Atmospheric Environment 82 (2014) 351-363



Contents lists available at ScienceDirect

# Atmospheric Environment

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

# Implementation of a high-resolution Source-Oriented WRF/Chem model at the Port of Oakland



ATMOSPHERIC



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# HIGHLIGHTS

• We develop a high resolution Source-Oriented WRF/Chem model (SOWC-HR).

- We predict PM<sub>2.5</sub> EC source contributions at 250 m resolution over Oakland CA.
- Higher resolution increased population-weighted EC exposure by 17% for some sources.

• Traffic, rail, and ships are dominant sources.

#### ARTICLE INFO

Article history: Received 17 June 2013 Received in revised form 25 September 2013 Accepted 28 September 2013

Keywords: WRF/Chem Source-oriented High resolution LES Elemental carbon Port of Oakland

# ABSTRACT

A version of the Source-Oriented WRF/Chem (SOWC) model with 250 m spatial resolution (SOWC-HR) was developed and implemented to perform high resolution simulations over the community of Oakland, California, during March 2010. A multiscale set of nested domains was used to predict contributions to airborne particulate elemental carbon (EC) concentrations from ships, trains, and on-road diesel trucks. The final domain at 250 m resolution used Large Eddy Simulation (LES) to predict turbulent mixing at scales where traditional first order closure models are not valid. Results of the high resolution simulation with the nested LES (HR case) and without the nested LES (non-HR case) were compared to speciated particulate matter (PM) measurements and source contributions calculated using Positive Matrix Factorization (PMF). The PMF results showed that on-road diesel traffic was a major EC contributor, a result consistent with previous studies for Oakland. The average EC concentration predicted at the site by the SOWC-HR model was 0.42  $\mu$ g m<sup>-3</sup>, with source contributions of 0.22  $\mu$ g m<sup>-3</sup> from on-road diesel, 0.05  $\mu g$  m  $^{-3}$  from ship fuel combustion, 0.08  $\mu g$  m  $^{-3}$  from trains, and 0.09  $\mu g$  m  $^{-3}$  from other sources. Both simulation cases predicted similar total EC concentrations and source contributions at the sampling sites, but more substantial differences were predicted at other locations in the study region. The HR case predicted higher average and maximum hourly EC contributions from all sources compared the non-HR case. The greatest relative increase of maximum hourly EC was seen in the onroad diesel source, which increased by nearly a factor of 2 (3.74  $\mu$ g m<sup>-3</sup> to 6.69  $\mu$ g m<sup>-3</sup>) when spatial resolution was increased from 1 km to 250 m. The SOWC-HR model predicted greater populationweighted EC concentrations from all sources when compared to the SOWC model without HR. The increase in period-averaged EC exposure from each source ranged from +1% to +17%, while the increase in maximum hourly EC exposure from each source ranged from +9% to +32%. This evaluation shows that resolving neighborhood scales through the representation of local mixing phenomena can significantly impact pollutant concentration predictions, especially when examining extreme exposures in a densely populated area with many sources and complex terrain.

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#### 1. Introduction

The San Francisco Bay Area in California is a densely populated metropolitan region with a variety of air pollution sources and complex topography. The West Oakland community within the Bay

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<sup>1352-2310/\$ -</sup> see front matter © 2013 Elsevier Ltd. All rights reserved. http://dx.doi.org/10.1016/j.atmosenv.2013.09.055



Fig. 1. Left: Map of LES domain (extent) and West Oakland area. Right: Map of West Oakland area, including locations of West Oakland community (red), major highways (orange), permitted point sources (green), Port of Oakland (yellow), Union Pacific Rail yard and lines (blue), Port of Oakland monitoring site (SITE 1), and BAAQMD West Oakland monitoring site (SITE 2). (©2013 TerraMetrics, Google). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Area has a population of 22,200 in a relatively small area of 7.7 km<sup>2</sup>, which lies adjacent to the Port of Oakland and the Union Pacific Rail yard, and is bounded by three major freeways (Di, 2008) (see Fig. 1). The terrain surrounding Oakland has elevation ranging from sea level to approximately 500 m in the hills 15 km to the east. Mesoscale circulation driven by differential heating over inland areas versus over the ocean produces a land—sea breeze wind system that interacts with the terrain to produce complex wind patterns and regions of micro-climates. High spatial resolution and sophisticated modeling treatments are needed to accurately predict population exposure to air pollution mixtures given these conditions.

