn seasons, respectively.

One test of the model is to compare the optimum parameter,  $\Delta z$ , the effective height of the plume throughout the day, predicted from the weekday data and from the weekend data separately, as the average plume height is not expected to be significantly different

between the two. Fig. 4 shows that the plume heights throughout the day are similar for weekends and weekdays. The plume heights are also highest during the middle of the day (reaching about 25 m) and lowest at night, consistent with what is expected in terms of variability throughout the day. This result gives us confidence that the model results are reasonable.

The advantage of including the emissions estimate into the model (in contrast to what was presented in the model of Dirks et al., 2002) is that it may be possible to use the optimum parameters for ‘average’ weekdays, for example, to predict concentrations for days such as holidays, when vehicle flows are significantly different from the average weekdays, or to look at what-if scenarios associated with planned or expected changes in traffic flow patterns. For example, for our site of interest, if the traffic flow rate during the morning rush hour increased by 20% from the present rate, the

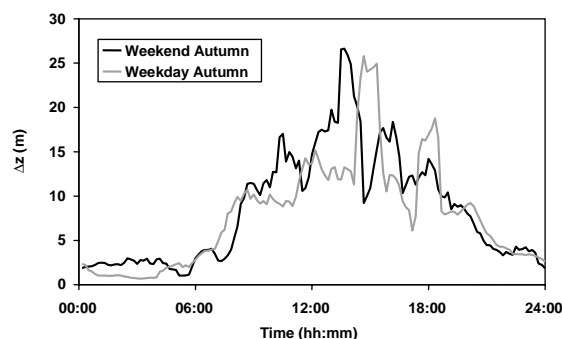


Fig. 4. Example of the effective plume height ( $\Delta z$ ) throughout the day based on the model-optimised parameters for weekend and weekday data.

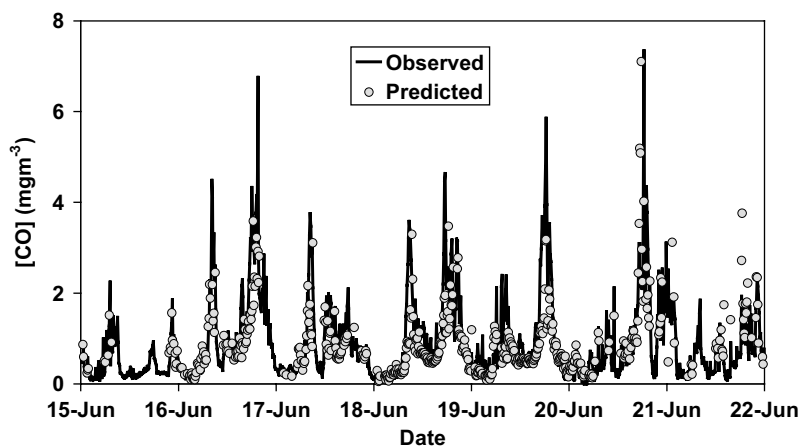


Fig. 3. One week of observed and predicted concentrations (leeward wind cases only) using independent emission estimates. Weekday parameters are used to predict for the weekend days and vice versa (15 June 1998 was a Monday).

emission rate for the road as a whole ( $Q_1$ ) would increase by 50%.

One of the main sources of error in the model predictions is believed to be the scavenging of carbon monoxide by rainfall as the peak concentrations and wet season in New Zealand coincide. Work is now underway to investigate the effect of rainfall rate on carbon monoxide and to include a component in the model that takes this into account.

The other source of error is that the emissions estimates were made based on only 23 vehicles and without the inclusion of any trucks. However, with the current procedure set in place, it is now possible to update the model estimates for the model as new emissions data become available. This will need to be done regardless, as the vehicle fleet and hence the emissions rates are constantly changing.

## 5. Conclusions

The source characteristics of vehicle emissions and the meteorology of the surface layer within suburban areas are highly complex. In order to investigate the effect of changes in meteorology and traffic flow patterns on air pollution concentrations, a simple semi-empirical model was developed based on standard traffic and meteorological information. Road emission rates were predicted based on vehicle emissions testing data collected in the laboratory and traffic flow information collected at the air quality monitoring site. This model allows the user to predict the expected concentration for days when the traffic flow patterns are significantly different or to investigate 'what-if' scenarios associated with changes in traffic flow patterns.

## Acknowledgements

The authors thank Environment Waikato for providing the air quality data required for this study and for their financial support throughout the project and the Hamilton City Council for providing the pneumatic counter data.

## References

- Cernuschi, S., Giugliano, M., Cemin, A., Giovannini, I., 1995. Model analysis of vehicle emission factors. *The Science of the Total Environment* 169, 175–183.
- Chock, D.P., 1978. A simple line-source model for dispersion near roadways. *Atmospheric Environment* 12, 823–829.
- Dirks, K.N., Johns, M.D., Hay, J.E., Sturman, A.P., 2002. A simple semi-empirical model for predicting missing carbon monoxide concentrations in records in the absence of emission or traffic data. *Atmospheric Environment* 36 (39–40), 5953–5959.
- Greenshields, B.D., 1943. The photographic method of studying traffic behaviour. *Proceedings of the 13th Meeting of Highway Research Board*.
- Kukkonen, J., Harkonen, J., Karppinen, A., Pohjola, M., Peitarila, H., Koskentalo, T., 2001. A semi-empirical model for urban PM10 concentrations, and its evaluation against data from an urban measurement network. *Atmospheric Environment* 35, 4433–4442.
- Mukherjee, P., Viswanathan, S., 2001. Contributions to CO concentrations from biomass burning and traffic during haze episodes in Singapore. *Atmospheric Environment* 35, 715–725.
- Raine, R., Blanchard, G., Jones, G., Elder, S., 1997. Measurement of emissions factors for New Zealand cars. *Transport and Air Pollution, Fourth International Scientific Symposium*, Avignon, France.
- Salter, R.J., 1989. *Highway Traffic Analysis and Design*, 2nd Edition. MacMillan, London, pp. 56–60.