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Assessing Concentrations and Health Impacts of Air Quality Management Strategies: Framework for Rapid Emissions Scenario and Health impact ESTimation (FRESH-EST)

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Abstract

In air quality management, reducing emissions from pollutant sources often forms the primary response to attaining air quality standards and guidelines. Despite the broad success of air quality management in the US, challenges remain. As examples: allocating emissions reductions among multiple sources is complex and can require many rounds of negotiation; health impacts associated with emissions, the ultimate driver for the standards, are not explicitly assessed; and long dispersion model run-times, which result from the increasing size and complexity of model inputs, limit the number of scenarios that can be evaluated, thus increasing the likelihood of missing an optimal strategy. A new modeling framework, called the "Framework for Rapid Emissions Scenario and Health impact ESTimation" (FRESH-EST), is presented to respond to these challenges. FRESH-EST estimates concentrations and health impacts of alternative emissions scenarios at the urban scale, providing efficient computations from emissions to health impacts at the Census block or other desired spatial scale. In addition, FRESH-EST can optimize emission reductions to meet specified environmental and health constraints, and a convenient user interface and graphical displays are provided to facilitate scenario evaluation. The new framework is demonstrated in an SO_2 non-attainment area in southeast Michigan with two optimization strategies: the first minimizes emission reductions needed to achieve a target concentration; the second minimizes concentrations while holding constant the cumulative emissions across local sources (e.g., an emissions floor). The optimized strategies match outcomes in the proposed SO_2 State Implementation Plan without the proposed stack parameter modifications or shutdowns. In addition, the lower health impacts estimated for these strategies suggest the potential for FRESH-EST to identify pollution control alternatives for air quality management planning.

Keywords

Air quality management; optimization; health impact assessment; FRESH-EST

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1 Introduction

In air quality management, the primary response to a known or potential exceedance of an air quality standard or guideline is to reduce emissions from local and sometimes regional emission sources. In the US, state agencies formalize such responses in State Implementation Plans (SIPs). For example, the 2010 promulgation of a more stringent National Ambient Air Quality Standard (NAAQS) for SO_2 caused 29 regions in 16 states to be in non-attainment (US EPA, 2016). The US Environmental Protection Agency (US EPA) suggests that emissions reductions form the basis of each state s attainment plan (US EPA, 2014). The allocation and magnitude of emissions reductions among polluting sources usually is determined by state agencies with the oversight of US EPA. Final allocations may require extended negotiations between these agencies and stakeholders, and may include consideration of costs, feasibility, legal requirements and public input. Central to air quality management and the development of emission reduction strategies are dispersion models used to predict pollution concentrations, allocate source contributions, and determine whether a specific strategy will meet ambient standards or other goals.

Despite broad success, challenges to air quality management remain (US EPA, 2011). First, for air quality managers, identifying emissions reduction strategies that avoid litigation and satisfy the public and other stakeholders can be difficult, requiring months of negotiation and perhaps years to implement, during which time sustained exposures occur to potentially harmful levels of pollution (NRC, 2004). Second, the health impacts and benefits of emission reduction strategies, the principal drivers for air quality management, are rarely assessed as part of the formal air quality management in the US or elsewhere. This absence can result in selection of strategies that minimize costs and avoid litigation but are not the most health protective. An approach limited to achieving air quality standards also ignores health effects that occur below the standards (Brook et al., 2010). Third, it is burdensome and complex to develop appropriate datasets, models, and interpretative outputs needed for dispersion modeling, health impact assessments, and other purposes. Fourth, this complexity results in long model run times that limits the number of scenarios that can be evaluated. As a result of these challenges, optimal strategies might not be identified, and in regulatory applications, missing such strategies could result in the rejection of the air quality plan or other undesirable economic, legal or health ramifications.

Many approaches have been used to address the challenges mentioned above. For the challenge of allocating emissions reductions among multiple sources, optimization approaches can identify strategies that minimize emissions reductions, control costs or other functions, while meeting technical and other constraints. Early studies focused on minimizing costs of emission controls while keeping pollutant concentrations below threshold values (Kohn, 1969; Kyan and Seinfeld, 1972; Cass, 1981). Others focused on administrative controls and optimized dispatch schedules to minimize pollutant concentrations during periods of adverse meteorology (Sullivan and Hackett, 1973). A game theory model balanced economic motivations of stakeholders (e.g., polluters, the public and regulators), rather than cost-minimization alone (Bird and Kortanek, 1974). Acid rain problems in Europe and the US were addressed with a suite of new optimization approaches. In Europe, the Regional Acidification INformation and Simulation (RAINS) model used optimization to meet several constraints including critical loads, which are spatially-varying deposition targets (Alcamo et al., 1990; Batterman, 1992). In the US, a multi-objective approach attempted to achieve an equitable distribution of impacts across stakeholders, as well as reduce deposition (Ellis, 1988). Markets for sulfur dioxide (SO_2) and nitrogen oxides (NO_x) emissions were evaluated using optimizations that incorporated costs and incentives of various abatement methods (Winebrake et al., 1995; Farrell et al., 1999). The growing concentrations of greenhouse gases stimulated the development of the Greenhouse Gas and Air Pollution INteractions and Synergies (GAINS) abatement optimization model (Wagner et al., 2007). Least-cost optimization at the regional scale has been used to address $PM_{2.5}$ and O_3 issues in several major eastern US cities (Liao and Hou, 2015). Overall, most optimized air quality management strategies have minimized emissions reductions or control costs, and to date few have considered public health impacts (Kan et al., 2004).

Air quality management analyses using health impact assessments (HIAs) and related techniques estimate the burden of disease attributable to air pollutant exposure. Spatially-resolved HIAs, which account for the susceptibility and vulnerability of subpopulations as well as the variation in concentrations, can apportion the burden to specific emission sources or source classes (Fann et al., 2013). The US EPA Benefits Mapping and Assessment Program (BenMAP), which is used in regulatory impact analyses (RIAs) to estimate impacts of changes in ambient air quality (US EPA, 2015a), might be customized to fit urban, regional or national scales and match available input data (Hubbell et al., 2009). However, incorporating HIA methods into air quality management is non-trivial. HIAs require spatially-resolved data regarding exposure, vulnerability, demographics, disease incidence rates and other information, which are collected at different scales using different geographic units (e.g., Census blocks and ZIP codes). These data often change over time, and quickly in some cases. The lack of suitable spatially- and temporally-resolved data can restrict the ability of HIAs to differentiate the health impacts of alternative emission scenarios (Hubbell et al., 2009). In addition, these analyses can be computationally intensive, requiring estimates and mapping of concentrations and other data at potentially high resolution over long periods of time.