The air pollutant of greatest concern in the Oakland region is airborne particles with diameter less than 2.5  $\mu$ m (PM<sub>2.5</sub>). PM<sub>2.5</sub> is composed of numerous solid and liquid chemical components in size fractions as small as a few nanometers (nm). The chemical components in PM<sub>2.5</sub> may be emitted directly to the atmosphere in the condensed form or they can be produced from atmospheric chemical reactions. The majority of the PM<sub>2.5</sub> in Oakland is thought to originate from various types of fuel combustion (Tanrikulu et al., 2011b), but the dominant sources are difficult to identify given the complex formation pathways and number of different sources. A lack of clear relationships between emissions sources and air pollution exposure makes it difficult to design control programs to protect public health.

Previous modeling studies have examined the sources of PM<sub>2.5</sub> and associated health risks in the Bay Area using a variety of multiscale regional air quality models, including CAMx, CMAQ, and WRF (Deng and Stauffer, 2011; Tanrikulu et al., 2009a, b). These simulations were performed at high spatial resolutions (4 km-1 km) and identified sharp spatial gradients of PM concentration around major sources. These sharp gradients lead to complex patterns of population exposure at the neighborhood scale, which can have a significant impact on health risks in these densely populated areas (Tanrikulu et al., 2011b). Higher spatial resolutions (250 m) have been used in receptor-based models to simulate annual average air pollution in Oakland (Di, 2008), but these receptor models use simplified treatments of meteorology, particle size distributions, and chemical reactions, and are not typically suited to predict population exposure over an entire city. A need exists to predict exposure to reactive air pollution mixtures at neighborhood scales in communities like Oakland across the US.

The use of high spatial resolution avoids numerical artifacts that can smooth fine spatial features in predicted concentration fields, but previous studies show that the accuracy of the overall model prediction is still influenced by the accuracy of the input data. Primary pollutants such as PM<sub>2.5</sub> EC have sharper spatial gradients than secondary pollutants such as ozone, but a study by Valari and Menut (2008) suggests that high resolution emissions input data is needed to capture these features. A study by Thompson and Selin (2012) suggests that increased model spatial resolution may not reduce uncertainties enough to recognize significant differences in health impact predictions for ozone exposure.

The objective of this study is to develop a method to predict source contributions to chemically reacting air pollution mixtures with sufficient spatial resolution to accurately calculate population exposure in the presence of sharp spatial concentration gradients. This method is applied to predict the spatial distribution of a primary pollutant (PM<sub>2.5</sub> EC) in a region where secondary transformations (condensation of nitrate, SOA, and other semi-volatile material) could influence the dry deposition rate and therefore the concentration field. A version of the Source-Oriented WRF/Chem (SOWC) model (Zhang et al., 2013) was modified to work at high resolution (HR) for this purpose. The model uses Large Eddy Simulation (LES) to predict source contributions to the size and composition distribution of airborne particulate matter at neighborhood scales of 250 m. The SOWC-HR model was implemented to simulate pollutant concentrations over the city of Oakland during the month of March 2010. Predictions of source-resolved elemental carbon (EC) concentrations were compared to receptor-based source apportionment results calculated using Positive Matrix Factorization at the Port of Oakland and at the West Oakland community monitoring location. Population-weighted EC exposure was also calculated to evaluate the differences caused by spatial variation ranging from 1 km down to 250 m.

Table 1Domain and model configurations.

Domain	Cell width	Grid mesh	PBL scheme?
1 2	12 km	45 × 45	On – YSU
	4 km	48 × 48	On – YSU
3	1 km	$\begin{array}{l} 56 \times 56 \\ 96 \times 96 \end{array}$	On – YSU
4	250 m		Off

# 2. Methods

# 2.1. SOWC-HR model description

The model used in this study was based on the SOWC model. which represents airborne particulate matter as a source-oriented external mixture in which particles emitted from different emissions sources are tracked separately rather than immediately averaged into a single internally mixed size distribution. The source-oriented approach supports size-resolved source apportionment calculations and it allows for more realistic calculations of optical properties compared to internally mixed approaches (Zhang et al., 2013). Chemistry is used in the current study to simulate the condensation of inorganic and organic secondary material onto primary PM, changes in PM hygroscopicity and water content, and associated changes in particle size, coagulation rates, and dry deposition, all of which have implications for PM2.5 EC concentrations. The SOWC model was developed from WRF/Chem V3.1.1, with source-oriented chemical mechanisms adapted from the UCD/ CIT source-oriented model (Zhang et al., 2013). The development history and formulation of these mechanisms have been described in detail elsewhere (Kleeman et al., 1997; Mysliwiec and Kleeman, 2002; Ying et al., 2004), and numerous studies and evaluations have been performed using the UCD/CIT source-oriented model (Ying et al., 2007, 2008; Zhang and Ying, 2010). This section will only emphasize recent model updates and features unique to the application of the SOWC model at high resolution.

