Sustainable Freight Infrastructure to Meet Climate and Air Quality Goals

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16. Abstract

This report examines the potential for freight modal shift from truck-to-rail in the upper Midwestern U.S. to improve air quality and reduce CO_2 emissions. Two scenarios were generated, one focusing on intra-regional freight movements within the Midwest and the second on through-freight movements into, out of, and through the region. Freight truck and rail emissions inventories were generated corresponding to each scenario and input to a regional air quality model (CMAQ). Results showed the intra-regional scenario had little impact on Midwest air quality, however the through-freight scenario greatly reduced concentrations of NO_2 and EC near roadways (up to 27% for NO_2 and up to 16% for EC), with corresponding increases near railways. The through-freight scenario also reduced CO_2 emissions 31% compared to baseline trucking. Reductions in $PM_{2.5}$ and O_3 were modest, up to 3%. We conclude that while truck-to-rail modal shift does improve regional air quality, the motivation for advocating rail over truck lies principally in reduced human exposure to near-roadway pollution, as well as reduction of carbon emissions.

17. Key Words Freight, air quality, emissions, modal shift, environment, sustainability, infrastructure, diesel pollution, truck, rail, greenhouse gases, carbon dioxide	18. Distribution Statement **No restrictions. This report is available through the Transportation Research Information Services of the National Transportation Library.**		
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Executive Summary

The majority of freight in the U.S. is transported by heavy duty diesel vehicles (HDDVs), trucks that are a major source of smog-producing nitrogen oxides and fine particulates – pollutants harmful to human health. A projected doubling of domestic freight tonnage by 2050 has caused concern both for transportation planners and air quality managers about how existing infrastructure will handle this growth, and what impact it will have on air quality and public health. Modal shift, or shifting freight away from truck towards more fuel-efficient freight transport options, such as barge and rail, has been proposed as a solution to increasing highway congestion and vehicle emissions.

In this analysis we examined the potential for freight modal shift from truck-to-rail in the upper Midwestern U.S. to improve regional air quality and reduce carbon dioxide (CO_2) emissions. Two scenarios were generated using national freight commodity flow data to both select commodities viable for rail (eg. base metals, motorized vehicles etc.), and transport distances longer than 400 miles, where rail is more economically competitive. One scenario focused on intra-regional (I-R) freight movements within the upper Midwest and the second on through-freight (T-F) movements into, out of, and through the Midwest region. We found 12 million tons of freight could be shifted in the I-R scenario, and 530 million tons in the T-F scenario. Freight truck and rail emissions inventories were generated for each scenario using geographic information system (GIS)-based freight activity datasets and a publicly available emissions model from the U.S. Environmental Protection Agency. Ground-level air quality impacts of each scenario were modeled with meteorology in the Community Multiscale Air Quality Model (CMAQ).

Results showed the Midwest I-R scenario exhibited only a small emissions reduction, and therefore little impact on regional air quality. However the T-F scenario greatly reduced emissions - 26% reduction of nitrogen oxides (NO_x) and 40% reduction of particulate sulfate (SO_4) relative to trucking. Surface concentrations were also significantly reduced, particularly nitrogen dioxide (NO_2) and elemental or black carbon (EC) near roadways in summer (up to 27% for NO_2 and up to 16% for EC), with corresponding increases near railways (23% and 22%, respectively). The T-F scenario also reduced CO_2 emissions 31% compared to baseline trucking. Reductions in regional fine particulate matter ($PM_{2.5}$) and ozone (O_3) were modest, about 3%.

Using more trains and fewer trucks to transport freight improved regional air quality in the Midwest, but not enough to affect designation of counties out of attainment with National Ambient Air Quality standards. The motivation for advocating more freight rail over truck lies principally in reducing human pollutant exposure near roadways, and decreasing CO_2 emissions.

1. Introduction

1.1 Freight Transport and Air Quality

Trucks, trains, ships and planes transporting freight are vital components of the U.S. economy, enabling producers to send products all over the world, and consumers to purchase everything from blue jeans to bananas in their local stores. However, the amount of goods transported, and the modes by which they are transported create problems for local and regional air quality. The majority of freight (73% [1]) in the U.S. is transported by freight trucks, which are classified as Heavy Duty Diesel Vehicles (HDDVs), and are a substantial source of smog producing nitrogen oxides (NO_x) and fine particulates ($PM_{2.5}$), pollutants that are harmful to human health [2].

Nitrogen oxides (NO_x), a group of pollutants including nitric oxide (NO) and nitrogen dioxide (NO_2), contribute to three separate health-relevant air pollutants. NO_2 is regulated by the U.S. Environmental Protection Agency (EPA) as a primary pollutant harmful to human health, responsible for airway inflammation and increased asthma symptoms [3]. NO_x is an ingredient in the formation of tropospheric ozone (O_3) [4]. Ozone, commonly known as "smog," is known to aggravate respiratory conditions like asthma, but can also damage crops, trees and vegetation [5]. Ozone is difficult to control because it forms in the atmosphere through the chemical reaction of NO_x and volatile organic compounds (VOCs) in the presence of sunlight. This chemical process also means O_3 pollution is expected to worsen with future climate change, as more warm days enhance O_3 production [6]. NO_x can also react chemically in the atmosphere with ammonia and other compounds to form small particulates that are components of $PM_{2.5}$.

Fine particulates are inhaled deep into the lungs, and have been linked with decreased lung function, aggravating asthma, and premature death in people with heart or lung disease [7,8]. The estimated monetary costs of health impacts in the U.S. due to $PM_{2.5}$ alone - not including missed days of school/work or loss of productivity - is on the order of billions of dollars per year [9].

1.2 Long-term Freight Planning

Targeting diesel vehicle pollutants, the U.S. EPA has mandated use of ultra-low sulfur diesel (ULSD), enabling application of after-treatment technologies to significantly reduce particulate and NO_x emissions from both trucks and trains. The new standards will greatly lower per-vehicle emissions, yet at the same time, increased international import and export activity is projected to double domestic freight tonnage by 2050 [1]. This freight will not only increase the number of trucks on the road, but demand for trucking may encourage continued use of older, dirtier trucks that lack after-treatment technologies – potentially diminishing regulatory impacts. A doubling of domestic freight transport also begs the question as to how our already congested transportation network will handle this growing traffic load.

To ensure a healthy economy, as well as a healthy environment now and in the future, it is necessary to examine current freight mode-share, and how distributing more freight to more fuel efficient - and less polluting modes - might enable freight growth while continuing to reduce pollution from the freight sector.

1.3 Freight Modes and Modal Shifts

As a solution to growing highway congestion and increasing vehicle emissions, several studies have proposed freight modal shifts away from truck toward more fuel-efficient, non-highway modes. To date, however, our study is the first to extend modal shift freight scenario analysis to consider air quality impacts.

In an economic analysis, Gorman [10] examined costs and benefits of modal shifts from truck-to-rail; concluding that 25% of freight could be shifted to rail at a lower cost if the infrastructure existed, resulting in an 80% reduction in social costs measured in pollution, congestion and safety. Targeting roadway congestion, Bryan et al. [11] found freight modal shift from truck to rail could significantly reduce congestion and advocated that if public investment in private infrastructure produced a public benefit, such an investment should be made. In considering a single interstate in California, Lee et al. [12] developed scenarios to replace 25% to 100% of freight truck volume with rail, and found 13% to 57% reductions in NO_x emissions, and 15% to 56% reductions in particulate matter (PM_{10}) emissions. Also in California, You et al. [13] investigated replacing truck drayage movements with rail at the ports of Long Beach and Los Angeles, concluding 22% to 28% reductions in emissions of NO_x and 8% to 22% reductions in emissions of $PM_{2.5}$ could be achieved. Finally, comparing fuel efficiency among freight modes in a report for the Federal Railroad Administration, ICF International [14] analyzed truck and rail movements on competitive corridors in the U.S., determining that rail was more fuel efficient on all 23 corridors, with additional potential for greatly reduced mobile emissions through future electrification of rail.

While all of these studies conclude mode shifts in freight transport will reduce emissions, and suggest subsequent improved air quality, none of them include an air quality modeling assessment of their transportation scenarios. Air quality models are based on the same models used to forecast weather and hurricanes, and are complex, mathematical tools capable of simulating the physical and chemical processes that dictate how emitted pollutants disperse and chemically react in the atmosphere. The use of models is important in evaluating policies aimed at improving air quality because many health-relevant pollutants, like O_3, are not emitted directly, but formed through chemical processes in the atmosphere.

The Midwest is the nation’s crossroads for freight transport, and an ideal location to investigate regional air quality impacts of a freight modal shift policy. Due to the lack of public data on in-land waterway freight transport at the level of detail necessary for air quality analysis, we focus solely on mode shifting from truck to rail. This study examines two scenarios for modal shift; the first looks at truck-to-rail shift of rail-competitive commodities on corridors originating and terminating within the Midwest, while the second scenario builds on the first, incorporating rail-competitive commodities moving *through* the Midwest as well.

2. Developing Modal Shift Scenarios

Two scenarios for truck-to-rail modal shift were explored in this analysis. The first, more conservative scenario - designated the Midwest intra-regional (I-R) scenario - considers freight on rail-competitive corridors originating and terminating within the Midwest study region defined by the Mid-America Freight Coalition (MAFC) member states (Illinois, Indiana, Iowa, eastern Kansas, Kentucky, Michigan, Minnesota, Missouri, Ohio, and Wisconsin). The second, broader modal shift scenario - designated the Midwest through-freight (T-F) scenario - incorporates the I-R scenario, as well as freight moving through the Midwest.

2.1 Commodities for Modal Shift

Freight commodity origin-destination and tonnage data were obtained from the Freight Analysis Framework (FAF) version 2.2 commodity database for 2002 [15] (the most recent version of the FAF at the commencement of this work). The FAF is a multi-commodity, multi-modal freight database and analysis tool developed by Oak Ridge National Laboratory's Center for Transportation Analysis and the Federal Highway Administration (FHWA). The FAF dataset includes spatial geographic information system-based data on freight flows (roadway-level freight activity, travel speeds, delays etc.), and a database of U.S. freight commodity movements, incorporating origin-destination, tonnage, value, transport mode and commodity information. The FAF commodity database was built from public data sources, including the 2002 Commodity Flow Survey (CFS), and represents the only freely available freight commodity database with accompanying spatial freight activity data necessary for the type of detailed air quality and transportation policy analysis presented here.

Commodities selected for modal shift in this study were limited to goods moving in the Midwest study region and currently transported by either truck or rail, as determined by comparing commodities and modes in the FAF database. This list of commodities was further narrowed by a literature review of commodity mode-choice for truck-rail competitive corridors [14,16-18]. Annual commodity tonnage was converted to truckloads using commodity-specific density values for railcars and trucks from FHWA's *Quick Response Freight Manual II* Table 4.18 [19]. These densities were generated by the Indiana Freight Model, and were selected because: 1.) Indiana is within the study region and therefore a reasonable representation of Midwest freight transport characteristics, 2.) densities were given by Standard Classification of Transported Goods (SCTG) code, matching the FAF commodity data, and 3.) density values were provided for both truck and railcar. It should be noted that most states have a gross vehicle weight limit of 80,000 pounds, and truck densities greater than 22.5 tons (eg. cereal grains and fertilizers) used in this analysis, may be unreasonable, or may represent illegal overweight hauling, permitted overweight hauling, or industries exempt from weight limits (eg. forest products in Wisconsin and farm commodities in Indiana [20,21]).

