Transportation Research Part D 59 (2018) 464–477

Contents lists available at ScienceDirect

Transportation Research Part D

journal homepage: www.elsevier.com/locate/trd

Development and evaluation of the R-LINE model algorithms to account for chemical transformation in the near-road environment

Alejandro Valencia[a], Akula Venkatram[d], David Heist[b], David Carruthers[c], Saravanan Arunachalam[a,*]

[a] Institute for the Environment, University of North Carolina at Chapel Hill, NC, USA
[b] US EPA, National Exposure Research Laboratory, Research Triangle Park, NC, USA
[c] Cambridge Environmental Research Consultants, Cambridge, UK
[d] University of California at Riverside, Riverside, CA, USA

ARTICLE INFO

Keywords:
Near-road
Dispersion modeling
R-LINE
GRS
Traffic emissions
Nitrogen oxides

ABSTRACT

With increased urbanization, there is increased mobility leading to higher amount of traffic-related activity on a global scale. Most NO_x from combustion sources (about 90–95%) are emitted as NO, which is then readily converted to NO_2 in the ambient air, while the remainder is emitted largely as NO_2. Thus, the bulk of ambient NO_2 is formed due to secondary production in the atmosphere, and which R-LINE cannot predict given that it can only model the dispersion of primary air pollutants. NO_2 concentrations near major roads are appreciably higher than those measured at monitors in existing networks in urban areas, motivating a need to incorporate a mechanism in R-LINE to account for NO_2 formation. To address this, we implemented three different approaches in order of increasing degrees of complexity and barrier to implementation from simplest to more complex. The first is an empirical approach based upon fitting a 4^{th} order polynomial to existing near-road observations across the continental U.S., the second involves a simplified Two-reaction chemical scheme, and the third involves a more detailed set of chemical reactions based upon the Generic Reaction Set (GRS) mechanism. All models were able to estimate more than 75% of concentrations within a factor of two of the near-road monitoring data and produced comparable performance statistics. These results indicate that the performance of the new R-LINE chemistry algorithms for predicting NO_2 is comparable to other models (i.e. ADMS-Roads with GRS), both showing less than ± 15% fractional bias and less than 45% normalized mean square error.

1. Introduction

Living, working, or attending school near major roadways has been associated with a range of health effects (Health Effects Institute, 2010; Vette et al., 2013). Additionally, it is estimated that as much 19% of the U.S. population are in the vicinity of roadways with significant traffic emissions (U.S. Census Bureau, 2007; Health Effects Institute, 2010; Rowangould, 2013). Therefore, understanding near-roadway pollutants and developing models for air quality prediction due to traffic-related emissions has been an area of ongoing research.

In the U.S, motor vehicles account for 60% of the nitrogen oxides ($NO + NO_2 = NO_x$) emissions (USEPA, 2010). In addition, exposure to NO_2 has been linked to adverse respiratory and cardiovascular effects (Samoli et al., 2006; Latza et al., 2009). Thus, the

* Corresponding author.
E-mail address: sarav@email.unc.edu (S. Arunachalam).

https://doi.org/10.1016/j.trd.2018.01.028

Available online 20 February 2018
1361-9209/

U.S. Environmental Protection Agency (USEPA) has established NO_2 as one of six principal pollutants with National Ambient Air Quality Standards (NAAQS) to protect public health. The U.S. EPA set a 1-h form of NAAQS for NO_2 in 2010 (set at 100 ppb for a 98th percentile value, averaged over 3 years) to address adverse exposure due to high short-term peaks in the vicinity of the near-road environment. To support NO_2 NAAQS attainment designations, the EPA has also required to set air quality monitoring sites for NO_2 within 50 m from major roads (USEPA, 2010). Considering that robust spatiotemporal monitoring efforts can be cost prohibitive, air quality models (AQMs) can aid to assess NO_2 near roads where measurements from monitors are limited.

Numerous studies have been published which aim to simulate NO_2 and its evolution in the general atmosphere (Gardner and Dorling, 1999; American Petroleum Institute, 2013; Hendrick et al., 2013; Podrez, 2015). The recent USEPA White Papers on Planned Updates to the AERMOD Modeling System discuss improvements to NO_2 modeling in AERMOD (USEPA, 2017). Due to the growing interest in understanding traffic-related air pollutants, several studies have focused on directly modeling NO_2 near roadways (Hirtl and Baumann-Stanzer, 2007; Kenty et al., 2007; Chaney et al., 2011; During et al., 2011; Wang et al., 2011; Kimbrough et al., 2017). Most of these studies predict NO_2 using dispersion models such as CALINE (Benson, 1984), AERMOD (Cimorelli et al., 2005), and ADMS-Urban (McHugh et al., 1997).