# 2.1.1. Nested Large Eddy Simulation

The capability to run large eddy simulations is available in the standard WRF/Chem model. A basic description of the LES options is provided in the Advanced Research WRF user guide (NCAR, 2010), and the numerical methods used are described in detail by Skamarock et al. (2008). LES has been used to simulate idealized cases, and has been applied in real data cases through multiscale nesting (Moeng et al., 2007; Talbot et al., 2012). Previous studies have evaluated the performance of the WRF-LES for various applications (Marjanovic, 2011; Zhu et al., 2010), but the LES

capability has not been used to investigate source-oriented pollutant concentrations. Modifications were made to the SOWC model to allow the nesting of the LES within multiscale parent domains using PBL parameterization schemes.

The 250 m spatial resolution employed in the current study does not resolve street canyon and building effects, as these are subgrid scale features. Explicit representations of flow and pollutant transport in street canyons typically require meter or sub-meter spatial scales (Cui et al., 2004; Liu et al., 2004). The WRF urban surface physics scheme accounts for the effects of buildings and urban land uses. The simulations in this study employed the Urban Canopy Model option, which accounts for urban geometry in surface energy budget and wind shear calculations.

#### 2.1.2. Adaptive time step

The 250 m grid scales used in the present study require very small time intervals to maintain numerical stability in the WRF advection scheme. These small time steps greatly increase simulation time, making it difficult to run continuous simulations over long time periods. WRF has the capability to employ an adaptive time step method based on the Courant–Friedrichs–Levy (CFL) stability criterion applied to both *u*- and *v*-wind speed fields (NCAR, 2010). This option was enabled in the current study, but additional input parameters were created to better control the adaptive mechanism. The original scheme can modify time steps to reach history output times, but an option was added to also modify time steps to reach data input times. This approach was required to maintain consistency between the simulation time steps and the predefined intervals for various meteorological and emissions inputs.

# 2.1.3. Bilinear interpolation scheme

A new interpolation scheme for nesting was introduced to solve numerical issues associated with sharp spatial gradients in sourceoriented pollutant fields. The standard WRF nesting function (bdy\_interp) uses the semi-Lagrangian interpolator (SINT) (Michalakes and Schaffer, 2004). This interpolation scheme is implemented as a collection of monotone interpolation routines



Fig. 2. Modeling domains used in SOWC model simulation over Oakland community. Horizontal resolution is 12 km (D01), 4 km (D02), 1 km (D03), and 250 m (D04). Population density in domains 3 and 4 corresponds to 2010 census.



Fig. 3. Factor profiles and CPF plots from source-apportionment analysis of BAAQMD West Oakland monitoring site data. From top to bottom: Factor 1 (secondary NH<sub>4</sub>NO<sub>3</sub>), Factor 2 (on-road traffic), Factor 3 (crustal/road dust), Factor 4 (sea spray), Factor 5 (ship fuel combustion).

(Chen, 2012). These routines apply a class of monotone advection algorithms to the interpolation problem, resulting in an advanced approach that can help maintain and preserve the shapes of interpolated fields (Grell et al., 1995). This method is derived in detail by Smolarkiewicz and Grell (1992).

The SINT approach is useful and, in some cases, necessary for many of the interpolated variables in the WRF model, but numerical issues arise when it is applied to the source-oriented pollutant variables with sharp spatial gradients in the SOWC model. The twomoment aspect of the SOWC model tracks number and mass throughout the simulation and uses these values to calculate particle radius at various points in the simulations. This requires particle number and mass to remain in agreement so that the model correctly calculates particle radius values. SINT fails to preserve identical spatial patterns for particle number and mass when sharp spatial gradients exist in these fields. Specifically, the nesting interpolation routines may produce a particle number concentration of zero and a non-zero species mass concentration in the same cell. This combination is physically impossible and leads to a calculated particle radius that is infinitely large.

A simplified bilinear scheme was implemented for nesting of the source-oriented pollutant variables to remedy this issue. This scheme uses a more straightforward and computationally inexpensive bilinear interpolation method (Press et al., 1989) that

	Table 2						
	Crustal	Enrichment	Factor	values	for	Factor	3
(	(road/c	rustal dust).					