SCTG	Commodity	Tons/Truckload	Tons/Railcar	I-R (2002 KT)	T-F (2002 KT)
2	Cereal grains	30.1	96.63	13.74	21,590.85
3	Other ag prods.	22.3	86.79	93.48	16,884.11
4	Animal feed	25.3	88.28	182.95	13,466.94
5	Meat/seafood	18.6	74.41	83.52	15,224.45
6	Milled grain prods.	21.4	85.5	501.42	15,014.75
7	Other foodstuffs	21	87.02	1,187.15	54,691.20
8	Alcoholic beverages	21	87.31	150.34	4,061.27
11	Natural sands	25.4	97.97	5.19	5,377.12
12	Gravel	24.1	97.97	146.32	16,346.23
13	Nonmetallic minerals	23.4	100.44	2.64	7,725.81
14	Metallic ores	21.4	95.91	29.72	435.85
15	Coal	22	109.36	134.32	6,445.62
17	Gasoline	28.2	84.04	287	8,615.98
18	Fuel oils	20	88.22	1.39	3,784.34
19	Coal-n.e.c.	23.5	73.66	166.43	11,858.28
20	Basic chemicals	17.5	98.66	273.01	9,988.78
22	Fertilizers	27.4	101.81	474.47	8,114.48
23	Chemical prods.	20.1	93.96	739.8	20,726.39
24	Plastics/rubber	13.3	94.3	638.85	23,896.29
25	Logs	29.2	64.11	3.3	4,515.65
26	Wood prods.	24.2	82.41	108.07	19,840.20
27	Newsprint/paper	23.5	82.75	331.37	16,748.49
28	Paper articles	17.2	7.09	216.49	8,669.26
30	Textiles/leather	13.3	14.17	44.63	5,135.58
31	Nonmetal min. prods.	21.2	98.64	1,115.57	42,923.93
32	Base metals	18.4	91.47	1,662.73	43,129.77
33	Articles-base metal	12.2	79.66	485.81	17,336.97
34	Machinery	13.8	49.77	470.5	19,522.28
35	Electronics	12.7	16.69	205.18	7,579.78
36	Motorized vehicles	13.3	21.73	1,048.76	24,547.60
37	Transport equip.	12.1	41.36	44.22	1,531.98
39	Furniture	10.7	15	107.62	6,308.93
40	Misc. mfg. prods.	14	65.22	231.34	11,771.11
41	Waste/scrap	20	79.86	161.7	12,474.26
43	Mixed freight	14.2	32.45	825.33	19,594.02
			TOTALS	12,174.36	525,878.55

Table 2.1.1 *Modal shift commodities and load factors for Midwest I-R and T-F scenarios. Modal Shift for the I-R scenario removes 2,534 trucks/day off Midwest highways, and adds 876 railcars per day, while the T-F scenario removes 103,450 trucks/day off Midwest highways and adds 34,854 railcars/day (both truck and railcar metrics assume 25% empty movements).*

Final commodities for both mode-shift scenarios are listed with their SCTG code and corresponding truckload and railcar load factors in Table 2.1.1. The most significant commodities (by tonnage) with potential to shift to rail in both scenarios were base metals, other foodstuffs, nonmetal mineral products, and motorized vehicles.

2.2 Midwest Intra-Regional Scenario

Previous studies addressing truck-to-rail mode-shift potential have established that rail freight movements are most cost-competitive with trucking beyond a minimum threshold transport distance. Rail freight has higher fixed costs than trucking, with comparatively low marginal costs, making rail more competitive on longer routes. The literature identifies this minimum competitive transport distance to be between 200 and 500 miles [14,16,18]. For this study, we set 400 miles as the minimum distance to consider modal shift to rail. Within the MAFC states, we identified 28 city pairs (see Table I.i in Appendix I) located more than 400 miles apart, all with access to freight rail service (see Figure 2.2.1).

While the FAF commodity database provides commodity origin-destination (O-D) and tonnage information, and the FAF network shapefile includes roadway activity and transport speeds, no data are given on what routes are used for which commodity O-D pairs. For this study, we chose truck freight routes according to the shortest *travel time* between city pairs. In addition, the cost of freight rail transport can significantly increase with rail carrier interchange. Rail routes corresponding to truck routes were selected first for the least number of carriers necessary for rail transport between city pairs (accounting for co-ownership and track rights), and next for shortest route. We also considered shipper options in choosing rail carriers by investigating the number of carriers serving each O-D city pair. Among the 28 Midwest city pairs, 8 rail routes had only one carrier option, 7 city pairs required carrier interchange (with multiple carrier options), while 13 pairs were served by several carriers and did not require interchange.

For the Midwest I-R scenario, our analysis found that Midwest truck routes longer than 400 miles transported 12,602 KT of freight - 4% of the intra-regional tonnage in the study domain. Of that, 12,174 KT (97%) were commodities eligible for mode shift, which corresponds to 2,534 removed HDDV trucks per day, or 1,337,602 removed HDDV VMT per day. This scenario, while significant for some routes, only amounts to a 1% reduction in total daily Midwest HDDV VMT, because most (80% by tonnage) of the

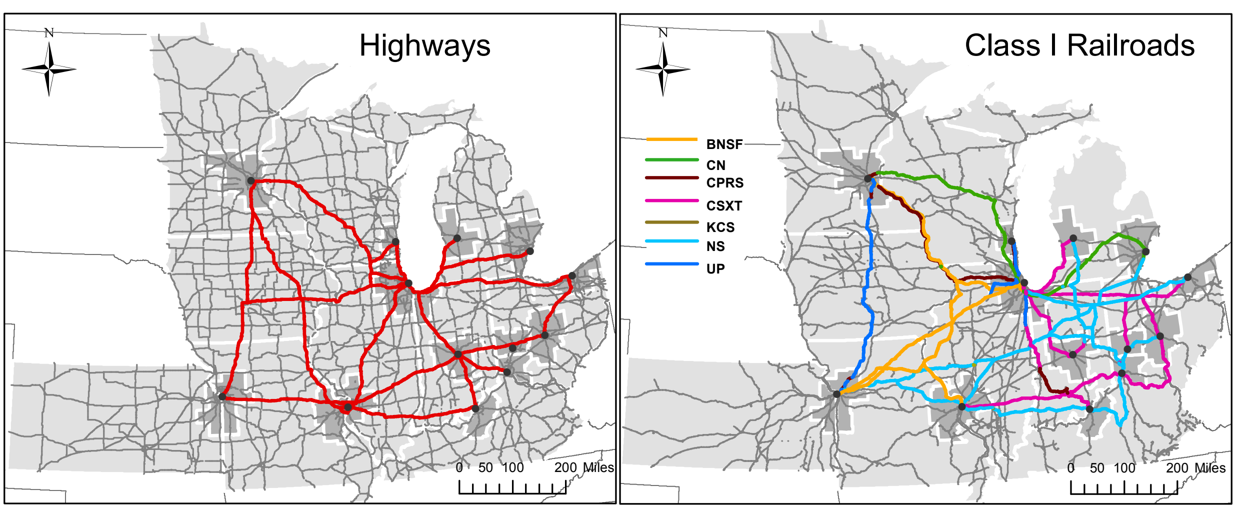

Figure 2.2.1 *Midwest Intra-Regional scenario cities, highway and railway corridors.*

intra-regional freight movements in the domain are also intra-state, and do not meet the 400 mile criteria. Such a scenario translates to adding 876 railcars per day, or 18,182,724 ton-miles to Midwest rail routes per day - a 5% increase in total Midwest rail freight tonnage.

Estimates of removed trucks and added railcars for both modal shift scenarios assume 25% of movements on both modes are empty. For rail, this value was taken from the literature [22] and used only to provide comparison against the number of trucks removed. The 25% empty assumption had no bearing on added rail activity or emissions, as emissions were based entirely on added rail activity in units of ton-miles, not railcars. For truck, the 25% empty value was taken from FAF documentation [23]. In FAF, the freight field containing annual average daily freight truck traffic excluded empty truck miles because they are not relevant for commodity flows. Empty truck miles are, however, relevant for air pollution, so we added them back in. Though percent empty miles vary by commodity and truck-type, the spread across truck types in the FAF analysis was relatively narrow (19% to 29% empty), so we assumed a mean value of 25% for all commodities and trucks.

2.3 Midwest Through-Freight Scenario

The Midwest T-F scenario expands on the I-R scenario by further incorporating freight traveling into-, out of-, passing through the region. Here we also expand slightly our definition of "Midwest" to incorporate the entire Lake Michigan Air Directors Consortium (LADCO) upper Midwest inventory domain, which adds portions of the states bordering the MAFC region (see Figure 3.3.1).

The FAF commodity database designates freight movement origins and destinations in terms of major metropolitan regions, for example, 'WI Milwa' for the Milwaukee-Racine-Waukesha, WI census statistical area, and remainder of state, 'WI rem'. While the I-R scenario focused on freight movements between metropolitan areas, for the T-F scenario, we wanted to include all U.S. freight movements through the Midwest region, including non-specific 'remainder of state' O-Ds. To approximate origins and destinations, and therefore estimate transport distances and routes, we used state centroids. We again set 400 miles as the minimum transport distance for mode shifting to rail, however since that 400 miles could primarily be outside the Midwest region – and thus a mode shift yield little to no local impact - we set mode shift criteria at travelling more than 400 miles in total, with at least 200 miles passing through the Midwest. We also removed any movements overlapping with the I-R scenario, to avoid double counting when incorporating the I-R mode shift scenario.

Total HDDV VMT removed from highways was calculated using FAF commodity tonnages, commodity-specific truck load factors, and estimated transport distances. Because actual freight origin-destinations were unknown, and using state centroids for every movement unrealistic, the removed HDDV VMT was distributed throughout the Midwest highway network, weighted by highway freight truck density. Similarly, ton-mileage added to railways was calculated using the same commodity tonnages and estimated transport distances. Rail ton-mileage was distributed to Midwest Class I freight rail lines, weighted by network freight densities obtained from the National Transportation Atlas Database (NTAD) 2009 rail shapefile.

For the Midwest T-F scenario, our analysis found that 526,789 KT per year could be shifted from truck to rail – 15% of all freight tonnage moving in the Midwest study region. This removes 103,450 trucks per day from Midwest highways, and 52,744,923 HDDV VMT per day. This scenario amounts to a 40% reduction of Midwest HDDV VMT. For freight rail, the T-F scenario adds 34,854 railcars per day, or 745,231,120 ton-miles per day to the Midwest freight rail network, doubling Midwest rail freight tonnage.

2.4 Scenario Assumptions

For both scenarios, we made several logistical assumptions. 1.) We assumed first and last mile transport would be provided by truck regardless of long-haul mode, and therefore did not add drayage activity. 2.) We did not account for emissions from freight rail switching activities. Switching engines can be electric, which would not add to rail emissions (but would slightly increase power plant load), or they can be diesel, which would directly add to rail emissions. Lacking detailed data on railyard activity and equipment, we assumed all switching activity to be electric, but not an appreciable increase to power plant emissions. 3.) For HDDV VMT and railcar estimates, we assumed 25% empty truckloads and carloads, in accordance with the literature [22,23] 4.) We assumed the existence of freight rail infrastructure to handle increased tonnage in both scenarios. The goal of our study is to evaluate the potential benefits of long-term infrastructure investments, so the assumption of sufficient rail infrastructure is part of the study design.

3. Developing Emissions Inventories

To evaluate air quality impacts of truck-to-rail modal shift scenarios in a regional air quality model, we developed heavy-duty diesel truck and Class-I freight rail inventories, using publicly available mobile emissions models, spatial activity data, emissions factors, and diesel speciation tables, described below.

3.1 Truck

Our HDDV truck freight inventory, the Wisconsin Inventory of Freight Emissions (WIFE), was built following the method described in detail by Johnston et al. ([24], in revision for Transportation Research Part D) and summarized here. Heavy-duty diesel vehicle emissions factors for pollutant species in Table 3.1.1 were calculated for 2005 using the U.S. EPA MOBILE6.2 motor vehicle emissions model [25]. Emissions factors in grams

Abbrev.	Pollutant
CO	Carbon Monoxide
CO2	Carbon Dioxide
NOx	Nitrogen Oxides
PMC	Particulate Matter - Coarse
PMFINE	Particulate Matter ($PM_{2.5}$) - Fine
PEC	Particulate Matter ($PM_{2.5}$) - Elemental Carbon
POC	Particulate Matter ($PM_{2.5}$) - Organic Carbon
PSO4	Particulate Matter ($PM_{2.5}$) - Sulfate
NH3	Ammonia
SO2	Sulfur Dioxide
VOC	Volatile Organic Compounds

Table 3.1.1 *HDDV truck pollutants from MOBILE6.2*

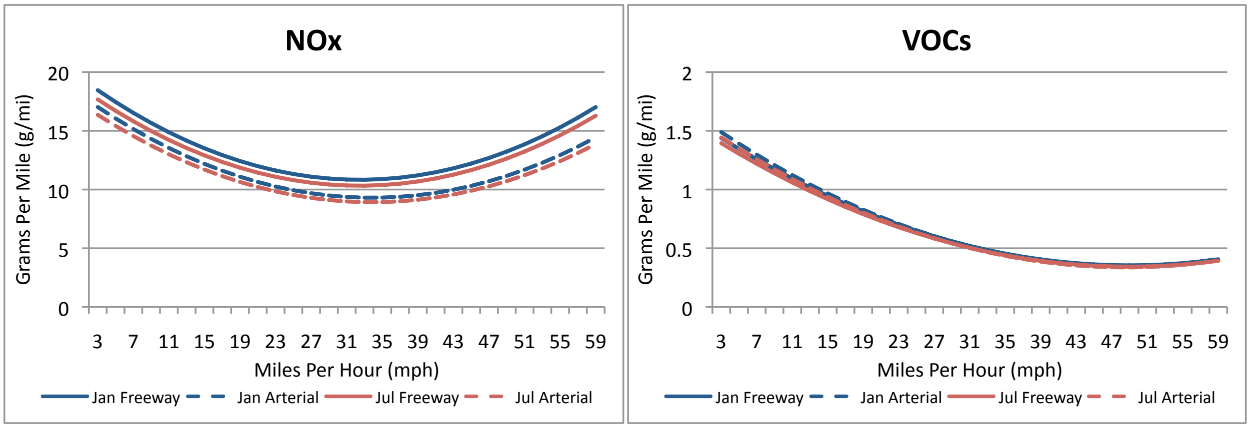

Figure 3.1.1 *HDDV emissions factor speed-curves for (a) NO_x and (b) VOCs.*

pollutant per VMT were generated at 2 mph intervals from 3 to 59 mph to create emissions factor speed-curves for January and July (see Figure 3.1.1). Emissions factor speed-functions were applied to roadway-level freight activity (in VMT) and speed data, in the FAF [15] highway network shapefile. Using GIS software, the link-level freight emissions inventory was assigned to grid-cells corresponding with the 12 km x 12 km LADCO Midwest emissions grid, and summed over grid-cells to convert roadway-level emissions to gridded emissions.