This paper presents a modeling framework, called the “Framework for Rapid Emissions Scenario and Health impact ESTimation” (FRESH-EST), which incorporates dispersion modeling, elements of HIA and optimization analyses into air quality management. FRESH-EST rapidly estimates concentrations and health impacts of alternate emissions scenarios at the urban scale, and gives results comparable to standard EPA models such as AERMOD. It incorporates optimization modules to identify strategies that meet cost, environmental and health constraints, and it provides a convenient user interface. This new framework is demonstrated using an SO_2 non-attainment area in southeast Michigan, as described in a recently proposed SIP (MDEQ, 2015).

2 Methods

2.1 Overview

FRESH-EST combines several database and modeling elements to simulate point-source emissions scenarios and the resulting concentrations and health impacts. In brief, the framework starts with pollutant source data (emissions inventory), utilizes dispersion modeling to predict concentrations at discrete locations ('receptors'), performs rasterization and spatial averaging to map receptor concentrations to geographic units of interest, e.g., Census blocks, and then combines concentrations at geographic units with demographic, epidemiologic and other data to estimate environmental and health impacts. An optimization module identifies emissions scenarios that meet economic, environmental or health goals. The formulation and programming implementation allow rapid calculations and facilitates the development of optimized strategies that attain concentration limits in a cost-effective manner, meet health goals, or address health inequities. This following presents the framework and several illustrative applications.

2.2 Source emissions and dispersion modeling

The concentration of a pollutant can be predicted from multiple emission sources at the urban scale as:

$$R_{i,t}=\sum_j S_{i,j,t} Q_j + B_{i,t} \quad \boldsymbol{R}=\boldsymbol{S}\,\boldsymbol{Q}+\boldsymbol{B} \tag{1}$$

where $R_{i,t}$ = concentration (μg/m^3) at receptor i (geocoded location) and time t (hour), Q_j = emission rate (g/s) at source j, $S_{i,j,t}$ = concentration (μg/m^3) at receptor i that results from dispersion modeling of unit emissions (1 g/s) from source j at time t, and $B_{i,t}$ = background concentration (μg/m^3) at receptor i at time t. Elements of matrix $\boldsymbol{S}$ are equivalent to the transfer coefficient representing the physical and chemical processes affecting the pollutant from release at source j to receptor i at time t. While any dispersion model can be used, the application and case study (below) applies AERMOD (Cimorelli et al., 2004), a "guideline" model recommended by US EPA. Eq. (1) estimates the contribution from local sources, and adds "background" concentration $B_{i,t}$ for other sources, e.g., those outside the modeled domain. Background levels can be significant (e.g., often the case for $PM_{2.5}$), or low and potentially negligible (e.g., CO, SO_2). Assumptions allowing the use of eq. (1) are that the modeled pollutant is conservative or first-order, and that emission rate changes do not substantially change pollutant dispersion. In this case, matrix $\boldsymbol{S}$ is independent of the emission rate. For conservative or nearly conservative pollutants (no significant transformation at the urban scale), the same $\boldsymbol{S}$ can be used. In this case, matrix $\boldsymbol{S}$ is also independent of pollutant. Otherwise, several sets of $\boldsymbol{S}$ may be required.

2.3 Estimating geographic unit concentrations

FRESH-EST estimates concentrations in the desired geographic units (e.g., ZIP codes, Census blocks) using spatial averaging or rasterization of receptor concentrations ($\boldsymbol{R}$). Several approaches are needed. For large geographic units (e.g., ZIP codes), simple spatial averaging can be used as each unit contains many modeled receptors (Pebesma, 2016). For small geographical units (e.g., Census blocks), such averaging may not be appropriate; some geographic units may contain few or no receptors within their borders. In this case, FRESH-EST uses a series of steps in a rasterization method similar to earlier work (Batterman et al., 2014). First, a modified inverse distance interpolation formula calculates distance weights between receptor *i* to centroids of raster grid *k* that has fine spatial resolution (Shepard, 1968):

$$D_{i,k}=(d^{p}{}_{i,k}\sum_{j'}\{1/d^{p}{}_{i*,k}\})^{-1} \quad (2)$$

where $D_{i,k}$ = unit-less distance weighting of receptor *i* to raster centroid *k*, $d^{p}{}_{i,k}$ = Euclidean distance *d* from receptor *i* to raster centroid *k* raised to power *p* (*p* = 2), and *i** = a receptor in the set of receptors *i'* that are within a user-defined range of each raster centroid (the default range is the largest nearest-neighbor distance in the receptor grid). Second, area-weights of raster cells to the geographic unit are found by dividing each raster cell into 100 sub-cells and counting the number of sub-cell centroids within the boundaries of nearby units (Hijmans, 2015). The percentage of each unit area attributed to nearby raster cells is calculated, and these area weights compose raster-unit mapping matrix ***A***. Finally, ***D***, the distance weight receptor-raster mapping matrix, and ***A***, the area weight raster-unit mapping matrix, are multiplied and transposed to create ***M***, the receptor-unit mapping matrix, which allows calculation of concentrations at the geographic unit of interest, ***C***, directly from receptor concentrations ***R*** in eq. (1):

$$\boldsymbol{C}=\boldsymbol{M}\ \boldsymbol{R}=(\boldsymbol{D}\ \boldsymbol{A})^{\mathrm{T}}(\boldsymbol{S}\ \boldsymbol{Q}+\boldsymbol{B}) \quad (3)$$

M depends only on the locations of receptors and geographic units and ***S*** reflects the transfer of emitted pollutants from emitting stack to receptor. Since ***M*** and ***S*** are independent and invariant of ***Q***, calculating ***C*** for a new scenario requires only a new ***Q***. Note that calculating ***R*** for a new scenario does require re-calculation of eq. (1).

For the greatest efficiency, eq. (3) can be expressed as:

$$\boldsymbol{C}=\boldsymbol{M}\ \boldsymbol{S}\ \boldsymbol{Q}+\boldsymbol{M}\ \boldsymbol{B} \quad (4)$$

An example using the case study application (described below) illustrates the efficiency of this formulation. In the case study, the dimensions of the matrices in eq. (3) are defined by 11 emission sources, 3,967 receptors, 3,242,001 raster cells, 74 geographical units (ZIP codes), and 8760 hours. Considering a moderately-sized problem, asthma exacerbations at the ZIP code level associated with annual average SO_2 concentrations, ***S*** is reduced to a 2-dimensional matrix of annual average receptor concentrations that result from unit emissions. Thus, the first group of variables on the right-hand side of eq. (3) becomes $(\boldsymbol{D}_{(3{,}967 \times 3{,}242{,}001)}\ \boldsymbol{A}_{(3{,}242{,}001 \times 74)})^{\mathrm{T}}\ \boldsymbol{S}_{(3{,}967 \times 11)}\ \boldsymbol{Q}_{(11 \times 1)}$. Precomputing and saving $(\boldsymbol{D}\ \boldsymbol{A})^{\mathrm{T}}$ ***S*** gives a matrix with dimensions of only (74 × 11), which requires only 814 multiplications for each optimization iteration, a tremendous computational savings over the 9.52×10^{11} multiplications required to compute eq. (3) and the 3.23×10^{6} multiplications required if $\boldsymbol{M} = (\boldsymbol{D}\ \boldsymbol{A})^{\mathrm{T}}$ is pre-computed.