Element	EF <sub>Crust</sub>
Fe	3.62
Pb	0.79
Mn	4.81
K	3.22
Na	57.59
S	1131.49
V	1.79



Fig. 4. Time trace of SOWC non-HR and HR model predictions against measurements and PMF results at the Port of Oakland sampling site. From top to bottom: total EC, on-road diesel traffic, and shipping contributions.

maintains consistency between particle number and mass in fields with sharp spatial gradients. The bilinear interpolation scheme remains positive definite so long as no negative values exist in the parent grid. Details of this approach are provided in the Supplemental information.

# 2.2. Model configuration and implementation

Model calculations were performed for the month of March 2010 over an area encompassing the Oakland community. The domain configuration uses two-way nesting and gradual down-scaling to increase spatial resolution from 12 km in Domain 1 (D01) to 250 m in Domain 4 (D04). As WRF does not currently

have a vertical refinement option for nested domains, vertical resolution remained the same in Domains 1 through 4. Vertical resolution at the surface was approximately 50 m, resulting in a D04 aspect ratio (horizontal grid size to vertical grid size) consistent with previous LES studies (Lundquist et al., 2010; Mirocha et al., 2010). The pressure-based vertical coordinate can evolve over time which makes it difficult to maintain a constant aspect ratio. LES performance has been shown to be much more sensitive to horizontal resolution than to vertical resolution (Talbot et al., 2012). The domain specifications and relevant model configurations are shown in Table 1 and Fig. 2. Meteorological inputs were prepared using the WRF preprocessing system (WPS) V3.1.1 with NARR data.



Fig. 5. Time trace of SOWC non-HR and HR model predictions against measurements and PMF results at the West Oakland Community sampling site. From top to bottom: total EC, on-road diesel traffic, and shipping contributions.

Two separate simulation cases were configured: (1) HR case – a full 4 domain simulation, with D01–D03 using the PBL parameterization scheme and D04 performing explicit LES calculations with no PBL scheme, and (2) non-HR case – a 3 domain simulation with D01–D03 using the PBL parameterization scheme. The HR calculations use the full 3-D diffusion option and the 3-D deformation option based on a Smagorinsky approach for K calculations (NCAR, 2010). The YSU PBL scheme is used for D01–D03. Four dimensional data assimilation (FDDA) was applied in D01 and D02.

# 2.3. Model emissions

The Source-Oriented WRF/Chem model and emissions preprocessor separate air pollutant emissions into different source type categories, which are tracked separately throughout the simulation. The current study tracks four airborne particle source types: (1) on-road diesel vehicles, (2) ships, (3) trains and rail yard activities, and (4) all other sources.

Emission inputs for the on-road diesel vehicle source type were created using two different sets of raw emissions data. Emissions for D01 and D02 were created using the 4 km resolution emissions data provided by the California Air Resources Board (CARB) as described by Ying et al. (2008). For D03 and D04, higher resolution on-road diesel vehicle emissions were developed using a fuel-based approach with data from Caltrans census truck counts, BAAQMD diurnal factors, a BAAQMD survey of port traffic, and updated emissions for vehicles in the San Francisco Bay Area (Dallmann et al., 2012, 2011; Lau et al., 2009).

The emissions for the ship, train, and other source categories were created from the 4 km resolution emissions data provided by CARB with modifications for domains D03 and D04. Shipping emissions were modified to be treated as point source emissions with stack height, diameter, temperature, and exhaust velocity based on previously reported studies (CARB, 2000; Mason et al., 2008). Train emissions were downscaled to the 1 km and 250 m resolution using the location of rail lines as the spatial surrogate.

Emissions from off-road diesel construction and industrial equipment included in the "other" source type were adjusted based on local fuel-based analyses by the BAAQMD (Tanrikulu et al., 2011a) and the revised PM and NO<sub>x</sub> estimates for these sources presented by Millstein and Harley (2009). The CARB emissions for these "other" source categories were multiplied by scaling factors to reflect these revised estimates of PM. The PM scaling factors selected were 0.30 for off-road industrial sources and 0.05 for off-road diesel construction and mining sources. This latter scaling factor is lower than the nominal value suggested by Millstein and Harley but still within the estimated uncertainty bounds of the emissions bias.