The Research LINE source (R-LINE) model was specifically developed for these types of studies (Snyder et al., 2013). To better simulate mobile source pollutant dispersion, it has an emphasis on near-surface releases and near-source dispersion, and models traffic-related sources as line segments. However, R-LINE was designed to simulate primary, chemically inert pollutants. Even though R-LINE has been shown to adequately estimate near-road dispersion (Heist et al., 2013), it does not have the ability to simulate chemically reactive species such as NO_2. Thus, we will develop three methods that will allow R-LINE to simulate the chemical evolution of NO_2 in the atmosphere, and present inter-comparisons of these when compared to observations from a near-road case study.

The first is a linear regression method based on the Dixon-Middleton-Derwent (DMD) method (Dixon et al., 2001) that uses NO_x and NO_2 data from near-road monitors in the U.S. The second approach used to simulate NO_2 consists of a simplified (Two-reaction) chemistry scheme as described in Hess and Cope (1989). The third involves a more robust approach, using the Generic Reaction Set (GRS). All methods are driven with R-LINE, the Research LINE-source dispersion model specifically designed to simulate the dispersion of traffic-related emissions from roadways. NO_2 predictions from all three approaches are compared against near-road measurements along a section of Interstate 96 (I-96) in Detroit, Michigan, USA.

2. Methods

2.1. Study domain and field measurements

Foremost, to evaluate our study, we use data from a field campaign developed to assess the relationship between near-roadway air pollutant exposure and the respiratory outcomes of asthmatic children in the vicinity of major roadways in Detroit, MI (Vette et al., 2013). This study describes the design and methods to support the Near-Road Exposures and Effects of Urban Air Pollutants Study (NEXUS), and additional details about the measurements are available in Kimbrough et al. (2013). From this study, we use a section of I-96 just west of Detroit city limits, to model traffic-related air pollutants and compare against measurements from the field campaign.

Four monitoring sites were commissioned at locations 10 m, 100 m and 300 m north (and downwind) of I-96 around the Eliza Howell Park and another site 100 m south (and upwind) of I-96 (Fig. 1 shows the site locations). Measurements were recorded every 5 min from September 26, 2010 to June 20, 2011 for NO_x and NO_2. Traffic volume (activity) and speed measurements were also collected for each lane of I-96 from September 25, 2010 to April 27, 2011. From these traffic volume measurements, an average annual daily traffic (AADT) of approximately 140,000 vehicles per day was calculated.

Another monitoring station used in this study includes the AQS site at East 7 Mile Road with ID 26-163-0019 (Fig. 1) where hourly NO_2, NO_x, and O_3 concentrations were collected. This site is 22 km away from the I-96 measurement locations. At this distance, it is inside the Detroit metro area, but not influenced by major roads, since it is approximately 4 km away from any primary road and 2 km away from any secondary road. This monitor is used as urban background site to aid in the NO_x to NO_2 conversion schemes. Each conversion scheme uses this background site differently. More details follow in Section 2.3. Several plots describing the background site and how they compare to the I-96 sites have been included in Supplementary Information (Figs. S1, S2, and S5).

2.2. Dispersion models

2.2.1. R-LINE

As previously mentioned, we used the R-LINE dispersion model for this study. R-LINE is a research grade dispersion model developed for near-roadway assessments. The model uses a Gaussian, steady-state plume-dispersion formulation that incorporates newly developed algorithms for predicting concentrations from road sources at receptors near roads. Unlike AERMOD (EPA's recommended dispersion model), R-LINE was specifically designed to model roadways as line segments. A considerable number of models that simulate dispersion of roadways are analytical approximations to the integral associated with modeling a line source as a set of point sources. Nonetheless, these approximations can cause large errors when the winds are light and variable, when the wind direction is close to parallel to the road, and when the source and receptor are at different heights. R-LINE uses a Romberg numerical integration to compute the contribution of the point sources used to represent a line source. This approach incorporates governing processes without including errors associated with approximations of the underlying model framework (Snyder et al., 2013). Finally,