2.4 Estimating health impacts

Health impacts for selected health outcomes and populations are derived using established health impact assessment methods (US EPA, 2015a). Health impact functions (HIFs), which estimate the number of cases attributable to pollutant exposures, are derived from expressions for relative risk and four parameters: the concentration-response (CR) coefficient for the pollutant-outcome pair; the baseline incidence rate for each health outcome; the exposure concentration; and the number of people exposed. Inputs should be spatially-resolved to the finest scale to reflect variability among subpopulations in a study area (Hubbell et al., 2009), but coarser data can be downscaled if necessary.

The form of the HIF is typically log-linear or logistic, depending on the underlying model used to generate the CR coefficient. For log-linear models, the estimated number of cases ΔY_u in geographic unit u attributable to ambient concentration C_u is:

$$\Delta Y_u = y_{0,u}(1 - \mathrm{e}^{-\beta\, C_u})\, P_u \quad (5)$$

where $y_{0,u}$ = unit-level health outcome baseline incidence rate (e.g., asthma exacerbations per person), β = CR coefficient for the pollutant-outcome pair (e.g., units are 1/ppb in the case study), C_u = unit concentration for unit u (e.g., units are ppb in the case study), and P_u = relevant exposed population in geographic unit u (US EPA, 2015a). For logistic models, the number of attributable cases is:

$$\Delta Y_u = y_{0,u}(1 - 1/\{[1 - y_{0,u}]\,\mathrm{e}^{\beta\, C_u} + y_{0,u}\})\, P_u \quad (6)$$

Both log-linear and logistic models are incorporated into FRESH-EST.

2.5 Optimizing air quality management strategies

FRESH-EST employs non-linear optimization modules, available through nlopt (Johnson, 2010) and accessed using the R package nloptr (Ypma, 2014), to optimize emission scenarios subject to economic, concentration and health constraints. The case study described below demonstrates the following two optimization strategies.

First, to minimize emission reductions required to meet a target concentration, R^*, e.g., an air quality standard, at all receptors, the objective function, constraints and bounds are:

$$min \sum_j (Q_{j,0} - Q_j) \quad (7a)$$

$$f_4\,(\boldsymbol{R}^{'}) \le R^* \quad (7b)$$

$$0 \leq Q_j \leq Q_{j,0} \quad \text{(7c)}$$

where $f_4(\cdot)$ = function returning the largest 4th highest daily 1-hour maximum concentration across all non-fence-line receptors (i.e., the “design” concentration), and $Q_{j,0}$ and Q_j = the initial and current emission levels at source *j*. This formulation considers receptor concentrations only, thus, mapping matrix ***M*** is not used. The use of f_4 reflects the current form of the SO_2 NAAQS.

The second optimization minimizes the maximum concentration under a constraint that the emissions summed across the facilities are not less than those in the proposed SIP case, designated as Q^* (g/s). In this case, the optimization tries to obtain a better environmental outcome for the same level of emissions, with the following objective function and constraint:

$$min\ f_4\ (\boldsymbol{R}^{'}) \quad \text{(8a)}$$

$$\sum_j Q_j \geq Q^* \quad \text{(8b)}$$

The same bounds on emissions at each source in eq. (7c) are also used. The rationale behind these two optimization strategies is further described in Section 4.1.

Both optimization strategies used the Constrained Optimization BY Linear Approximation (COBYLA) non-linear optimization algorithm (Powell, 1994) with a relative emission tolerance of 10^{-4} (stopping the optimization if each emission value changed by less than 10^{-4} in an iteration), and a relative constraint tolerance of 10^{-8} (similar to the relative emission tolerance). No stopping criteria were used for the absolute emission tolerance, objective function stopping value, absolute or relative changes in objective function value, number of iterations, or optimization time.

2.6 Interface and implementation

FRESH-EST uses an R-Shiny (Chang et al., 2015) interface to interact with primary framework components. To generate ***R*** , this interface packages together the desired metric, i.e., annual average, daily 24-hour average, or daily 1-hour maximum concentrations, the pollutant, daily background concentrations (***B***), and a vector of emission factors (***Q***). These inputs are passed to a FORTRAN subroutine that applies ***Q*** to the unit emission concentration matrices (***S***) and generates new spatial profiles. FORTRAN was selected to maximize processing speed and because it allows simultaneous references to a single file, which enables the subroutine to run efficiently on multiple cores or clusters (using the R package parallel (R Core Team, 2015)). The emission factor application subroutine returns a matrix of (hourly) concentrations at receptors in the receptor grid (***R***).

Options for the objective function and constraints of the optimization subroutine also are accessed using the R-Shiny interface.

The R-Shiny interface incorporates functions to calculate and map health outcomes and potentially affected populations. These functions access user-prepared comma separated files containing concentration-response coefficients, unit-level population counts and health data, and other data. The generated maps allow for quick visual screening of results and can be easily saved for use in presentations or papers.

3 Case study

3.1 Overview

A full scale "real-world" demonstration of FRESH-EST is presented for Detroit and areas of southeast Michigan. This area is highly industrialized, densely populated, and a portion has been classified as non-attainment for SO_2. A proposed SO_2 SIP (MDEQ, 2015) presents several SO_2 emission scenarios. Detroit residents are susceptible to adverse effects of pollutants, e.g., 13.7% of adults in 2005 had asthma (much higher than state and national norms (Wasilevich et al., 2008; US Census Bureau, 2015a, b; DeGuire et al., 2016)). Many Detroit residents are vulnerable, e.g., 32.5% of residents earned below the federal poverty level and subsequently may be less able to respond to or mitigate high exposures (O'Neill et al., 2012). Further, over 80% of Detroit residents are non-white, and minority populations, especially children, in urban areas can suffer increased risk of health effects associated with air pollution (Pope and Dockery, 2006). This situation warrants examination of a comprehensive set of emission scenarios and associated health impacts.