#### 2.4. Positive Matrix Factorization analysis of measurements

Source apportionment analysis was performed on speciated PM measurements from the BAAQMD West Oakland monitoring site using EPA Positive Matrix Factorization (PMF) version 3.0. The details of the sampling site and monitoring network are provided by Malone et al. (2012). The data were analyzed for the period from 2/12/2009 to 12/28/2010, and the results were used to evaluate model performance for source apportionment calculations. An overview of the software and algorithm have been provided in EPA's user guide for EPA PMF 3.0 (Norris et al., 2008), and the details of the Positive Matrix Factorization method have been described at length elsewhere (Paatero, 1997; Paatero and Tapper, 1994). Model configuration and analysis details are provided in the Supplemental information.

The optimal PMF solution yielded five factors, which are illustrated in Fig. 3 along with their conditional probability function (CPF) (Kim et al., 2003) showing dominant wind direction. Crustal Enrichment Factors (cEFs) were also calculated to help differentiate natural versus anthropogenic sources on PMF factor profiles and will be discussed below.

Factor 1 contains a majority of the  $NO_3^-$  and  $NH_4^+$  in the PM samples and is generically called secondary ammonium nitrate

(NH<sub>4</sub>NO<sub>3</sub>). CPF results show that the factor is associated with winds from the north and northeast inland directions, which originate from the rural North Bay and the Central Valley. These regions are home to considerable agricultural activity and emissions that likely act as the ammonia source for the formation of ammonium nitrate in the Bay Area (Tanrikulu et al., 2009b).

Factor 2 accounts for a majority of the EC. OC. Fe. and Cu in the PM samples. These species are indicative of on-road traffic. High EC and OC are consistent with on-road fuel combustion (Watson et al., 2001), and Fe and Cu are commonly used as tracers for brake wear (Lough et al., 2004). Factor 2 makes minor contributions to total S, which is expected because of the low sulfur content of on-road fuels. CPF results do not reveal a dominant wind direction. This is consistent with on-road traffic, as Oakland is surrounded by major freeways. Similarities between on-road diesel and train emission profiles complicate the identification of Factor 2 as a unique source type. Significant Fe, Cu, and EC concentrations are also consistent with train and railroad emissions (Friend et al., 2011; Kim et al., 2004) and train emissions are difficult to separate from on-road diesel emissions in PMF analyses (Kim and Hopke, 2005; Lee et al., 2006). Factor 2 may contain some railroad contributions that cannot be resolved using PMF in the current study.

Factor 3 contained significant Si and Mn contributions, as well as a moderate Fe signal, suggesting crustal material or windblown dust. CPF results indicate that the dominant source of this material is northwest of the monitoring site, which is consistent with windblown dust originating from open rail yards in this direction. Fe and Mn are major components of railroad-related PM (Bukowiecki et al., 2007). The calculated cEF values for Factor 3 are reported in Table 2. Fe, Pb, Mn, K, and V had low cEFs in Factor 3, indicating a strong natural contribution. Large cEF values for Na and S are likely a result of background contributions from sea salt deposited onto the ground in coastal regions. The S/Na ratio for Factor 3 is 5.54, which is similar to the S/Na ratio of 2.94 associated with Factor 4 (fresh sea spray). Mn/Fe ratios have been used to investigate railroad-related mass contributions in PM samples (Bukowiecki et al., 2007). The Mn/Fe ratio of 0.025 for Factor 3 is more consistent with crustal dust (0.019) than railroad-related emissions (0.009), suggesting a windblown dust source (Chillrud et al., 2003; Finlayson-Pitts and Pitts, 2000).

Factor 4 contains significant amounts of Na, Cl, Mg, and Br with a CPF pointing to the San Francisco Bay, leading to the identification of Factor 4 as fresh sea spray.



Fig. 6. Model predicted and PMF resolved EC contributions at the West Oakland community monitoring site over simulation period (March 2010). Note that no PMF result is available for the "train" source. PMF signal for "other" includes secondary ammonium nitrate, road dust, and sea spray.



**Fig. 7.** Period-averaged EC concentrations from on-road diesel (A–C), shipping (D–F), and trains (G–I) in non-HR and HR cases. From left to right: non-HR 1 km results (A, D, G), HR 1 km results (B, E, H), and HR 250 m results (C, F, I). HR domain results are presented within D03 parent domain results for comparison with non-HR results over the same geographical extent. Scales are in  $\mu$ g m<sup>-3</sup>.