3.2 Rail

Rail emissions developed for the modal shift scenarios were based on rail activity using grams pollutant per revenue ton-mile, and applied to a Class-I rail network shapefile built from the NTAD rail shapefile. Emissions factors for Class-I rail for 2005 were obtained from LADCO [26], the U.S. EPA [27] and the U.S. Energy Information Administration (EIA) [28]. Emissions factors given in grams per gallon of diesel fuel were converted to grams per revenue ton-mile using the Association of American Railroads (AAR) average 2005 Class-I fuel efficiency of 414 revenue ton-miles per gallon of diesel fuel [29] (see Table 3.2.1). Our rail inventory includes only rail emissions added as a result of the modal shifts. Baseline rail emissions were provided by LADCO, as part of their 2005 Midwest emissions inventory. Using the same GIS method as the truck inventory, link-level rail emissions were gridded to 12 km x 12 km.

Pollutant	g/ton-mile	Source
CO	0.06	LADCO
NO_X	0.44	LADCO
PMC	0.00	LADCO & EPA
$PM_{2.5}$	0.02	LADCO & EPA
SO_2	0.04	LADCO
NH_3	0.00	LADCO
VOC	0.02	LADCO & EPA
CO_2	24.51	EIA

Table 3.2.1 *Class-I Rail Emissions Factors Per Revenue Ton-Mile*

Though MOBILE6.2 truck emissions factors differ by season, no such seasonality for rail emissions was found in the literature, nor did we find any documentation for emissions factor speed-dependence. In fact, detailed emissions, and in particular, activity data are very difficult to obtain for rail. Unlike freight trucking, which operates on public infrastructure such that freight truck movements on any given highway segment are reasonably anonymous regarding carriers, freight rail operates on infrastructure privately owned by individual rail companies such that rail activity on any given railway segment directly reveals the carrier and how much business they are doing on that route. The result is a lack of publicly available, detailed rail activity data, in order to prevent rail carrier competitors from having open access to one another's commercial activities.

The lack of detailed emissions information can partly be explained by rail's relatively small freight mode share (18% [1]) compared to trucking over the least few decades, resulting in more emphasis being placed on truck emissions data than rail. There is also greater expense and difficulty in researching locomotive emissions factors under various operating conditions (eg. number of engines in the train, number of cars in the train, density of freight in the cars, summer, winter, high speed, low speed, uphill, downhill etc.), compared to trucks, where emissions data are often gathered in controlled laboratory settings, and empty load, maximum load, average load and seasonal impacts on operating conditions can be more easily tested.

3.3 Modal Shift Emissions Change

The net emissions change – removed truck emissions plus added rail emissions – from each scenario, for representative summer (July) and winter (January) months are shown in Table 3.3.1. Percent emission changes are relative to baseline (B-L) trucking emissions. While changes for the I-R scenario are small, <1% reductions, changes for the T-F scenario are much more significant, ranging from 3% for elemental carbon, to 40% for particulate sulfate. In addition to the air pollutant reductions, emissions of carbon dioxide (CO_2), the greenhouse gas most responsible for global climate change, are reduced 31% in the T-F scenario.

In both scenarios, sulfur dioxide (SO_2) emissions increase. This is due to the difference in diesel fuels used by trucking and railroad industries. In 2005, fuel standards for highway diesel contained 500 ppm sulfur [30], while railroad diesel contained 2600 ppm [26], causing more freight rail use to yield increased SO_2 emissions. Since 2005, new EPA regulations have targeted reduction of sulfur in diesel fuel; the 2007 Heavy Duty Highway Diesel Rule, and the 2008 Clean Air Nonroad Diesel Rule step down both highway and rail diesel sulfur levels to 15 ppm by 2015.

Figures 3.3.1a-d show the spatial pattern of net emissions changes for July primary NO_2 and fine $PM_{2.5}$ (note: $PM_{2.5}$ = PEC + PMFINE + POC + PSO_4), for each modal shift scenario. Emissions reductions occur on highways (blue), while emissions increases occur on railways (yellow-red). In the I-R scenario, primary NO_2 emissions are reduced as much as 17 kg per day per 12 km x 12 km grid on highways, and increase as much as 7 kg per day per 12 km x 12 km grid on railways, while primary $PM_{2.5}$ emissions decrease as much as 3 kg per day on highways, and increase as much as 2 kg per day on railways. In the T-F scenario, primary NO_2 emissions are reduced as much as 160 kg per day, and increase as much as 62 kg per day, while primary $PM_{2.5}$ emissions decrease as much as 31 kg per day on highways, and increase as much as 21 kg per day on railways.

Pollutant		July					January				
		B-L	I-R		T-F		B-L	I-R		T-F	
	Abbrev.	Tons/day	ΔTons /day	%	ΔTons /day	%	Tons/day	ΔTons /day	%	ΔTons /day	%
Carbon Monoxide	CO	540.46	-4.62	-0.86	-168.09	-31.1	547.14	-4.71	-0.86	-168.02	-30.71
Carbon Dioxide	CO_2	202,992.73	-1,610.75	-0.79	-62,752.75	-30.91	202,992.73	-1,610.75	-0.79	-62,752.70	-30.91
Ammonia	NH_3	3.84	-0.03	-0.89	-1.34	-34.85	3.84	-0.03	-0.89	-1.34	-34.85
Nitrogen Oxides	NO_X	2,441.03	-17.01	-0.7	-631.81	-25.88	2,178.89	-14.25	-0.65	-305	-14
Particulate Elemental Carbon	PEC	25.49	-0.03	-0.12	-0.86	-3.39	26.41	-0.04	-0.15	-1.24	-4.7
Particulate Matter - Coarse	PMC	7.12	-0.06	-0.9	-2.52	-35.46	7.22	-0.07	-0.91	-2.57	-35.53
Particulate Matter - Fine	PMFINE	1.69	0	-0.16	-0.08	-4.97	1.69	0	-0.16	-0.08	-4.97
Particulate Organic Carbon	POC	12.16	-0.07	-0.6	-2.79	-22.96	12.57	-0.08	-0.61	-2.96	-23.55
Particulate Sulfate	PSO_4	4.41	-0.04	-1.02	-1.77	-40.02	4.41	-0.04	-1.02	-1.77	-40.02
Sulfur Dioxide	SO_2	63.05	0.16	0.25	7.39	11.72	63.09	0.16	0.25	7.37	11.69
Volatile Organic Compounds	VOC	67.46	-0.23	-0.34	-7.52	-11.15	70.61	-0.27	-0.38	-9.4	-13.31

Table 3.3.1 *Midwest Modal Shift Emissions Change by Scenario and Season. Percentage changes are relative to baseline (B-L) trucking.*

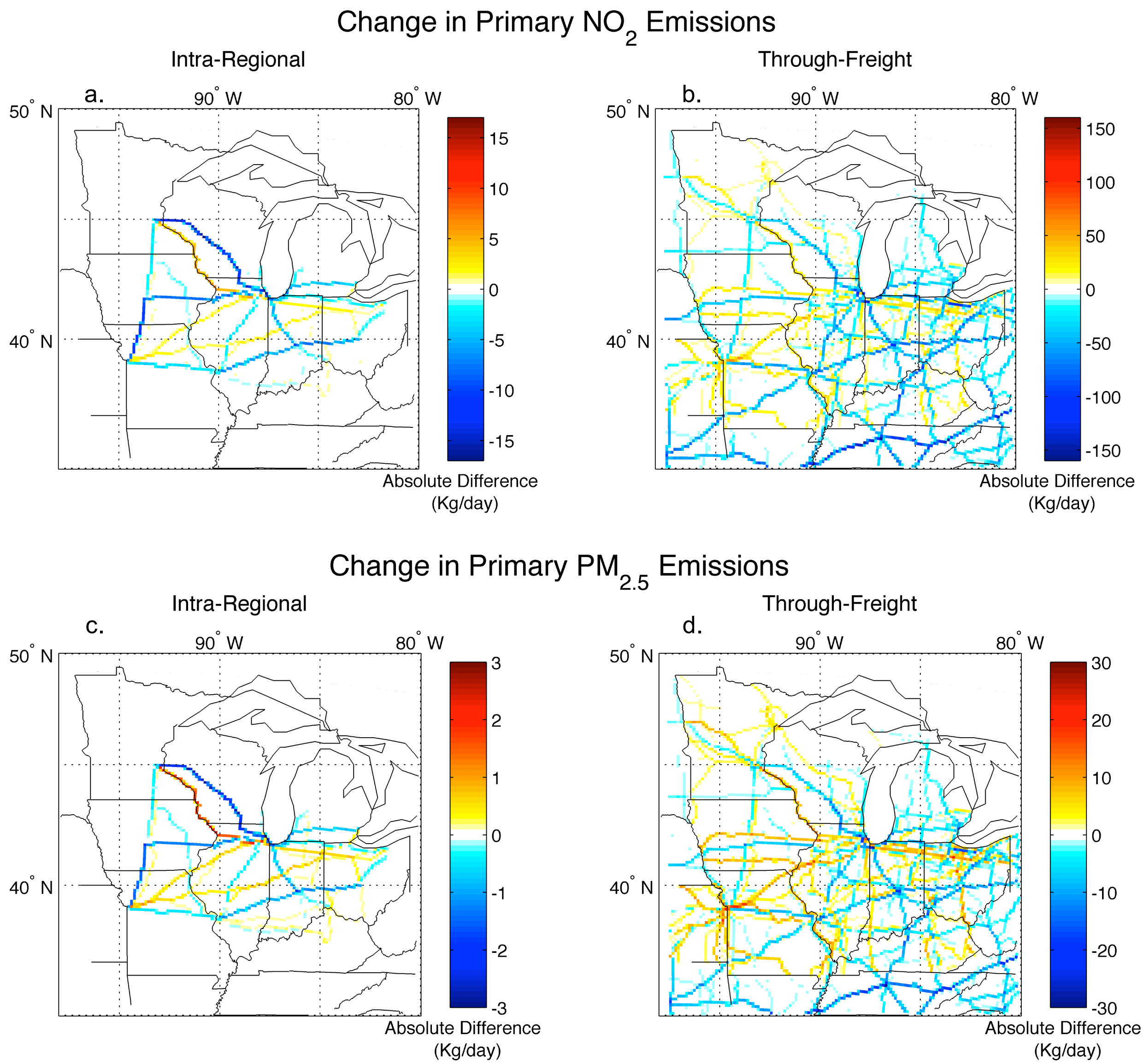

Figure 3.3.1 *Daily July Emissions Change from Modal Shift Scenarios. (a-b) Primary NO_2 emissions on highways are reduced as much as 17 kg/day (-28%) and 160 kg/day (-54%), for the I-R and T-F scenarios, respectively, while emissions on railways increase as much as 7 kg/day (I-R) and 62 kg/day (T-F). (c-d) Primary $PM_{2.5}$ emissions on highways are reduced as much as 3 kg/day (-28%) and 31 kg/day (-54%), for the I-R and T-F scenarios, respectively, while emissions on railways increase as much as 2 kg/day (I-R) and 21 kg/day (T-F). Regionally, net NO_2 emissions decrease by 1,513 kg/day (I-R), and 57,317 kg/day (T-F), while net $PM_{2.5}$ emissions decrease by 137 kg/day (I-R) and 4,995 kg/day (T-F).*

3.4 Emissions Inventory Speciation

The EPA's Sparse Matrix Operator Kernel Emissions (SMOKE) model [31] speciates aggregate pollutants (eg. NO_x, $PM_{2.5}$ and VOCs) into sub-species required by air quality models. At this time, SMOKE is unable to process gridded emissions for mobile sources; it allocates them to the county-level. To maintain the spatial integrity of our 12 km x 12 km gridded freight inventories, both the truck and rail inventories were speciated manually using tables for the Carbon-Bond 5 chemical mechanism [32,33] within the SMOKE model. Appendix II includes speciation tables and methods used in this analysis.