FRESH-EST is used to simulate four cases: the base case (2012 emissions), the proposed SIP case (SIP), and two optimized strategies (OPT1 and OPT2). Changes in emissions, concentration, and health benefits (i.e., reduction in adverse health outcomes) are compared for these four cases. We also evaluate the computational efficiency of FRESH-EST.

3.2 Emissions cases

Sources in the case study were drawn from an emission inventory generated by the Michigan Department of Environment Quality (MDEQ) as part of the SO_2 SIP process (MDEQ, 2015). The inventory contains allowable and actual (2012) emissions for 70 stacks at the 9 largest SO_2 facilities in the southeast Michigan area. These facilities are major sources (annual actual emissions in 2012 exceeding 100 tons of SO_2). The inventory included stack location, height, diameter, exit gas temperature and velocity, and annual average emission rate. The proposed SIP case reduced emissions at 20 of 70 stacks; of these 20, we identified the 11 largest and closest sources to Detroit. The design concentration, i.e., the largest 4th highest daily 1-hour maximum concentration at non-fence-line receptors, predicted using the 11 stacks closely matched the design concentration that was predicted using all 70 sources. The 11 stacks represented 79% of the actual 2012 emissions from the MDEQ SIP inventory (90% by excluding DTE Monroe, a distant source which contributes only modestly to SO_2 in the non-attainment area) and includes large stacks at the Carmeuse Lime & Stone manufacturing plant, DTE River Rouge and DTE Trenton Channel coal-fired power plants, and the Hot Strip Mill (HSM) reheat furnaces at the US Steel steelmaking plant in Ecorse. The 9 blast furnaces at the US Steel facility on Zug Island were modified in the proposed SIP but were excluded in our analysis (these sources totaled only 919 tons SO_2/year. The 11 stacks modeled for the case study emitted a total of 94,394 tons SO_2/year.

Case 1 (“Base”) used maximum allowable emissions, and thus represented current worst-case conditions. Case 2 (“SIP”) used the proposed SIP strategy, developed by MDEQ using Reasonably Achievable Control Technology (RACT) analyses, AERMOD dispersion modeling, emissions limitations negotiated between MDEQ and polluters (summarized in Table 1) (MDEQ, 2015), and maximum allowable emissions under the proposed emission limits; this represents a future worst-case condition designed to attain the NAAQS. Case 3 (“OPT1”) minimized total emission reductions from the base case (summed across the modeled sources) with the constraint that R* (design concentration from the proposed SIP case) was not exceeded (eqs. 7a-c). Case 4 (“OPT2”) minimized the design concentration, subject to an emission floor Q* (the total modeled emissions from the SIP case) (eqs. 8a-b).

3.3 Dispersion modeling

Hourly concentrations (coefficients of transfer matrix $\boldsymbol{S}$) were predicted using AERMOD (Version 8.1.0) and pre-processed 2012 AERMET (minute) meteorological data from the Detroit Metro Wayne County Airport. The receptor network (3967 receptors) combined two grids: a grid with 200 m spacing near SO_2 sources in southwest Detroit, and a grid with 1000 m spacing that spanned most of Wayne County containing Detroit (Figure 1). Following MDEQ’s implementation, certain sources were designated as urban. The “source group” function of AERMOD was used to generate unformatted binary files of hourly concentrations at the receptors for each of 70 stacks (resulting in 70 files totaling 18.1 GB).

3.4 Health impact estimation

Health impacts were estimated for SO_2 concentrations due to local point sources following methods in the recent SO_2 RIA (US EPA, 2010); exposures and health impacts from secondary $PM_{2.5}$ were not considered. Due to data availability, ZIP codes were chosen as the geographical unit. The study domain contained 74 ZIP codes. The average concentrations within the ZIP code was obtained using the “simple spatial averaging” option of FRESH-EST.

Health outcomes, HIFs and CR coefficients were selected on the weight of evidence of a causal relationship with SO_2 (US EPA, 2008, , 2015a) and included asthma exacerbations (as one or more asthma-related symptoms, children ages 6-14), emergency department (ED) visits for asthma (children ages 0 – 17), asthma hospitalizations (ages 0 – 64), and chronic obstructive pulmonary disease (COPD) hospitalizations (ages ≥ 65 years) (Table 2). Each HIF uses 24-h average SO_2 concentrations. ZIP codes-specific baseline rates of asthma hospitalizations and ED visits in Detroit used the Epidemiology of Asthma in Michigan report (DeGuire et al., 2016); county-specific rates were used for ZIP codes outside of Detroit (MDHHS, 2014, 2016). For asthma exacerbations (6 – 14 years), an incidence rate of 0.412 cases per person-day is used (Batterman et al., in preparation). Population data were obtained from the 2010 Census (US Census Bureau, 2015a). The population of each ZIP code was age-stratified using 2010 Detroit data (MDHHS, 2015). The prevalence of asthma in Wayne County was used to estimate the population with asthma (AIM, 2014). Asthma or COPD hospitalizations, asthma ED visits, and asthma exacerbations attributable to SO_2 exposure were calculated for subpopulations in age groups of 6 – 14, 0 – 17, 0 – 64, and 65 and older years of age, depending on the outcome.

4 Results

4.1 Emissions comparisons

The final emission reductions in the proposed SIP (Table 3) resulted from months of negotiations involving discussions of feasibility, legal considerations and RACT analyses, while OPT1 and OPT2 are solutions to a set of emission and concentration constraints. In this regard, these alternative emissions reduction strategies are not directly comparable. However, the purpose of the case study was to demonstrate the utility of FRESH-EST using a realistic full-scale application, which OPT1 and OPT2 provide. OPT1 converged after 485 iterations to a final cumulative emission rate slightly below that of the SIP case (2.1% difference, 1,113 tons/year); OPT2 converged after 216 iterations with the same cumulative emission rate as the SIP case.

As expected, the largest differences in emission reductions came at Carmeuse Lime and DTE Trenton Channel, i.e., the only facilities that proposed physical modifications. Under the proposed SIP, Carmeuse Lime would construct a new and taller stack to vent the combined emissions from its two kilns. The short existing stacks at Carmeuse Lime were identified as a cause for the high SO_2 concentrations near the facility, thus a taller stack was proposed that will increase dispersion, reduce local impacts and permit a higher combined emission rate from both kilns (MDEQ, 2015). The RACT analysis in the proposed SIP indicates that constructing a new stack is the most cost effective strategy for this facility; our analysis did not consider the cost to the polluter. Stack construction has different implications compared to the emission reduction strategy in the FRESH-EST; OPT1 and OPT2 strategies reduced the combined emissions from the two kilns by 511 and 693 tons/yr, respectively (representing 45 and 61% reductions from the base case).