Factor 5 accounts for the majority of V and a large fraction of S and  $SO_4^{2-}$  in the samples with a CPF pointing to the Port of Oakland and San Francisco Bay, strongly suggesting that Factor 5 is associated with shipping emissions. V has traditionally been used a tracer for heavy fuel oil, which is commonly used by ships. The BAAQMD implemented a program to use cleaner ship fuels within 24 nautical miles of shore starting in 2009. Concentrations of S,  $SO_4^{2-}$ , and V all decreased in the Bay Area in response to this change (Tao et al., 2013), but the current results indicate that even cleaner fuels act as the dominant source of V in airborne PM in Oakland.

The factors identified at the West Oakland community monitoring site in the current study are generally consistent with the factors determined at the Port of Oakland by Kuwayama et al. (2012). Both analyses found that on-road traffic, ships, windblown dust, and sea spray are prevalent sources in the Oakland area. Neither study identifies trains or rail yard activities as significant, distinguishable contributors, possibly because the factor profile is confounded with the signal for on-road vehicles.

# 3. Results and discussion

HR and non-HR results were evaluated by comparing predicted EC source contributions with source apportionment results, examining predicted source contributions over the region, and calculating population-weighted concentration values. The USEPA's "Report to Congress on Black Carbon" (2012) provides an overview of studies exploring short-term exposure to EC and associated health effects. These studies examine different averaging periods of exposure, varying from minutes to days, and generally document

Table 3 Highest predicted period average and maximum hourly EC concentrations ( $\mu$ g m<sup>-3</sup>) over Oakland for non-HR and HR cases.

		Non-HR	HR	
			1 km resolution	250 m resolution
Average EC	On-road diesel	0.41	0.41	0.53
	Shipping	0.09	0.12	0.14
	Trains	0.22	0.25	0.34
Maximum EC	On-road diesel	3.74	6.69	9.94
	Shipping	0.62	0.76	1.07
	Trains	1.84	2.30	3.35

consistent associations between short-term exposure to EC and cardiovascular effects.

Where applicable, the HR case results are analyzed at both the native 250 m resolution and at the parent domain resolution of 1 km. The 1 km grid cell values are automatically calculated from the average of the 250 m cells that occupy the same space as the 1 km cell as part of the two-way nesting feature of the WRF model. The 1 km resolution results can be used to compare the HR and the non-HR cases at the same spatial resolution, eliminating the effect of dilution.

# 3.1. EC source contributions at sampling sites

The predicted surface level 24-h average EC concentrations were compared to the total measured EC at the West Oakland and Port of Oakland sampling sites (Figs. 4 and 5). Predicted EC contributions from individual source types and comparable PMF results are also shown. For the HR case, results at 250 m and 1 km resolution are presented. The non-HR results are presented at the native 1 km resolution. Train contributions are omitted in this analysis because PMF failed to resolve this source at either site.

At the Port of Oakland site, PM<sub>2.5</sub> EC concentrations predicted by the SOWC-HR model are consistently lower than measured concentrations by an average of 59% in the non-HR case and 45% in the HR case. As expected, much of this under prediction in total EC can be attributed to the under prediction of EC contributions from the on-road diesel source. The Port of Oakland sampling site was located within a few meters of a surface road heavily traveled by diesel trucks, making it useful for characterizing emissions from those trucks but not ideal for comparison to models that instantaneously dilute the truck emissions in a 250 m grid cell. The comparison between SOWC-HR and PMF calculations for shipping contributions to EC concentrations at the Port of Oakland are appropriate because the monitoring location is located more than 250 m away from the emissions source. SOWC-HR and PMF estimates of shipping EC contributions are closer than traffic contribution estimates, although PMF signals are still under predicted by 36% in the non-HR case and 31% in the HR case.

Both HR and non-HR model predictions are generally in better agreement with the PMF results at the West Oakland community site. The model performs well in predicting the total EC and PMF signals, although total EC and shipping contributions show slight over prediction. Because the measurements at this site are less impacted by nearby localized emissions, more in-depth analysis of model performance is appropriate. Model predictions and site measurements of average total EC and source contributions over the simulation period at this site are shown in Fig. 6. On-road diesel is under predicted in all cases by  $0.04-0.06 \ \mu g \ m^{-3}$  (16–23%, respectively). Shipping PMF contributions are over predicted by the model, but contributions are below  $0.05 \ \mu g \ m^{-3}$ . Model predictions show that the train source contributes more to EC than ships, with an average contribution of  $0.1 \ \mu g \ m^{-3}$ . In all cases, the over

prediction of total EC can be predominantly attributed to an over prediction of almost 0.2  $\mu g~m^{-3}$  in the "other" source category contribution.