4. Air Quality Modeling

4.1 Air Quality Model – CMAQ

The EPA's Community Multiscale Air Quality Model (CMAQ) [34] is a state-of-the-science photochemical model that takes meteorological data and emission inventories as inputs, and calculates ambient air pollutant concentrations based on atmospheric chemistry, meteorological transport and numerical processes. The CMAQ model is widely used for policy analysis in the U.S. and abroad [35-38], and many states use CMAQ to develop their state implementation plans (SIP) in accordance with the Clean Air Act. These types of complex numerical models are the only way to effectively estimate how energy and transportation choices affect health-relevant air pollution.

4.2 Methods and Data

4.2.1 Meteorology

We used the Weather Research and Forecasting (WRF) model version 3.0 with North American Regional Reanalysis (NARR) input data to simulate meteorology for December 2004, January 2005, June 2005, and July 2005. Daily meteorology files output by WRF were processed for CMAQ using the Meteorology-Chemistry Interface Processor (MCIP) version 3.6.

4.2.2 Emissions Inventories

Emissions inventories for freight truck emissions (WIFE inventory), and added rail emissions were calculated, speciated, and gridded for CMAQ as part of this research (see Section 3). Emissions data for all other sectors including power plants, gasoline vehicles, industrial facilities, agriculture, natural emissions etc., came from LADCO's 2005 12 km x 12 km Midwest emissions inventory. Emissions files were grouped for processing in CMAQ with the merge component of the SMOKE model.

4.2.3 CMAQ Experimental Runs

Three scenarios were modeled for this analysis: 1.) A baseline scenario, 2.) The I-R scenario and, 3.) The T-F scenario. To capture atmospheric chemistry differences between winter and summer months, all scenarios were run for both January and July 2005, each using 10 days of model spin-up. The model ran at 12 km x 12 km resolution over the Midwestern U.S. using CMAQ version 4.6.

4.3 Results

4.3.1 Model Validation

To verify pollution estimates produced by CMAQ reasonably represent "real world" conditions, 2005 July and January baseline CMAQ runs were compared against surface measurements obtained from the EPA's Air Quality System (AQS) database. Table 4.3.1.1 displays statistical results of the model validation, comprised of the mean correlation between modeled and observed pollutant concentrations, normalized mean bias (NMB) of the model, and normalized mean error (NME) of the model. Equations for these metrics can be found in EPA documentation for CMAQ model evaluation [40]. Appendix III contains spatial maps of CMAQ pollutant concentrations overlaid with AQS measurements, and scatter plot comparisons of CMAQ and AQS monthly mean pollutant concentrations.

Results of the baseline CMAQ-AQS analysis are similar to documented CMAQ performance in studies by Eder & Yu [41], O'Neill et al. [37], Liu et al. [35], Sarwar et al. [33] and Zhang et al. [42], also shown in table 4.3.1.1. In July, elemental carbon (EC), $PM_{2.5}$ and O_3 perform as well, or better, than was found in other studies. No literature values were found for either NO_2 or SO_2. In January, EC again performs well, while $PM_{2.5}$ exhibits a negative NMB in opposition to literature values, though NME for $PM_{2.5}$ is within the literature range. These model performance differences for the same species between July and January demonstrate the varying ability of the model to simulate atmospheric chemistry for species between summer and winter meteorological conditions.

There are currently no universally accepted, or EPA-recommended quantitative criteria for judging acceptability of model performance. That statistics from model-observation comparisons in this study generally agree with values from published model performance analyses indicate there were no serious errors in model meteorological and emissions inputs, nor in the model's numerical operations. While lower NMB and NME values would be preferable, particularly for SO_2, model performance in this study is on par with the state of the science of air quality modeling. Further, because the focus of this study is on surface pollutant concentration *differences* between baseline and modal shift scenarios, model pollutant bias and error are somewhat less significant because over- and under-prediction of pollutant formation are removed when the difference between the modal shift scenario and the baseline scenario is taken.

4.3.2 Midwest Intra-Regional Scenario

Consistent with the relatively small emissions reductions resulting from the smaller scale I-R truck-to-rail mode shift scenario, modeled regional air quality changes were also very small. Net regional changes, relative to the baseline modeled scenario, were mostly less than 0.01% with the exception of NO_2, which regionally decreased an average 0.1% in both months. The highest reductions, up to 6% for NO_2, were found along I-94 in Wisconsin, I-88 between Illinois and Iowa, and I-35 in Iowa. Interstate-94

July	NO_2	Lit.	EC		Lit.	$PM_{2.5}$		Lit.	SO_2	Lit.	O_3		Lit.
mean r	0.47	N/A	0.49	0.47	Eder & Yu, 2006	0.56	0.5 to 0.7	Eder & Yu, 2006	0.34	N/A	0.67	0.69	Eder & Yu, 2006
NMB (%)	9.21	N/A	-10.15	-37.5 to 97	Eder & Yu, 2006; O'Neill et al, 2006; Liu et al, 2010	-10.52	-51.2 to 45.4	Eder & Yu, 2006; O'Neill et al, 2006; Liu et al, 2010	87.42	N/A	12.24	8.1 to 12.4	Eder & Yu, 2006; Sarwar et al, 2008
NME (%)	55.03	N/A	48.64	58 to 104	Eder & Yu, 2006; O'Neill et al, 2006; Liu et al, 2010	42.43	38 to 52.8	Eder & Yu, 2006; O'Neill et al, 2006; Liu et al, 2010	132.06	N/A	20.29	17.7 to 21.8	Eder & Yu, 2006; Sarwar et al, 2008
January	NO_2	Lit.	EC		Lit.	$PM_{2.5}$		Lit.	SO_2	Lit.			
mean r	0.45	N/A	0.5	N/A		0.57	N/A		0.45	N/A	–	–	–
NMB (%)	-14.66	N/A	-20.87	-49.6 to 17.5	Liu et al, 2010; Zhang et al, 2009	-35.58	1.3 to 29.7	Liu et al, 2010; Zhang et al, 2009	4.81	N/A	–	–	–
NME (%)	42.63	N/A	58.58	40.8 to 67.8	Liu et al, 2010; Zhang et al, 2009	43.96	32 to 59.6	Liu et al, 2010; Zhang et al, 2009	72.99	N/A	–	–	–

Table 4.3.1.1 CMAQ validation statistics for 2005 baseline CMAQ July and January runs with EPA AQS measurements, compared to validation statistics in the literature. Table contains mean correlation r, normalized mean bias (NMB) and normalized mean error (NME). Because ozone is of concern only during summer in the Midwest, we omitted January statistics for ozone .

leads to and from the Minneapolis metropolitan area, which was an origin or destination in 11 of the 28 Intra-Regional city pairs. I-88 and I-35 lead to and from Kansas City, which was also an origin or destination in 11 of the 28 I-R city pairs. Emissions increases occurred along the Mississippi river border between Iowa, Minnesota and Wisconsin, where the Burlington Northern and Santa Fe (BNSF) and Canadian Pacific (CPRS) rail lines run to and from the Minneapolis area (see figure 2.2.1).

4.3.3 Midwest Through-Freight Scenario

In contrast to the I-R scenario, the considerably larger tonnage of freight transferred from truck to rail in the T-F scenario resulted in some significant pollutant concentration reductions, particularly near roadways. Maps depicting percent and absolute pollutant changes for July and January for the I-R scenario are shown in figures 4.3.3.1 – 4.3.3.5.

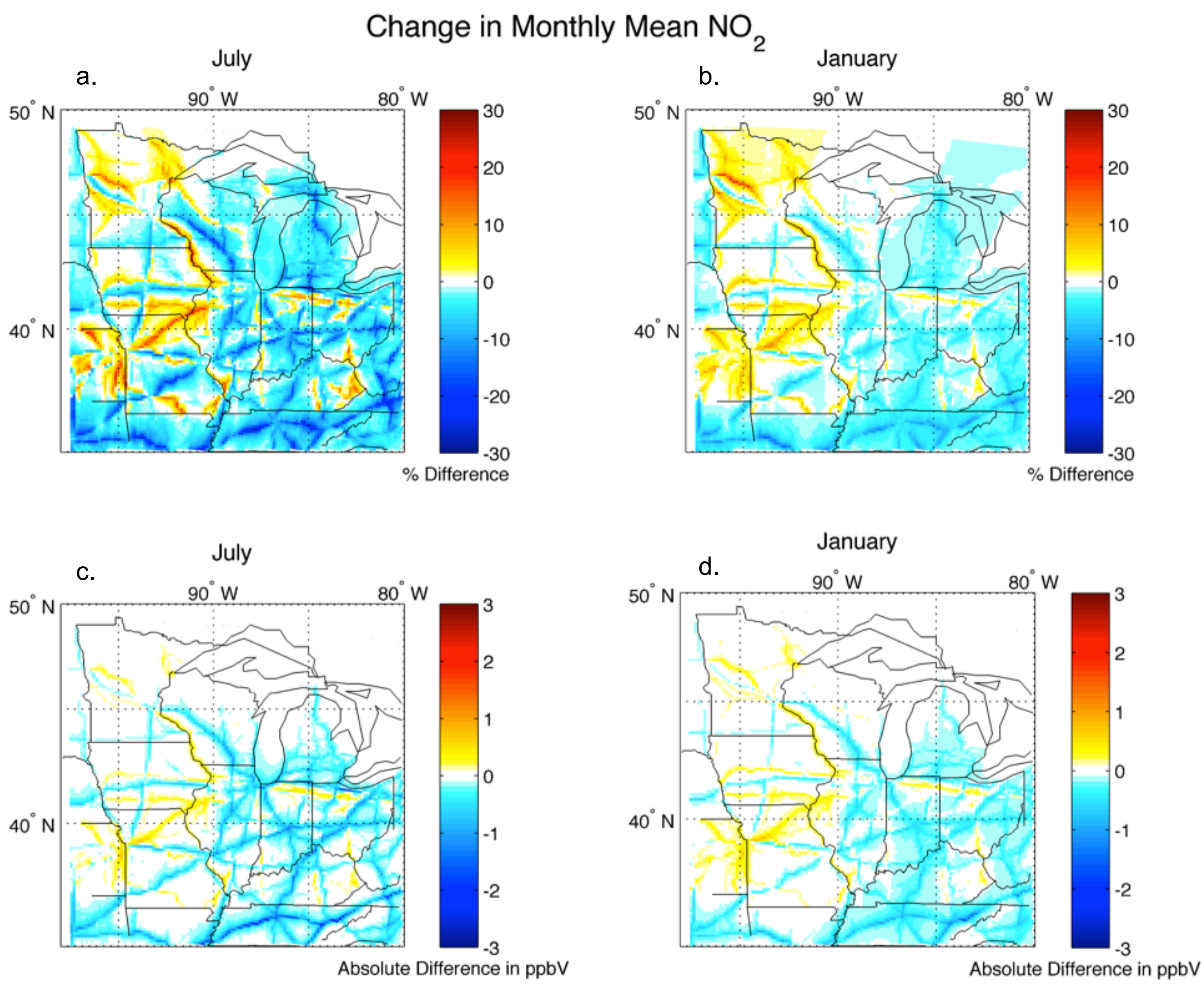

Figure 4.3.3.1 *Through-Freight scenario (a-b) percent and (c-d) absolute change in July and January surface nitrogen dioxide (NO_2) concentration as a result of shifting freight from truck to rail. Regionally, NO_2 concentrations decrease 3.5% (1800 ppbV) in July, and 1.4% (1200 ppbV) in January. In July (a) NO_2 is reduced up to 27% on highways, and increased up to 23% on railways while in January, (b) NO_2 is reduced up to 16% on highways, and increased up to 18% on railways.*

Figure 4.3.3.1 shows changes in surface NO_2 concentrations, in percent and absolute change, for both July and January. The T-F scenario yielded significant reductions in NO_2 concentrations near roadways with a maximum reduction of 27% in July and 16% in January. Added rail freight activity increased NO_2 emissions along rail lines up to 23% in July, and 18% in January. The balance of reduced highway emissions and increased rail emissions yields a net regional change in surface NO_2 of 3.5% in July, and 1.4% in January.