At the DTE Trenton Channel electrical generating unit, the proposed SIP would shut down four of the smaller coal-fired boilers (boilers 16-19, total capacity of 3,012 MMBTU/hr); emissions at the fifth and largest boiler, called 9A (4,530 MMTBU/hr), would be unaffected. Although the SIP does not describe the shuttering of boilers, recent MDEQ dispersion modeling files and proposed permits show boilers 16-19 being replaced by five natural gas units (MDEQ, 2016). By comparison, OPT1 reduced emissions at boilers 16-19 and 9A by 30 and 66%, respectively; OPT2 reduced emissions by 37 and 58%, respectively. As at Carmeuse Lime, the optimized strategies did not involve cost estimates. The impending Mercury and Air Toxics Standards regulations (MDEQ, 2016) may make shuttering and replacing these boilers the most cost effective option for the utility.

Both optimization scenarios achieved concentration reductions comparable to those in the SIP without building or modifying emission sources. This indicates the potential for optimized strategies to expand the set of alternatives considered in emission reduction negotiations.

4.2 Concentration comparisons

The predicted SO_2 design concentration in the proposed SIP case was 79.2 ppb, designated R^* and used in OPT1. R^* exceeds the current NAAQS (75 ppb), and is only used to compare the base case and alternative emission scenarios. Several factors affect the determination of R^*. First, the case study did not consider background concentrations; the proposed SIP derived a background concentration of 15 ppb to be added to modeled design concentrations ((MDEQ, 2015). Second, the NAAQS is defined as a three-year average of the annual 4th highest daily 1-hour maximum concentration at a monitor, not a 1-year value. Third, placement of fence-line receptors can influence whether the standard is attained, and the SIP and case study use slightly different receptor grids. Fourth, MDEQ s justification for allowing some receptors to exceed the standard is that not all sources will emit maximum emissions, and that all facilities are unlikely to simultaneously emit at the maximum rate. This said, the case study was intended to demonstrate capabilities of FRESH-EST and not to demonstrate strategies that attain NAAQS compliance.

The distributions of concentrations across receptors in optimized and SIP cases are compared in Table 4. The maximum 4th highest 1-hour concentrations show similar distributions, e.g., percentile values for the SIP, OPT1 and OPT2 cases were different by an average of 4.6% (3.6 ppb). Differences were greater for daily 24-hour average concentrations, e.g., the SIP case decreased concentrations from the base case by an average of 46% (excluding the minimum and maximum concentrations); OPT1 and OPT2 decreased concentrations by an average of 52 and 58%, respectively. While the SIP, OPT1 and OPT2 strategies all achieved the same design concentration, the optimized strategies also reduced daily average concentrations, an important metric since it is used to calculate health impacts attributable to SO_2 exposure (Section 4.3).

The spatial pattern of average daily 24-hr (non-fence-line) concentrations at the ZIP code level is shown in Figure 2. The greatest reduction in near major sources, e.g., in the 48217 ZIP code, which has been called Michigan's (and at times, the nation's) "most polluted" ZIP code (Lam, 2010). The two optimizations reduced average 24-hr SO_2 levels in this area by 52 to 56%, compared to 44% for the SIP case.

4.3 Health impacts

The numbers of cases of adverse health outcomes attributable to SO_2 exposure for the four cases are shown in Table 5. SO_2-related health effects were calculated using average daily SO_2 concentrations, so the spatial pattern of avoided health impacts matches the concentration reductions (Figure 2). Compared to the baseline, both SIP and optimized strategies reduce impacts significantly (by 45 to 52%). Benefits of the optimized strategies are most evident for avoided asthma exacerbations, e.g., OPT1 and OPT2 result in 2,613 and 3,859 fewer asthma exacerbations than the SIP case, representing reductions of 9.2 and 13.6%, respectively. These differences are a consequence of the spatial pattern of SO_2 exposure at the ZIP code level (Figure 2) applied to the population density and vulnerability risk factors in Detroit. Although both optimized strategies resulted in fewer health impacts than the SIP case, they do not account for the political and legal factors issues in the SIP case. Nevertheless, these results indicate the potential for optimized strategies to expand the set of alternatives considered in emission reduction negotiations.

4.4 Computational efficiency

FRESH-EST calculations are far faster than the routine implementation of AERMOD, GIS, and R calculations. For example, each iteration of the case study optimization (applying FRESH-EST with 11 sources, 3967 receptors, and 8760 hours) required 11 sec on a workstation (equipped with 8 GB RAM, 64 bit Windows 7 ™ OS, Intel® Core™i7-2600 CPU operating at 3.40 GHz with 4 physical cores and 8 logical cores; roughly 1 sec per source). In comparison, about 6 min was required for the comparable AERMOD run (33 sec per source). While an initial AERMOD run is required to calculate $\boldsymbol{S}$, FRESH-EST does not require further AERMOD runs (if stack parameters other than emission rate do not change significantly). Additional efficiencies are attained by common use of the mapping matrix $\boldsymbol{M}$ for each receptor-unit pairing for health impact calculations; this implementation shortens a calculation conventionally requiring hours to a few minutes. Gains are greatest in health or inequity optimization problems that require concentrations in geographic units like Census blocks or ZIP codes, e.g., using an existing $(\boldsymbol{D}\,\boldsymbol{A})^{\mathrm{T}}\,\boldsymbol{S}$ matrix allows several thousand iterations in minutes. The FRESH-EST approach makes relatively complex and large scale optimizations feasible on an individual workstation.

4.5 Case study limitations

The case study was intended to demonstrate the capability of FRESH-EST to develop and evaluate emission strategies. The case study has several limitations that may restrict the broader relevance of certain conclusions. First, generating optimized emissions scenarios using goals or constraints based on emissions summed across stacks and facilities does not account for differences in control costs, technical feasibility, and economic and political viability. These factors that will vary by stack, facility and context, but cost or other functions and constraints could be added to the optimization to increase realism. Second, the spatial resolution of health impacts used ZIP codes, with the implicit assumption that these are homogenous geographic units, mainly due to limitations in the health data. Spatial distance weighting, rasterization and other approaches to increase the spatial resolution were not attempted. Third, health impact estimates were conservative, and did not consider effects of secondary particulate matter (PM) due to SO_2 emissions, or emissions and exposures of other pollutants emitted by the same facilities. This is important since the relationship between $PM_{2.5}$ exposure and asthma (and other outcomes) is stronger than for SO_2, and nationwide impacts due to secondary $PM_{2.5}$ may exceed those of SO_2 alone (US EPA, 2010). Future versions of FRESH-EST may be able to estimate health effects due to secondary PM, as modeling of SO_2 to particle formation is a potential option in future AERMOD versions (US EPA, 2015b). Health impacts from additional pollutants are easily incorporated into FRESH-EST. In addition, the health impact estimates utilized baseline health rates at the county- or study-wide level, which may not reflect the variability in health and vulnerability at the ZIP code (or finer) level. Fourth, we did not consider equity implications of the emission control strategies. Fifth, the case study considered only four facilities, three of which were close together. While representing the configuration of the major SO_2 sources in Detroit, this situation will limit differences between optimized control strategies and those with other goals. Potentially much larger differences may result if the emission sources are more broadly distributed. Finally, a single point estimate is used for each CR coefficient. Incorporating the uncertainty of these coefficients would increase the magnitude the health impacts, especially for those CRs using log-linear models (Chart-Asa and Gibson, 2015).