It is difficult to judge if the HR model predicts EC concentrations more accurately than the non-HR model at either the Port of Oakland or the West Oakland community measurement sites, as the two models are in strong agreement at these locations. As seen in Fig. 6, the HR and non-HR predictions (1 km resolution) at West



**Fig. 8.** Difference in average EC concentrations between non-HR (1 km) and HR (1 km feedback) for period from 3/11/10 to 3/18/10. Top to bottom: (A) on-road diesel, (B) ships, (C) trains. Scales are in  $\mu$ g m<sup>-3</sup>.

Oakland differ by less than 9% for total EC and source contributions from on-road diesel, trains, and other sources. Shipping contributions differ by 21% in these cases, but the absolute difference is only 0.009  $\mu$ g m<sup>-3</sup>, making quantitative comparisons to ambient measurements difficult. The non-HR and HR cases diverge on select dates, but neither model can be consistently determined to be more accurate at the measurement sites, especially given the uncertainties associated with the measurements and PMF analysis.

#### 3.2. Regional EC source contributions over Oakland community

The EC concentrations over D03 and D04 were analyzed to observe the impact of the model spatial resolution across the entire region of interest. This analysis focuses on an 8-day period from 3/ 11/2010 to 3/18/2010, during which elevated EC concentrations are

observed at the Port of Oakland and West Oakland sites. For each source, spatial plots of the 8-day average EC concentration and the maximum hourly EC concentration were constructed. Non-HR results are presented at 1 km resolution. HR results are presented at the native 250 m and at 1 km resolution to examine any bias or dilution effects that may be introduced by the different grid cell size.

#### 3.2.1. Average 8-day EC concentrations

Fig. 7 compares spatial fields of 8-day averaged  $PM_{2.5}$  EC concentrations for the non-HR case at 1 km resolution and the HR case at 1 km and 250 m resolution. The HR case resolves higher EC concentrations around each source. The highest predicted EC concentrations over Oakland are summarized in Table 3. Both simulations predict that on-road diesel sources make the largest



**Fig. 9.** Maximum hourly EC concentrations from on-road diesel (A–C), shipping (D–F), and trains (G–I) in non-HR and HR cases. From left to right: non-HR 1 km results (A, D, G), HR 1 km results (B, E, H), and HR 250 m results (C, F, I). HR domain results are presented within D03 parent domain results for comparison with non-HR results over the same geographical extent. Scales are in  $\mu$ g m<sup>-3</sup>.



**Fig. 10.** Difference in maximum hourly EC concentrations between non-HR (1 km) and HR (1 km feedback) for period from 3/11/10 to 3/18/10. Top to bottom: (A) on-road diesel, (B) ships, (C) trains. Scales are in  $\mu g m^{-3}$ .

contribution to 8-day average EC concentrations, but the HR simulation predicts average contributions up to 0.53  $\mu$ g m<sup>-3</sup> while the non-HR simulation predicts average contributions up to only 0.41  $\mu$ g m<sup>-3</sup>.

Fig. 8 shows the difference in 8-day averaged EC concentrations between the non-HR and HR cases at 1 km resolution. These results demonstrate that the HR predictions produced at 250 m resolution shown in Fig. 7 do not exactly match the non-HR predictions produced at 1 km resolution, even when the HR results are averaged back to the coarser 1 km resolution. The explicit large eddy calculations used in the HR case predict different concentration fields than the boundary layer parameterizations used in the non-HR case. The numerical diffusion introduced by these parameterizations in the non-HR model at coarser grid resolution produces secondary effects in vertical mixing and particle deposition that fundamentally change the predicted concentration fields. The HR and non-HR predictions mainly diverge near sources where spatial gradients are sharpest.

#### 3.2.2. Maximum hourly EC concentrations

Fig. 9 shows the spatial distribution of maximum hourly average PM<sub>2.5</sub> EC concentrations predicted by the non-HR simulation at 1 km resolution and the HR simulation at 1 km and 250 m resolution. Once again, higher maximum hourly EC concentrations are predicted over the Oakland community in the HR simulations for all sources (see Table 3 for a summary). The largest difference is observed for the on-road diesel source, which increases by nearly a factor of 2, from 3.75  $\mu$ g m<sup>-3</sup> in the non-HR case at 1 km resolution to 6.69  $\mu$ g m<sup>-3</sup> in the HR case at 1 km resolution. The 250 m HR model predicts a maximum hourly concentration up to 9.94  $\mu$ g m<sup>-3</sup>.