Elemental Carbon (EC), commonly referred to as "Black Carbon" or "soot", is a component of fine $PM_{2.5}$ that causes respiratory and cardiovascular health problems, in addition to contributing to climate change by scattering and absorbing incoming solar radiation [43-45]. Figure 4.3.3.2 shows changes in surface EC concentrations for July and January. Roadway emissions of EC were reduced up to 16% in July, and 15% in January. Added rail activity increased railway EC emissions 23% in July and 28% in

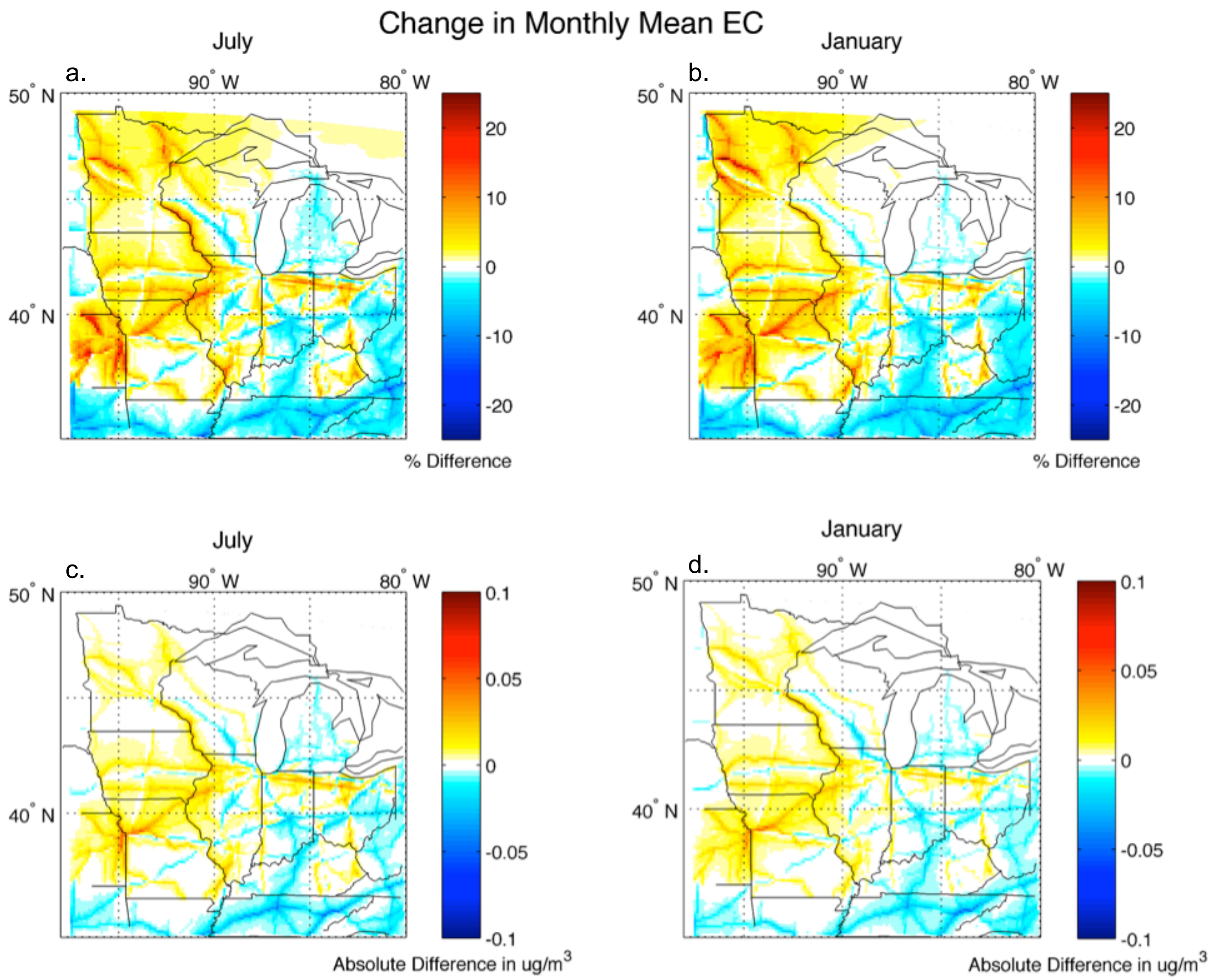

Figure 4.3.3.2 *Through-Freight scenario (a-b) percent and (c-d) absolute change in July and January surface elemental carbon (EC) concentration as a result of shifting freight from truck to rail. In both July and January, regional net EC concentrations increase slightly, 0.2% (7 ug/m^3). In July (a) EC is reduced up to 16% on highways, and increased up to 22% on railways while in January, (b) EC is reduced up to 15% on highways, and increased up to 28% on railways.*

January, resulting in a small net increase in regional EC emissions of 0.2% for July and January.

Figure 4.3.3.3 shows July and January monthly mean changes in $PM_{2.5}$ resulting from the T-F scenario. Near roadway emissions of $PM_{2.5}$ were reduced up to 3% in July, and 2% in January, while near-railway emissions increased up to 1% in July and January. The net change in regional $PM_{2.5}$ is small, a 0.5% reduction in July and 0.1% reduction in January. Though $PM_{2.5}$ decreases regionally, it is not significant enough to bring any counties into regulatory attainment.

Figure 4.3.3.4 shows regional changes in SO_2. While near-roadway concentrations of SO_2 decrease up to 3% in July, and 2% in January, near railway concentrations increase up to 7% in July and January. Region-wide concentrations increase slightly,

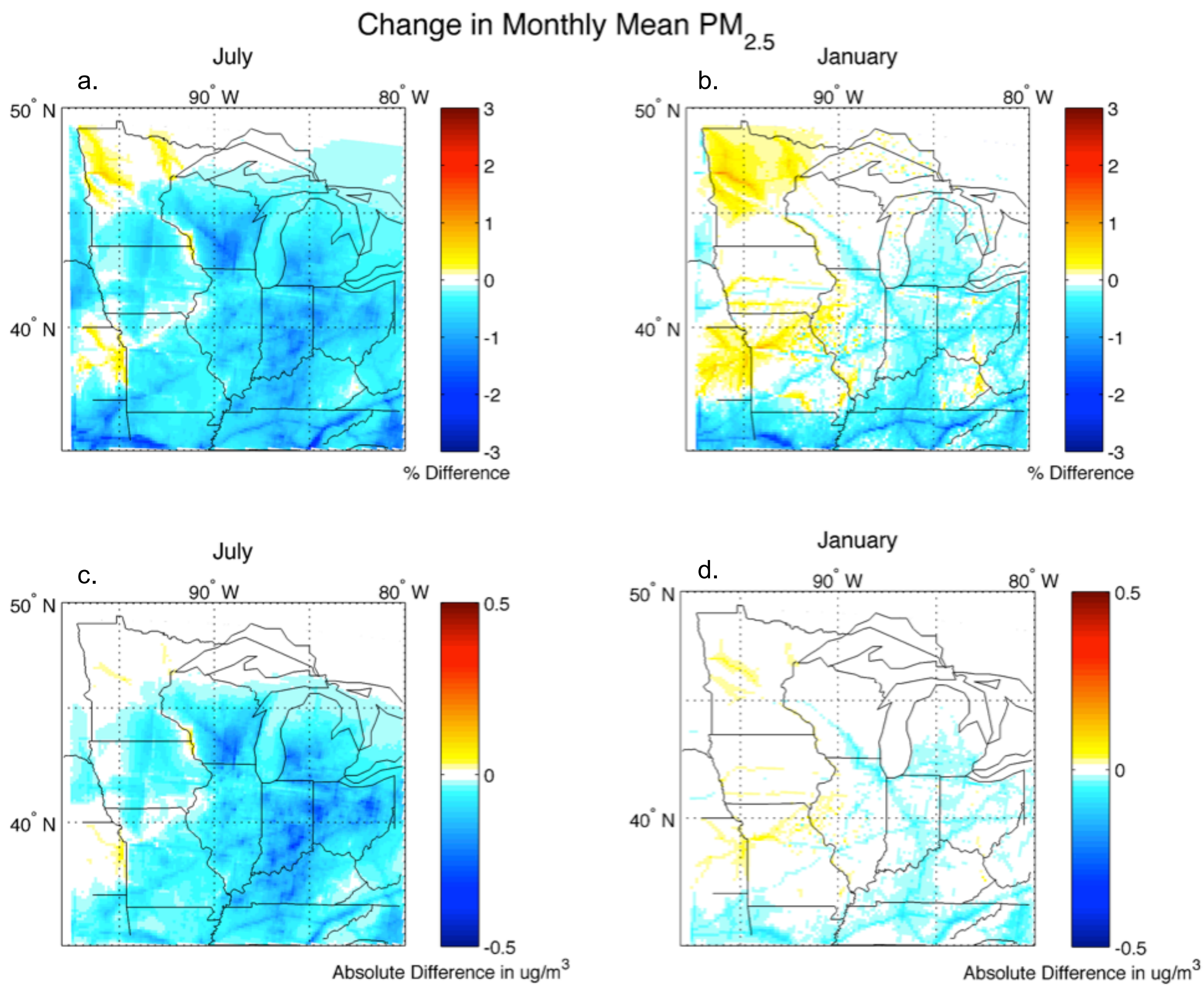

Figure 4.3.3.3 *Through-Freight scenario (a-b) percent and (c-d) absolute change in July and January surface fine particulate matter ($PM_{2.5}$) concentration as a result of shifting freight from truck to rail. Regionally, $PM_{2.5}$ concentrations decrease 0.5% (900 ug/m^3) in July, and 0.1% (90 ug/m^3) in January. In July (a) $PM_{2.5}$ is reduced up to 3% on highways, and increased up to 0.7% on railways while in January, (b) $PM_{2.5}$ is reduced up to 2.1% on highways, and increased up to 1.1% on railways.*

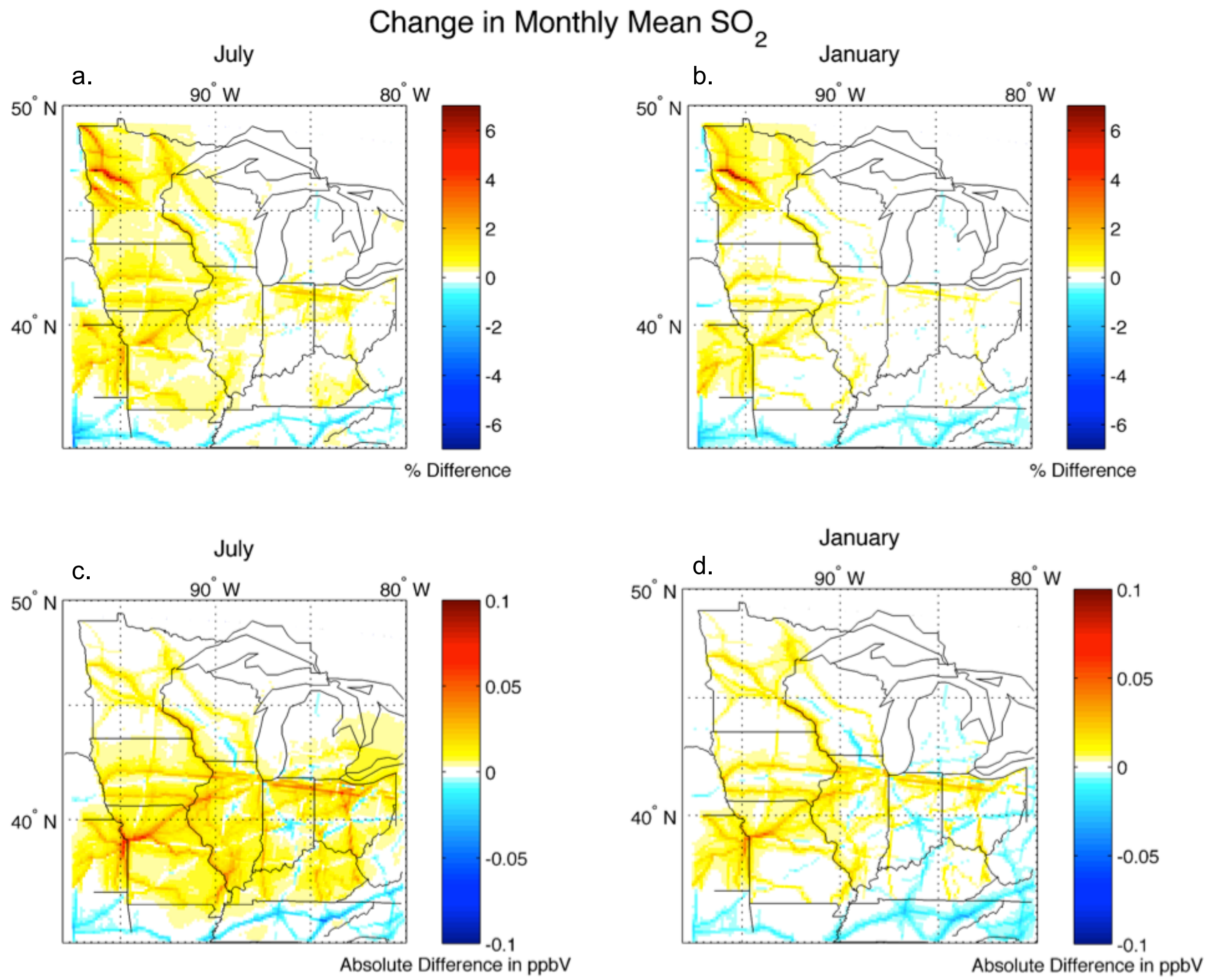

Figure 4.3.3.4 *Through-Freight scenario (a-b) percent and (c-d) absolute change in July and January surface sulfur dioxide (SO_2) concentration as a result of shifting freight from truck to rail. Regionally, SO_2 concentrations increase 0.2% (80 ug/m^3) in July, and 0.1% (20 ug/m^3) in January. In July (a) SO_2 is reduced up to 3.2% on highways, and increased up to 6.9% on railways while in January, (b) SO_2 is reduced up to 2.1% on highways, and increased up to 7% on railways. This increase in SO_2 is due to the much higher allowable sulfur levels in locomotive diesel fuel compared to highway diesel (2600 ppm compared to 500 ppm).*

0.2% in July and 0.1% in January. This increased SO_2 concentration is attributable to diesel fuel sulfur content differences between highway and rail grade fuels (discussed in section 3.3), which will be negated once the transition to ULSD is completed in 2015.