5 Discussion

5.1 Overview

FRESH-EST varies from standard tools in several ways. It is not equivalent to the "source group" option in AERMOD that allows apportionments of pre-designated outputs. Rather, FRESH-EST evaluates the influence of sources and gives substantial flexibility with respect to emission rates. FRESH-EST also minimizes emission reductions, concentrations, or health effects using non-linear rather than linear optimization; linear optimization has been used in nearly all previous emission scenario modeling efforts (Amann et al., 2011; Thorneloe et al., 2007).

5.2 Advantages of FRESH-EST

The reduction in computational burden in FRESH-EST allows analyses that can enhance dispersion modeling applications. As examples: dispersion model applications might use simple uniform receptor grids rather than multi-tiered nested grids to identify hotspots; Monte Carlo-type uncertainty analyses addressing emission variability become much more feasible; and model runs using variable (e.g., historical) hourly emissions will run rapidly.

Similarly, the optimization module in FRESH-EST provides opportunities to examine and design emissions scenarios in novel ways, including ways that might be missed by conventional modeling setups. Optimization results can highlight differences between typical abatement strategies and other specific strategies. For example, some health effects in the case study were driven by emissions from smaller sources with poor dispersion that were close to vulnerable populations, rather than by emissions from much larger and distant sources with elevated stacks. Such results depend on city- and site-specific factors, and FRESH-EST can quickly reveal such relationships. Further, since essentially any set of optimization objectives and constraints can be applied, including considerations of emissions, concentrations and health, optimization results can better fit the goals and constraints informed by scientific, economic, and regulatory considerations.

FRESH-EST fills several regulatory needs in current frameworks and models. It simultaneously performs dispersion modeling, quantitative health impact estimation, optimization, mapping and tabulation functions, which normally require the use of various specialized software programs. Further, it allows users to perform "what if" analyses. Stakeholders do not need additional software or technical training to run FRESH-EST; rather, state agencies need only provide the modeling components: receptor grid, unformatted unit-emission binary outputs, and initial stack-level emissions. This added flexibility allows for expanded exploration of alternative emission scenarios and facilitates stakeholder involvement in the SIP process.

FRESH-EST provides an alternative to estimating health impacts from existing health risk assessment tools (Anenberg et al., 2015). Both FRESH-EST and the current EPA Regulatory Impact Assessment method, BenMAP (US EPA, 2015a) can be customized for analyses of health impacts at various spatial and temporal resolutions, including short time periods that are relevant for outcomes like asthma exacerbations and ED visits, and both can be used to design strategies that comply with specific design values relevant to the NAAQS. However, FRESHEST may be the preferred tool for SIP development and other applications for several reasons: it generates results for many emissions alternatives without requiring multiple modeling runs; it includes additional health impact metrics that may be of interest for urban-scale analyses, e.g., DALYs and inequality metrics; and its optimization module offers greater flexibility in the development of control alternatives. Compared to other health risk assessment tools (Anenberg et al., 2015), FRESH-EST uses user-defined local concentration-response relationships to estimate a range of health outcomes due to exposures to primary pollutants on the city-level to regional scale.

Spatially-resolved estimates of the health burden due to air pollutants, like those produced in FRESH-EST, provide information that can be used to identify emissions reduction strategies with the largest public health impact. This is particularly important for areas like metropolitan Detroit that have significant emissions sources and large vulnerable populations. For researchers and public health practitioners, FRESH-EST can generate information on the potential health impacts of exposures to ambient air pollutants at fine-grained scales and help inform plans to mitigate these impacts. An expanded discussion and analysis of FRESH-EST for use in regulatory frameworks and quantitative HIAs is forthcoming (Martenies et al., in preparation).

5.3 Limitations of FRESH-EST

Like any modeling system, FRESH-EST has a number of limitations. First, with respect to emissions, only point sources are considered, cost functions associated emission reductions are not used, and emission rates are time invariant. All of these limitations can be relaxed with appropriate inputs. FRESH-EST assumes that stack parameters are independent of emission rate, as discussed earlier. The verity of this assumption depends on the pollutant, local meteorology and emission magnitude. For example, dry electrostatic precipitators used to control PM emissions can operate at high temperatures (up to 700 °C (US EPA, 2003a)), and thus stack temperatures at the power plants in the case study (which range from 138 to 288°C) would not need modification. Wet flue-gas desulfurization systems used to control SO_2 emissions can operate from 149 to 371°C (US EPA, 2003b), and, similarly, stack temperatures would not require changes. In other cases, large temperature changes might affect plume rise and alter pollutant dispersion. Such changes, as well as changes in physical stack height, can be accommodated in FRESH-EST using a different transport matrix $\boldsymbol{S}$.

FRESH-EST does not model reactions among pollutants since eq. (1) linearizes the source-receptor relationship. Thus, concentrations of secondary pollutants that depend on atmospheric chemistry (e.g., O_3) cannot be modeled. Generally, this does not pose a significant limitation at the urban scale for SO_2, CO, PM_{10}, $PM_{2.5}$, Pb and many other pollutants. As noted earlier, first-order transformations that produce secondary pollutants may soon be modeled by AERMOD and thus could subsequently be incorporated in transfer matrix ***S***.

The HIA calculations in FRESH-EST (and most similar work) make several assumptions that may limit some applications. FRESH-EST does not consider population and disease dynamics (including trends). It omits health effects for which causal associations with air pollutant exposure have not been determined or which are highly uncertain (e.g., birth defects, cancer, and mortality). At present, only a single pollutant is considered in the optimization, although multiple pollutants may be evaluated using multiple runs.