Fig. 10 shows the difference in maximum hourly EC concentrations between the non-HR and HR simulations at 1 km resolution. The largest differences in these values occur over the Oakland community for the on-road diesel source, but ship and train sources show divergence over much of the simulation domain.

# 3.3. Population-weighted results

A quantitative summary of the differences between HR and non-HR predictions over the community of Oakland was created by calculating population-weighted values from the 8-day average and hourly maximum EC concentrations. Tract level 2007 census data were aggregated to the 1 km and 250 m resolution simulation domains for use in the population weighting calculations within the Oakland city boundaries (see Fig. 2 inset). The calculations were performed for the period from 3/11/2010 to 3/18/2010.

The results of the population-weighted analysis shown in Table 4 are consistent with the results displayed in the EC spatial plots (Figs. 7-10). The increase in population-weighted 8-day average EC source contributions ranged from 1% to 17% when the

#### Table 4

Population-weighted values for 8-day average and maximum hourly average PM<sub>2.5</sub> EC concentrations by source for non-HR and HR cases.

		Population-weighted EC concentration ( $\mu g m^{-3}$ )				
		Non-HR (1 km resolution)		HR		
			1 km resolution	% Difference from non-HR	250 m resolution	% Difference from non-HR
8-day average EC	On-road diesel	0.152	0.155	2%	0.153	1%
	Shipping	0.025	0.029	16%	0.028	13%
	Trains	0.089	0.104	17%	0.103	16%
Hourly maximum EC	On-road diesel	1.187	1.466	23%	1.566	32%
	Shipping	0.242	0.264	9%	0.275	14%
	Trains	0.681	0.795	17%	0.829	22%

nested HR was used. Population-weighted maximum hourly EC contributions also increased by 9%–32% when HR was used.

The use of HR within a regional air pollution model allowed for clearer identification of locations of maximum concentration and showed increased estimates of population-weighted exposures to different sources of PM<sub>2.5</sub> EC, but it did not change the relative importance of major sources under the conditions studied. On-road diesel traffic makes the largest contribution to EC levels in Oakland, followed by the train and ship sources. This result is consistent with the receptor-based PMF analysis carried out at the West Oakland monitoring site (this study) and the Port of Oakland site (Kuwayama et al., 2012). A health risk assessment of diesel PM in the West Oakland community also found on-road trucks to be the largest contributor to the West Oakland community potential cancer risk from diesel PM (Di, 2008).

### 4. Conclusions

The Source-Oriented WRF/Chem (SOWC) model was adapted to utilize high spatial resolution (HR). Large Eddy Simulation (LES) was used to increase spatial resolution from 1 km to 250 m so that exposure to complex mixtures of air pollution can be carried out at the neighborhood scale. The model was applied to the community of Oakland as a case study where a population with high spatial density exists in close proximity to industrial sources in a region with complex terrain. The SOWC-HR model performed well at the West Oakland community site when comparing predicted PM<sub>2.5</sub> EC concentrations to total measured EC and when comparing predicted source contributions to PMF results for traffic sources, and ship sources. The total EC concentration and traffic source contribution at the Port of Oakland were consistently under predicted by the model due to the proximity of the measurement location to a busy road, but the predicted shipping contributions at this site matched well with source apportionment results. The higher resolution nested simulation did not significantly change predicted concentrations everywhere in the study domain. Predictions of EC concentrations at the measurement locations were similar with or without the HR approach, but HR simulations did resolve locations with extremely high EC concentrations that were not identified in the non-HR simulations with lower spatial resolution. Populationweighted concentrations increased in all cases where HR predictions with 250 m resolution were used in comparison to non-HR predictions generated at 1 km resolution. These concentration differences were not just a result of the higher spatial resolution (as shown by HR results averaged back to the coarser 1 km resolution), but rather they are also due to the explicit large eddy calculations that can be performed at this scale.

The relative importance of source contributions to EC concentrations predicted with the SOWC-HR model in the current study are consistent with the findings from previous Bay Area modeling studies, with on-road diesel traffic being the dominant contributor (Deng and Stauffer, 2011; Tanrikulu et al., 2009a,b, 2011b). The identification of focused locations with extremely high concentrations can help identify populations with higher exposure who may suffer disproportionate health effects. Further analysis should be performed to determine the associated change in public health impacts and risks, and more spatial analysis of the results may be done to investigate if these different predictions have implications for policy or mitigation strategies.

# Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.atmosenv.2013.09.055.

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