Figure 4.3.3.5 shows the modal shift's impact on regional O_3 for July. Near-roadway O_3 concentrations decrease up to 3%, while near-railway concentrations increase up to 1%. Region-wide ozone decreases 0.5%, also not significant enough to impact county attainment status.

5. Discussion

We found 12 million tons of intra-regional freight, and 530 million tons of all freight moving through the upper Midwest region could be shifted off of truck and onto train. Emissions impacts for the I-R scenario were small, on the order of 1% or less, while emissions impacts for the T-F scenario were considerably larger, including a 26% reduction in NO_x emissions, and 31% reduction in CO_2 emissions. Subsequent ground-level air quality impacts of the modal shift scenarios were again modest for the I-R scenario, exhibiting a maximum pollutant reduction of 6% for NO_2. For the T-F scenario, while concentrations of both O_3 and $PM_{2.5}$ diminished due to modal shift, the reductions were on the order of 3% or less, not significant enough for county attainment status. The T-F scenario reduced CO_2 emissions 31% compared to baseline trucking, and greatly reduced concentrations of NO_2 and EC near roadways (up to 27% for NO_2 and up to 16% for EC), with corresponding increases near railways (up to 23% and 22%, respectively). These near-road concentration reductions could have significant impacts on human pollutant exposure and health. Research has shown that people who live or work near highways, and are consistently exposed to high concentrations of NO_2, EC and other motor vehicle pollutants have increased incidence of reduced lung function, impaired lung development in children, asthma, cardiovascular disease and premature death [9,46-48].

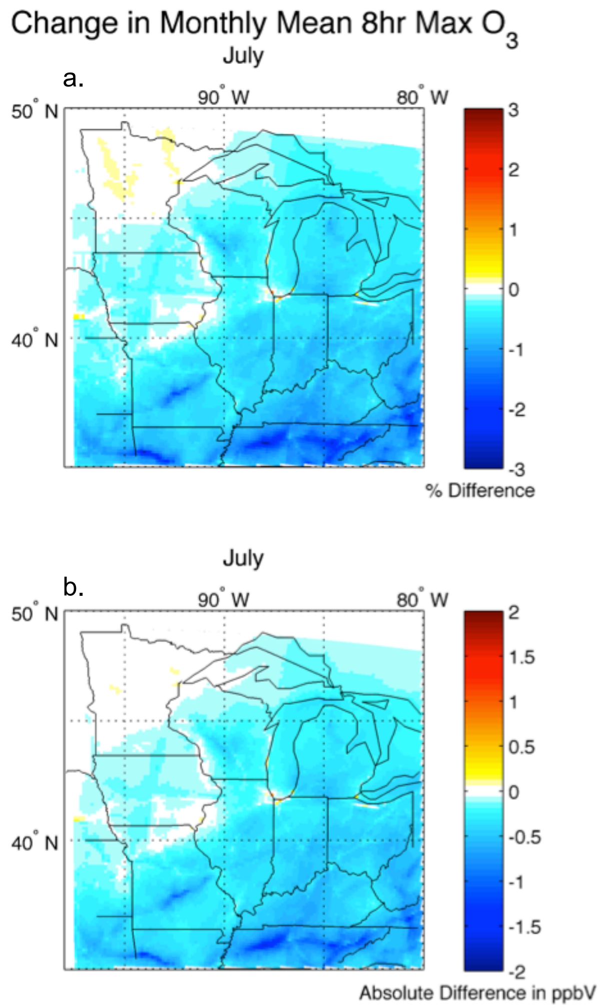

Figure 4.3.3.5 *Through-Freight scenario (a) percent and (b) absolute change in July surface ozone (O_3) as a result of shifting freight from truck to rail. Ozone decreases across the region, with a net change of 0.5%. Summer O_3 decreases as much as 2.8% in some regions, while increasing as much as 1.2% in others.*

Several studies have examined emissions impacts of freight truck-to-rail modal shift, highlighting the increased fuel efficiency of rail over truck for its potential to both improve air quality and reduce carbon dioxide emissions [10,12-14,49]. Table 5.1 summarizes emissions change results for NO_x and PM from this study, compared to other freight truck-to-rail mode shift analyses. In a study of the I-710 freight corridor in California, Lee et al. [12] found shifting 25% to 100% of truck volume to rail lead to a 13% to 57% reduction in NO_x, with a 15% to 56% reduction in PM_{10}. Comer et al. [1],

	NO_x	$PM_{2.5}$	PM_{10}	CO_2	**Study Summary**
CFIRE (2011)	-26%	-13%	-16%	-31%	Midwest truck to rail mode shift, where 40% of truck freight VMT is replaced with rail freight.
Lee et al, 2009	-13% to -57%	--	-15% to -56%	--	California I-710 freight corridor truck to rail mode shift where 25%-100% of truck volume is replaced by rail.
Comer et al, 2010	+58% to +283%	--	+12% to +30%	-59%	Great Lakes truck to rail mode shift. Study assumes new freight trucks adhering to newewst emissions standards while rail is assumed to be tier 2, with maximimum allowable NOx and PM10 emissions factors.
You et al, 2010	-22% to -28%	-8% to -22%		--	Truck to Rail mode shift for drayage movements at ports of Long Beach and Los Angeles.

Table 5.1 *Emissions change comparison with truck-to-rail modal shift studies in the literature.*

looking at truck-to-rail modal shift in the Great Lakes region and assuming HDDVs with the newest pollution control technologies, found emissions increases for both NO_x (58% to 283%) and PM_{10} (12% to 30%), although CO_2 emissions decreased 59%. You et al. [50], focusing on shifting drayage movements to rail at the ports of Long Beach and Los Angeles found 22% to 28% reductions of NO_x and 8% to 22% reductions of $PM_{2.5}$. With the exception of the Comer et al. [49] study, where the authors' assumption of comparatively "clean" HDDV trucks, and relatively "dirty" locomotives resulted in emissions increases for NO_x and PM, emissions reductions found in this study's T-F scenario are inline with reduction ranges found in other truck-to-rail studies.

While other studies assume significant emissions reductions lead to significantly improved air quality, we find in modeling air quality with meteorology in a regional photochemical model that the actual on the ground impacts of emissions reductions on that scale is limited to primary pollutants. For secondary pollutants, like O_3 and the secondary components of $PM_{2.5}$, relative emissions contributions from other anthropogenic and biogenic sectors coupled with meteorology and atmospheric chemistry can confound the effectiveness of policies aimed at single-sector emissions reductions.

Although truck-to-rail modal shift in this analysis did not greatly improve air quality in counties out of attainment with National Ambient Air Quality Standards, by significantly decreasing highway pollutant concentrations, using fewer trucks and more trains could yield valuable benefits by reducing human pollutant exposure (A health impact analysis of the scenarios used in this study is currently in progress). In addition, modal shift in the T-F scenario decreased CO_2 emissions 23 million tons per year, which amounts to 1% of U.S. transportation carbon emissions, or the equivalent of taking four million passenger cars off the road. If at some point in the future the EPA does regulate carbon emissions, or the cost of diesel fuel continues to increase, the superior fuel-efficiency of rail and/or lower CO_2 emissions may serve as a primary motivator for moving more freight by rail, with reduced human roadway pollutant exposure and marginally improved regional air quality serving as co-benefits.

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Appendix I: Intra-Regional Scenario Modal Shift City Pairs

	Origin	Destination		Origin	Destination
1	Chicago	Minneapolis	15	Detroit	Minneapolis
	Minneapolis	Chicago		Minneapolis	Detroit
2	Chicago	Kansas City	16	Detroit	Kansas City
	Kansas City	Chicago		Kansas City	Detroit
3	Cincinnati	Minneapolis	17	Detroit	St. Louis
	Minneapolis	Cincinnati		St. Louis	Detroit
4	Cincinnati	Kansas City	18	Grand Rapids	Minneapolis
	Kansas City	Cincinnati		Minneapolis	Grand Rapids
5	Cleveland	Minneapolis	19	Grand Rapids	Kansas City
	Minneapolis	Cleveland		Kansas City	Grand Rapids
6	Cleveland	Kansas City	20	Grand Rapids	St. Louis
	Kansas City	Cleveland		St. Louis	Grand Rapids
7	Cleveland	St. Louis	21	Grand Rapids	Louisville
	St. Louis	Cleveland		Louisville	Grand Rapids
8	Cleveland	Milwaukee	22	Indianapolis	Minneapolis
	Milwaukee	Cleveland		Minneapolis	Indianapolis
9	Columbus	Minneapolis	23	Indianapolis	Kansas City
	Minneapolis	Columbus		Kansas City	Indianapolis
10	Columbus	Kansas City	24	Louisville	Minneapolis
	Kansas City	Columbus		Minneapolis	Louisville
11	Columbus	St. Louis	25	Kansas City	Louisville
	St. Louis	Columbus		Louisville	Kansas City
12	Columbus	Milwaukee	26	Kansas City	Milwaukee
	Milwaukee	Columbus		Milwaukee	Kansas City
13	Dayton	Minneapolis	27	Minneapolis	St. Louis
	Minneapolis	Dayton		St. Louis	Minneapolis
14	Dayton	Kansas City	28	Kansas City	Minneapolis
	Kansas City	Dayton		Minneapolis	Kansas City

Table I.i *Intra-Regional Scenario City Pairs. Note that city names represent metropolitan areas which may overlap state boundaries (eg. Chicago extends to Indiana, and St. Louis extends to Illinois, etc). See Figure I.i for metropolitan regions.*

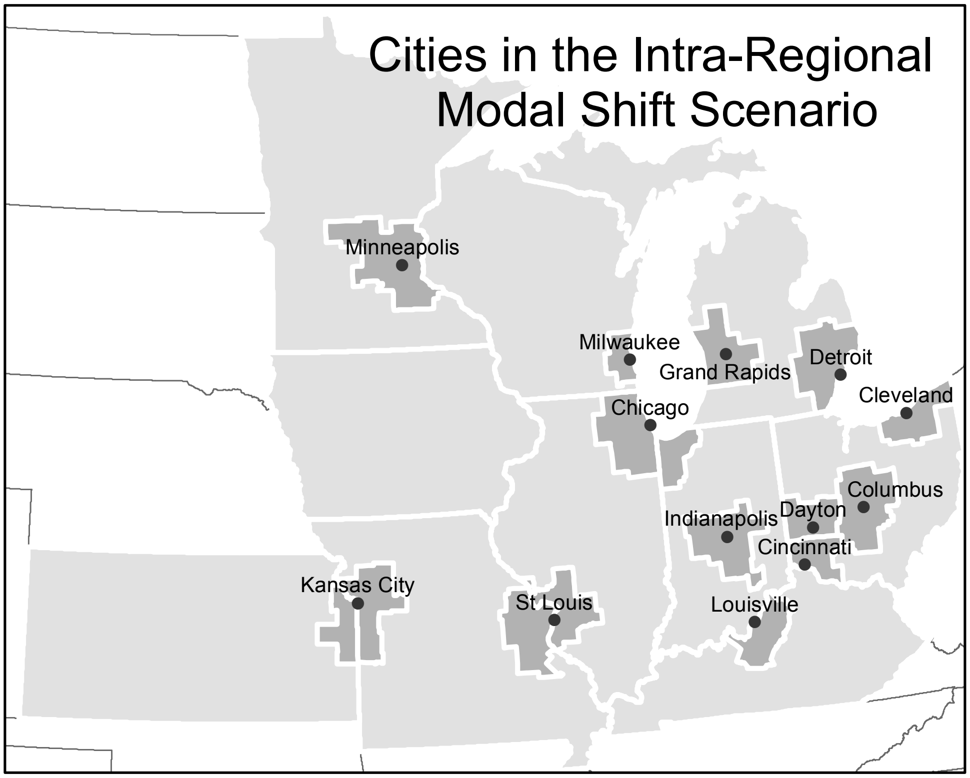

Figure I.i *Shows Midwest City metropolitan regions used for the Intra-Regional (I-R) modal shift scenario. Areas shaded in dark grey show the spatial extent of the metropolitan region around each city, as determined by FAF. In the case of Kansas City, St. Louis, and Chicago, the metropolitan areas cross state lines. Commodity flows selected for modal shift in this scenario incorporate movements originating and terminating within these metropolitan areas.*

Appendix II: Diesel Emissions Speciation Methods for Truck and Rail

Methods employed in this analysis for speciating heavy-duty diesel vehicle (HDDV) and Class-I locomotive emissions are described in Appendix II. Though speciation in this analysis was performed manually, all conversion and speciation factors were obtained from EPA documentation [27] and SMOKE [31] model speciation tables. All references to “gspro” and “gsref” files refer to speciation and source reference tables for the Carbon Bond 5 [32] (CB05) chemical mechanism included with the SMOKE model. Speciation profiles were identified using SMOKE’s source classification codes (SCC) in Table II.i.