5.4 Lessons from FRESH-EST development

The implementation of FRESH-EST involved several challenges with quickly reading and aggregating many gigabytes of binary data. Several examples are given. First, even the simplest FRESH-EST setup involved filling a large 3 dimensional matrix ($N_{SOURCES} \times N_{RECEPTORS} \times N_{HOURS}$); however, the workstation used could not allocate enough memory for the case study problem (options involving writing sections of the matrix to the hard-drive would drastically increase computation time and thus were not considered). Therefore, the algorithm was modified to read concurrently from several binary files using a local cluster (using cores of the local machine as cluster nodes), and create a new ***S Q*** matrix for each scenario. Second, using the above setup (i.e., each core on the local machine reading from a different binary file) the number of concurrent hard-drive reads exceeded the threshold that could be sustained at rapid speed. Ultimately, applications worked fastest when set up on a cluster consisting of 1 node that read from one binary file at a time. The remaining time-savings were accomplished by pre-calculating all matrices that were emission-invariant.

6 Conclusions

FRESH-EST is a flexible modeling tool that facilitate rapid tests of emissions and health scenarios and is suitable for a wide range of regulatory and scientific applications. In addition to developing strategies that meet NAAQS or other concentration objectives, FRESH-EST can be used in conjunction with health impact analysis or risk assessment techniques to investigate emission reductions strategies that best reduce the burden of disease while considering vulnerability factors, e.g., the population density, demographic factors, and existing disease rates. The case study results, in particular, the optimized emission strategies, can meet regulatory goals and improve health. Forthcoming work will apply FRESH-EST to develop air quality management strategies that improve health and equity (Martenies et al., in preparation), and we intend to distribute FRESH-EST (please email the corresponding author). This will permit additional applications, including those relevant to developing emission strategies, evaluating health impacts of alternative scenarios, and expediting the SIP process by the rapid development and evaluation of alternative control options.

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Highlights

- An integrated model, FRESH-EST, rapidly generates concentrations and health impacts
- FRESH-EST optimizes emission reduction strategies for environmental and health goals
- FRESH-EST optimizations met agency goals in a case study of an SO_2 SIP in Detroit, MI
- Optimized strategies can contribute to development of emission reduction scenarios

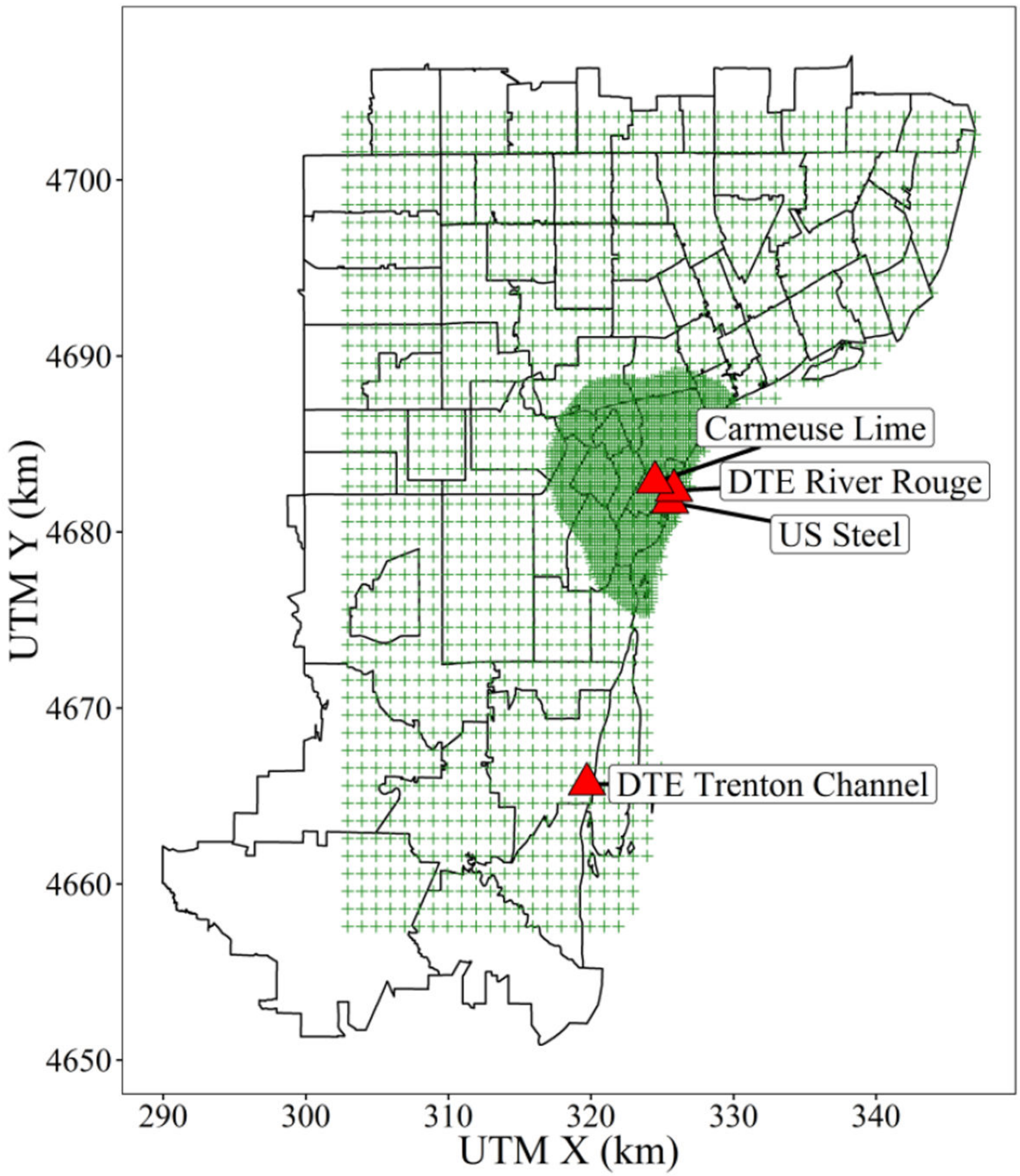

Figure 1.
The ZIP codes, receptors (+) and facilities (▲) containing the 11 modeled stacks in the case study.

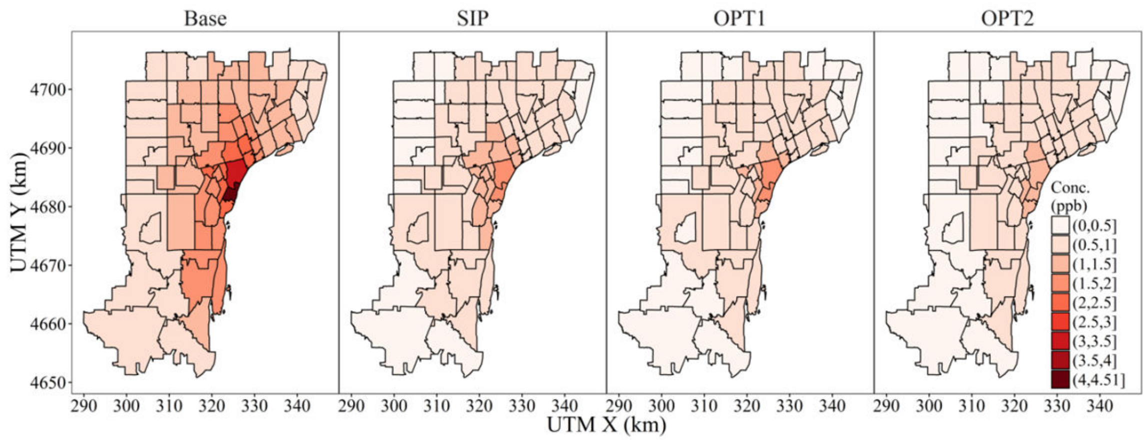

Figure 2.
Maps showing annual average SO_2 concentrations (ppb) at the ZIP code level for Base, SIP and two optimized cases.

Table 1

Summary of relevant control strategies employed and MDEQ-assigned average monitor violation contribution in the proposed SIP (MDEQ, 2015).

Source (% Contribution)	Control strategy
Carmeuse Lime (0.6%)	Construct a 100-foot standalone stack to vent emissions from both kilns. This taller stack will provide additional dispersion and accommodate a higher SO_2 emission rate.
US Steel Ecorse (42.0%)	The company proposal, to shut down boiler 4 in boiler house 1 and cap the coke oven gas used per month, was not accepted. As such, MDEQ gives with Draft Rule 430, which limits the combined emission rate from the HSM furnaces to 648 tons/year, among other constraints.
DTE River Rouge and Trenton Channel (38.4%)	Employ emission limits based on a 720-hour rolling average. DTE demonstrated that these longer term average limits were as stringent as the associated 1-hour limit. Lower sulfur coal will also be used.

Table 2

Adverse health outcomes, “at risk” population age groups (in years), HIF form, and concentration response (CR) coefficients (and standard errors, SE) included in the FRESH-EST health impact assessment database for SO_2. These SO_2-related outcomes use 24-h average SO_2 concentrations.

Outcome	Age group	HIF form	CR (SE)	Reference
Asthma hospitalizations	(0 – 64)	Log-linear	0.00203 (0.00259)	(Sheppard, 2003)
COPD hospitalizations	(65+)	Log-linear	0.02081 (0.01113)	(Yang et al., 2005)
Asthma ED Visits	(0 – 17)	Log-linear	0.00825 (0.00190)	(Ito et al., 2007)
Asthma ED Visits [†]	(0 – 17)	Log-linear	0.00976 (0.00287)	(Li et al., 2011)
Asthma exacerbations [a]	(6 – 14)	Logistic	0.00392 (0.00196)	(Schildcrout et al., 2006)
Asthma exacerbations [a†]	(6 – 14)	Logistic	0.01695 (0.00660)	(Batterman et al., in preparation)

[†]Detroit-specific concentration-response (CR) coefficients used in the Health Impact Functions (HIFs)

[a]Total cases of asthma exacerbation (as noted by cough, shortness of breath, wheeze etc.) Acronyms: COPD = Chronic obstructive pulmonary disease; ED = Emergency department

Table 3

SO_2 emission rates (tons per year, rounded to the nearest integer) for modeled stacks in the base, negotiated, and optimized (OPT1 and OPT2) cases.

Facility	Stack	Base	SIP	OPT1	OPT2
Carmeuse Lime [†]	Kiln 1	552	2,059	119	319
	Kiln 2	583	-	505	122
DTE River Rouge	Unit 2	15,768	9,021	9,040	7,813
	Unit 3	18,431	11,026	9,925	13,317
DTE Trenton Channel	HS Boilers [α]	22,110	-	7,506	9,368
	Unit 9	33,143	29,753	23,180	20,959
US Steel (Ecorse)	Furnaces [β]	3,807	653	1,125	614
Cumulative Emission Rate		**94,394**	**52,512**	**51,399**	**52,512**

[†] In the proposed SIP, the emissions from both kilns are channeled to a single taller stack

[α] The emissions from High Side (HS) Boilers 16-19 at DTE Trenton Channel are released from a single stack

[β] In the SIP case, each of the 5 Hot Strip Mill (HSM) Furnaces emits ~20% of the emissions from US Steel (Ecorse). In OPT1 and OPT2, HSM furnace emissions were optimized separately.

Table 4

SO_2 concentrations (ppb) at selected percentiles for daily 24-hour average and annual 4th highest daily 1-hour maximum concentrations at non-fence-line receptors for base, SIP, OPT1 and OPT2 cases.

	Daily 24-hour average							4th highest 1-hour maximum						
Scenario	**Min**	**10th**	**25th**	**50th**	**75th**	**90th**	**Max**	**Min**	**10th**	**25th**	**50th**	**75th**	**90th**	**Max**
Base	0.005	0.041	0.120	0.83	2.8	5.5	155.9	26.7	49.0	72.1	87.6	97.1	107.4	283.2
SIP	0.001	0.021	0.062	0.45	1.6	3.0	27.0	15.3	27.5	39.5	49.3	54.7	59.9	79.2
OPT1	0.002	0.019	0.056	0.39	1.4	2.7	40.5	14.3	26.2	38.4	46.4	51.2	56.3	79.2
OPT2	0.001	0.016	0.050	0.32	1.3	2.5	27.7	14.4	27.1	39.2	48.1	53.3	58.8	79.2

Table 5

Annual cases (rounded to the nearest integer) of various health outcomes resulting from SO_2 exposures in base, negotiated and optimized (OPT1 and OPT2) cases.

Health outcome	Age group	Base	SIP	OPT1	OPT2
Asthma hospitalizations	(0 – 64)	13	7	7	6
COPD hospitalizations	(65+)	84	47	43	41
Asthma ED Visits	(0 – 17)	166	92	83	79
Asthma ED Visits [†]	(0 – 17)	196	108	98	94
Asthma exacerbations [a]	(6 – 14)	12,006	6,588	5,981	5,692
Asthma exacerbations [a†]	(6 – 14)	51,681	28,415	25,802	24,556

[†] Detroit-specific concentration-response (CR) coefficients used in the Health Impact Functions (HIFs)

[a] Total cases of asthma exacerbation (as noted by cough, shortness of breath, wheeze etc.)

Acronyms: COPD = Chronic obstructive pulmonary disease; ED = Emergency department