SMOKE Diesel SCCs	
Heavy-Duty Diesel Vehicles	223007*
Class-I Linehaul Locomotives	2285002006

Table II.i *SMOKE Source Classification Codes, where * is a 4-digit road-type code.*

II.i Particulate Matter (PM)

For HDDVs, PM was speciated in MOBILE6.2, and therefore no further pre-processing was necessary. Following EPA Locomotive Emissions Factor Guidance, the PM_{10} emissions factor was first speciated into PMC (coarse PM) and $PM_{2.5}$, with the assumption that $PM_{2.5}$ comprises 97% of PM_{10} by mass [27].

Equation II.i.i $PM_{2.5} = 0.97 \times PM_{10}$

Equation II.i.ii $PMC = PM_{10} - PM_{2.5}$

$PM_{2.5}$ was further broken out into its sub-species following speciation tables for Class-I locomotives in SMOKE (see Table II.i.i).

CB05 PM2.5 Speciation for Locomotives				
Units: grams		**Split Factor**	**Divisor**	**Mass Fraction**
PM2.5	PEC	0.7712	1	0.7712
PM2.5	PMFINE	0.0491	1	0.0491
PM2.5	PNO3	0.0011	1	0.0011
PM2.5	POC	0.1756	1	0.1756
PM2.5	PSO4	0.0029	1	0.0029

Table II.i.i *$PM_{2.5}$ Speciation for Class-I Locomotives, taken from* gspro_cb05_notoxics_cmaq_poc_30jan2007_v0.txt file in SMOKE.

Particulate matter, measured by mass (grams), was separated into its sub-species by mass fraction with the following equation.

Equation II.i.iii PM sub-species (grams) = $PM_{2.5}$ (grams) x Mass Fraction

II.ii Volatile Organic Compounds (VOCs)

While MOBILE6.2 produces emissions factors for VOCs, organic pollutant emissions for locomotives are given as hydrocarbons (HCs). Per EPA guidance on locomotive emissions, HCs may be converted to VOCs using a constant conversion factor [27].

Equation II.ii.i VOCs = 1.053 x HCs

To speciate both HDDV and locomotive VOC emissions, the table for total organic gases (TOG) from SMOKE was used. For CB05, a conversion factor is applied to convert VOCs to TOG. For both HDDVs and locomotives, that conversion factor is 1. Therefore VOCs were speciated according to the TOG table (see Table II.ii.i).

CB05 TOG Speciation for Medium Diesel Trucks				
Units: grams		**Split Factor**	**Divisor**	**Mass Fraction**
TOG	ALD2	0.1633	43.9898	0.1633
TOG	ALDX	0.1072	36.0727	0.1072
TOG	ETH	0.0327	28.0532	0.0327
TOG	FORM	0.0965	28.5778	0.0965
TOG	IOLE	0.0048	56.4485	0.0048
TOG	NVOL	0.0047	14.1436	0.0047
TOG	OLE	0.0389	34.154	0.0389
TOG	PAR	0.3642	15.9027	0.3642
TOG	TERP	0.0097	164.9627	0.0097
TOG	TOL	0.0673	103.8384	0.0673
TOG	UNK	0.0022	226.4412	0.0022
TOG	UNR	0.0631	14.8645	0.0631
TOG	XYL	0.0456	116.8771	0.0456

Table II.ii.i *TOG and VOC Speciation for HDDVs and Class-I Locomotives, from gspro_cb05_notoxics_cmaq_poc_30jan2007_v0.txt in SMOKE. Note that gsref_2002_cb05_cap4_11dec2007_v3.txt assigns both HDDV and Class-I locomotive TOG (VOC) speciation to medium duty diesel vehicles.*

Unlike $PM_{2.5}$, VOCs as gases are measured in moles, rather than mass. Therefore speciating VOCs requires division by molar mass to convert from grams to moles.

Equation II.ii.ii

VOC sub-species (moles) = VOCs (grams) x Mass Fraction / Divisor

II.iii Nitrogen Oxides (NO_x)

For CMAQ version 4.6 with the CB05 mechanism, NO_x is speciated into two species: NO and NO_2. Nitrogen oxides are speciated in a standard way for all sources, so the same method was used for HDDVs and locomotives (see Table II.iii.i).

CB05 NOx Speciation				
Units: grams		**Split Factor**	**Divisor**	**Mass Fraction**
NOX	NO	0.9	46	0.9
NOX	NO2	0.1	46	0.1

Table II.iii.i *NO_x Speciation for HDDVs and Class-I Locomotives from* gspro_cb05_notoxics_cmaq_poc_30jan2007_v0.txt in SMOKE.

Nitrogen oxide emissions are also quantified in moles, and therefore speciation of NO_x follows Equation II.ii.ii.

Appendix III: CMAQ Validation Figures

Basecase 2005 CMAQ model runs were validated against surface observations from the EPA's Air Quality System (AQS) (see section 4.3.1 for statistics). Appendix III contains spatial maps of modeled monthly mean (or mean 8-hour maximum for ozone) pollutant concentrations with observations overlaid (in circles), as well as scatter plots of monthly mean observations plotted against corresponding modeled grid cells.

2005 July Mean 8hr Maximum O_3

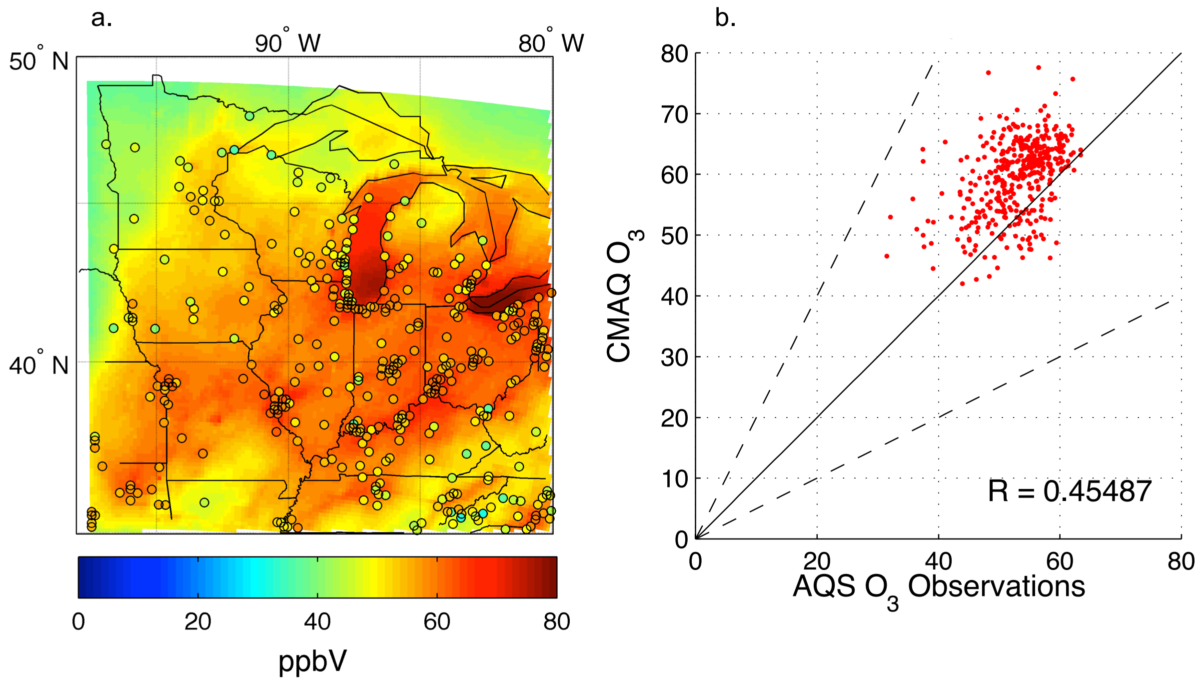

Figure III.i *(a) CMAQ modeled July 2005 monthly mean 8-hour maximum O_3, overlaid with monthly mean 8-hour maximum AQS O_3 observations. (b) CMAQ modeled July 2005 monthly mean 8-hour maximum O_3 (y-axis) plotted against monthly mean 8-hour maximum AQS O_3 observations (x-axis), with a 1:1 line (solid), a 2:1 line (dashed), a 1:2 line (dashed), and correlation value R. Modeled O_3 for much of the domain is on the order of 10 ppbV too high (12% NMB) with the exception of northwestern Minnesota, where the model is 10 ppbV lower than observations.*

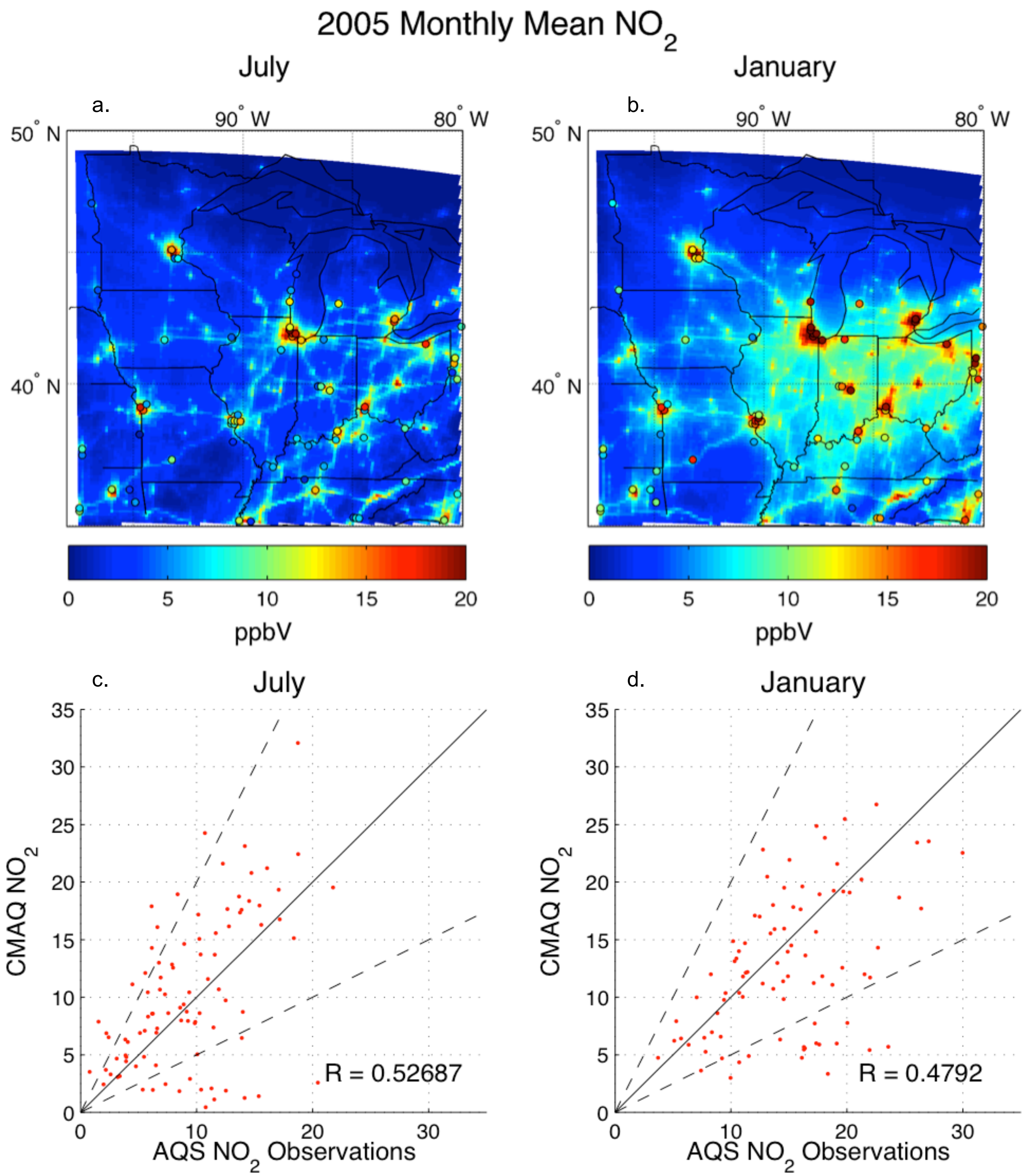

Figure III.ii *CMAQ modeled (a) July and (b) January 2005 monthly NO_2 overlaid with monthly mean AQS NO_2 observations. CMAQ modeled (c) July and (d) January 2005 monthly mean NO_2 (y-axis) plotted against monthly AQS NO_2 observations (x-axis), with a 1:1 line (solid), a 2:1 line (dashed), a 1:2 line (dashed), and correlation value R. Modeled NO_2 is in good agreement with observations. NO_2 is overpredicted over the domain (9% NMB in July, 15% NMB in January) however tends to be underpredicted in some urban areas.*

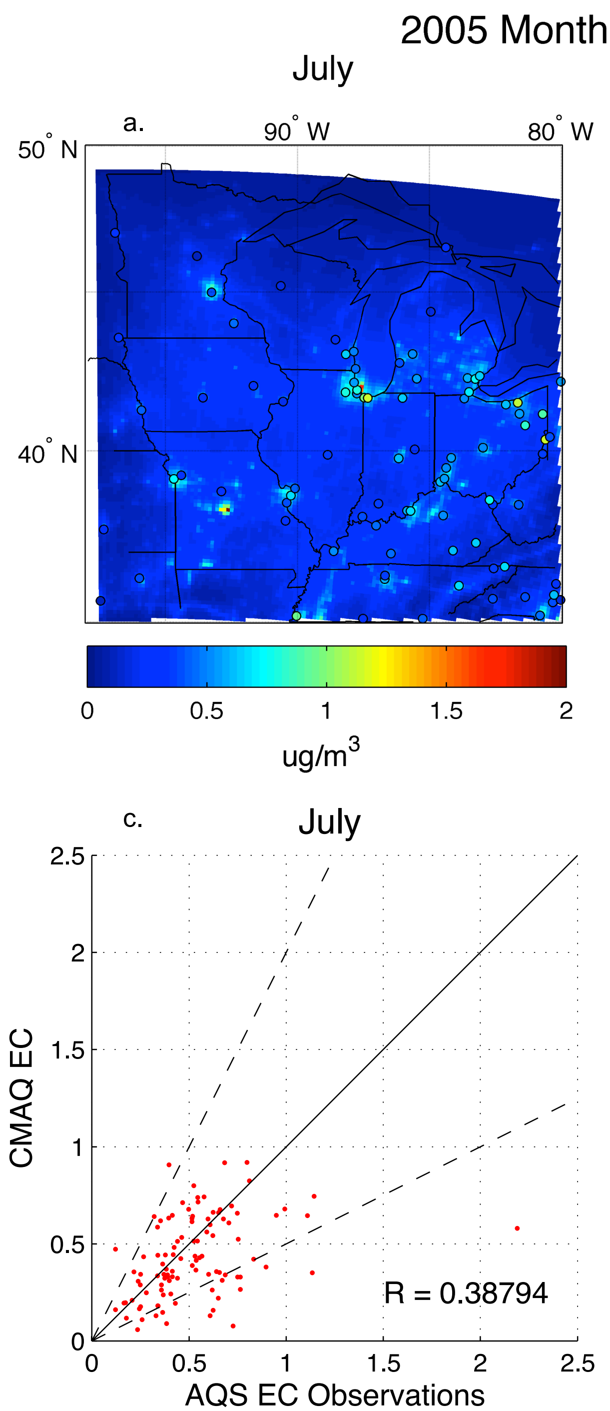

Figure III.iii *(a) CMAQ modeled July 2005 monthly mean EC, overlaid with monthly mean AQS EC observations. (b) CMAQ modeled July 2005 monthly mean EC (y-axis) plotted against monthly mean AQS EC observations (x-axis), with a 1:1 line (solid), a 2:1 line (dashed), a 1:2 line (dashed), and correlation value R. Modeled EC is in reasonable agreement with observations, however is under-predicted in both months (-10.2% NMB in July, -20.9% NMB in January), particularly in urban areas.*

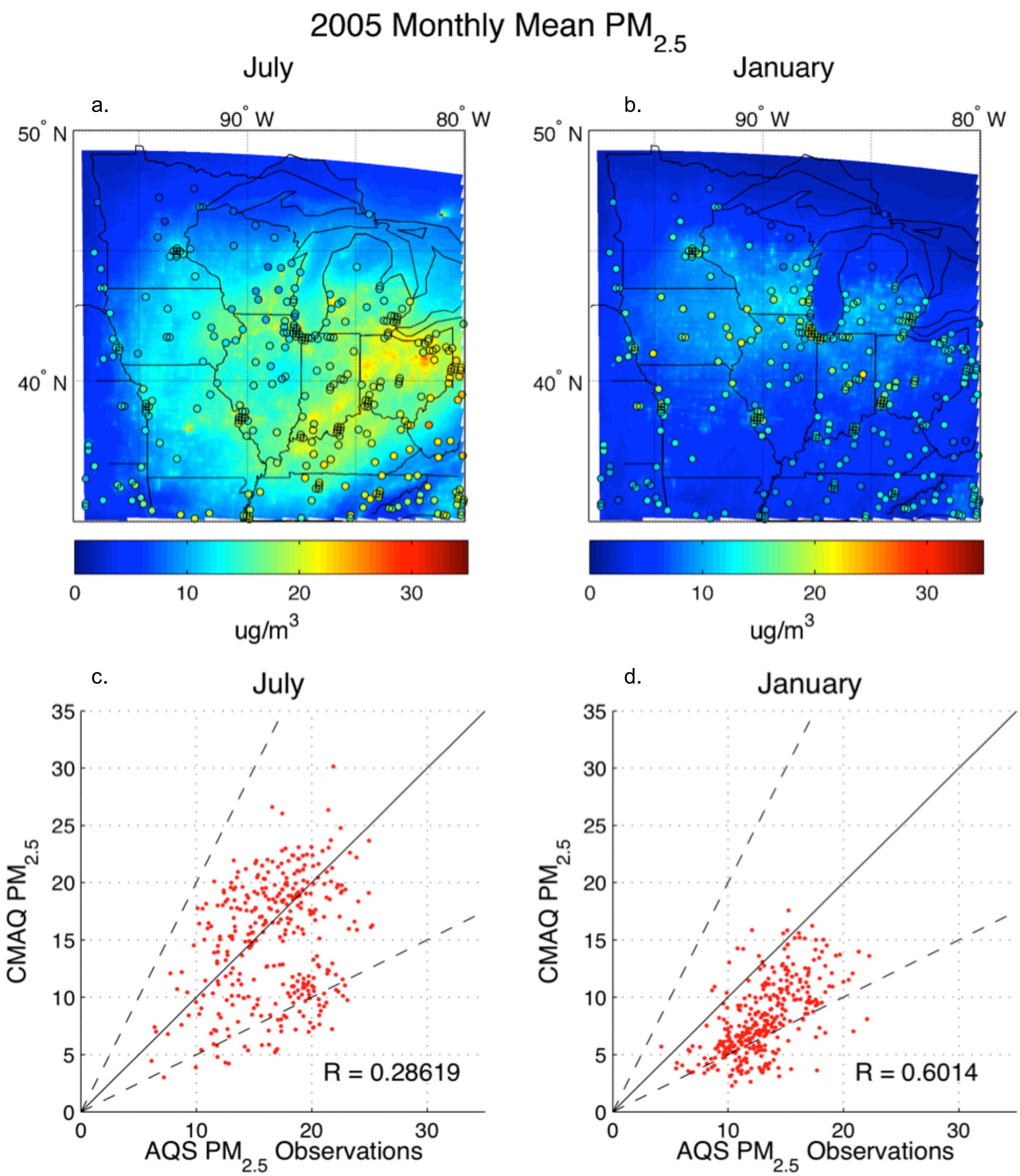

Figure III.iv *CMAQ modeled (a) July and (b) January 2005 monthly $PM_{2.5}$ overlaid with monthly mean AQS $PM_{2.5}$ observations. CMAQ modeled (c) July and (d) January 2005 monthly mean $PM_{2.5}$ (y-axis) plotted against monthly AQS $PM_{2.5}$ observations (x-axis), with a 1:1 line (solid), a 2:1 line (dashed), a 1:2 line (dashed), and correlation value R. Modeled $PM_{2.5}$ compares fairly well with observations, but tends toward underprediction, particularly in January (-36% NMB, -11% NMB in July).*

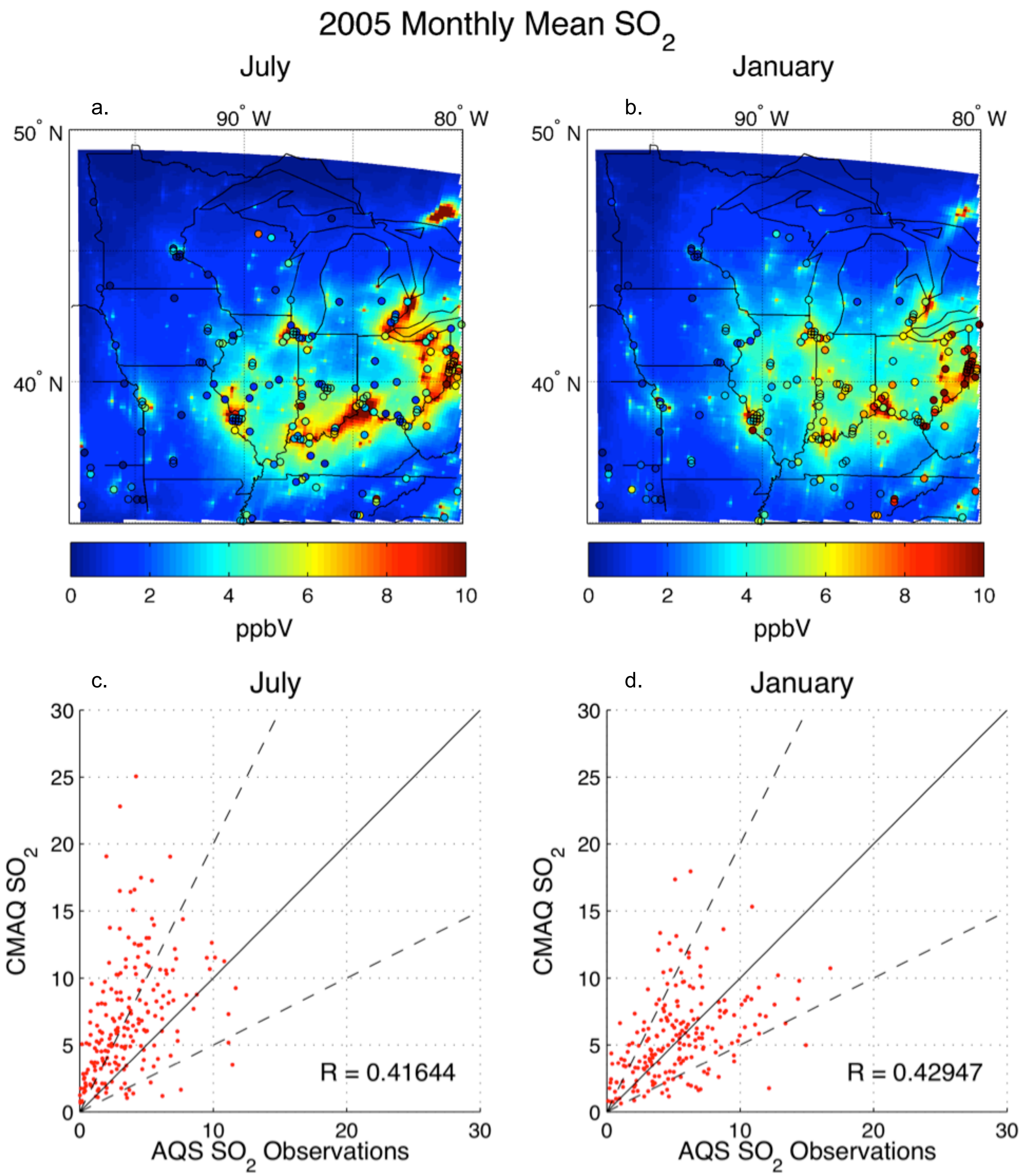

Figure III.v *CMAQ modeled (a) July and (b) January 2005 monthly SO_2 overlaid with monthly mean AQS SO_2 observations. CMAQ modeled (c) July and (d) January 2005 monthly mean SO_2 (y-axis) plotted against monthly AQS SO_2 observations (x-axis), with a 1:1 line (solid), a 2:1 line (dashed), a 1:2 line (dashed), and correlation value R. Modeled SO_2 correlates reasonably well with observations, yet overpredicts concentrations in urban regions, with scattered rural underpridction. Performance is better in January (4.8% NMB) than July (87% NMB).*

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