

InMAP: A Model for Air Pollution Interventions

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Abstract

Mechanistic air pollution modeling is essential in air quality management, yet the extensive expertise and computational resources required to run most models prevent their use in many situations where their results would be useful. Here, we present InMAP (Intervention Model for Air Pollution), which offers an alternative to comprehensive air quality models for estimating the air pollution health impacts of emission reductions and other potential interventions. InMAP estimates annual-average changes in primary and secondary fine particle ($PM_{2.5}$) concentrations – the air pollution outcome generally causing the largest monetized health damages – attributable to annual changes in precursor emissions. InMAP leverages pre-processed physical and chemical information from the output of a state-of-the-science chemical transport model and a variable spatial resolution computational grid to perform simulations that are several orders of magnitude less computationally intensive than comprehensive model simulations. In comparisons run here, InMAP recreates comprehensive model predictions of changes in total $PM_{2.5}$ concentrations with population-weighted mean fractional bias (MFB) of -17% and population-weighted $R^2 = 0.90$. Although InMAP is not specifically designed to reproduce total observed concentrations, it is able to do so within published air quality model performance

criteria for total PM_{2.5}. Potential uses of InMAP include studying exposure, health, and environmental justice impacts of potential shifts in emissions for annual-average PM_{2.5}. InMAP can be trained to run for any spatial and temporal domain given the availability of appropriate simulation output from a comprehensive model. The InMAP model source code and input data are freely available online under an open-source license.

Introduction

Ambient air pollution is estimated to kill over three million people per year globally [1, 2]. Reducing air pollution and its impacts is therefore an important policy goal. However, it is often unclear *a priori* which potential emission reductions would be most effective in improving air pollution and health because the chemical and physical relationships between emissions of air pollutants and the ambient concentrations that result can be complex [3]. To assist in decision-making, air pollution models are often used to estimate the health effects of a range of hypothetical changes in emissions.

Eulerian Chemical Transportation Models (CTMs; examples: CAMx, [4]; CMAQ, [5]; WRF-Chem, [6]; GATOR-GCMOM, [7]) are powerful tools that can simulate the effectiveness of emission reductions at reducing air quality-related health impacts. Running CTM simulations generally requires dedicated experts or teams, and often is computationally expensive and time consuming. For example, a single simulation for annual exposure in the contiguous US with a 12 km spatial resolution can take days to run on a high performance computing system (i.e., a “super-computer”) [8].

The computational intensity and high degree of difficulty inherent in performing CTM simulations is a bottleneck for the rate at which air quality strategies can be evaluated, for the number of people who can perform such evaluations, and also therefore potentially the rate at which policies for improving air quality can be investigated, evaluated, potentially enacted. Therefore, there is a need for air quality models that are simpler to use; provide results more quickly than CTMs, while minimizing losses in predictive accuracy; and potentially can be run by outside experts. Here, we describe such a model.

The design of our new model reflects current understandings of the health impacts of air pollution:

1. Of the three million global deaths per year attributed to ambient air pollution,
26 approximately 95 % are caused by fine particulate matter ($PM_{2.5}$) [1, 2]. The
27 strongest predictor for these deaths is chronic $PM_{2.5}$ exposure over periods of
28 a year or more [9–11]. Therefore, a prediction of chronic exposure to $PM_{2.5}$ is
29 a good indicator of overall health impacts from air pollution.
30
2. $PM_{2.5}$ can travel long (e.g., intercontinental) distances but can also be highly
31 spatially variable near emissions sources. Additionally, $PM_{2.5}$ can be both directly
32 emitted (“primary”) and formed in the atmosphere (“secondary”). Models that
33 predict $PM_{2.5}$ exposure should consider all of these aspects.
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3. Air pollution-mediated health damages can be a major driver of overall
35 environmental externalities [12, 13]. Therefore, air pollution models that can be
36 used by non-air-pollution-experts can be beneficial.
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Numerous air quality models already exist that have lower operational difficulty
38 than CTMs [14–30]. As discussed in S1 Appendix, while each model type is well-suited
39 to certain use-cases, none are ideal for the specific use-case we are interested in: an
40 adaptable and updatable model for human health impacts of changes in air pollutant
41 emissions that can resolve intraurban gradients in pollution concentrations near
42 emissions sources, can track the long-range transport of pollution, and can be used by
43 non-specialists.
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Here we develop and apply a new approach, which we implement as the Intervention
45 Model for Air Pollution (InMAP). InMAP is designed to provide estimates of air
46 pollution health impacts resulting from marginal changes in pollutant emissions, such as
47 those resulting from new regulations. InMAP combines spatially-resolved
48 annual-average physical and chemical information derived from a state-of-the-science
49 CTM (WRF-Chem) with simplifying assumptions regarding atmospheric chemistry for
50 cases of marginal changes in emissions. InMAP is developed here to predict changes in
51 annual average exposure to $PM_{2.5}$; as mentioned above, that outcome is estimated to
52 cause 95 % of air quality-related mortalities. The model is also able to predict changes
53 in concentrations of several other pollutants. Features of InMAP include reductions in
54 computational cost relative to CTMs, yet with more spatially detailed results than are
55 available with existing reduced-complexity models, a variable-resolution grid that
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focuses on human exposures by employing higher spatial resolution in urban areas and lower spatial resolution in rural and remote locations and at high altitude; and the ability to account for spatially variable aspects of secondary PM_{2.5} formation while also being amenable to running many scenarios and theoretically simple enough for use by non-experts. InMAP is designed to be informed by the default output of a single CTM run, so CTM runs that were originally created for other purposes can be used to create InMAP inputs. To our knowledge, the modeling approach developed here is the first of its kind for air pollution. It was inspired by recent advancements in reduced complexity sediment transport modeling [31, 32].

Methods

Model formulation

The fate and transport of pollution in the atmosphere can be represented by a reaction-advection-diffusion equation:

$$\frac{\partial C_i}{\partial t} = \nabla \cdot (D \nabla C_i) - \nabla \cdot (\vec{v} C_i) + \sum_{j=1}^n R_{i,j} + E_i - d_i \quad (1)$$

where C_i is the concentration of one of n model pollutant species, D is a molecular diffusion coefficient (neglected here as a negligible source of chemical transport in the atmosphere compared to advection), \vec{v} is the wind vector, $\sum_{j=1}^n R_{i,j}$ is the net formation rate of species i from species j , E_i is pollutant emission, and d_i is pollutant removal via wet and dry deposition. InMAP estimates pollutant concentrations by estimating a steady-state solution to Eq. (1), yielding annual average pollutant concentration results. To do so, we replace each of the terms on the right-hand side of Eq. (1) with parameterizations suitable for numerical solution as described below.

InMAP solves Eq. (1) for model chemical species comprised of primary PM_{2.5}, volatile organic compounds (VOCs), secondary organic aerosol (SOA), sulfur dioxide (SO_x), particulate sulfate ($p\text{SO}_4$), oxides of nitrogen (NO_x), particulate nitrate ($p\text{NO}_3$), ammonia (NH₃), and particulate ammonium ($p\text{NH}_4$). InMAP assumes that primary PM_{2.5}, VOCs, SOA, and SO_x, NO_x, and NH₃ can be emitted directly; the other species are secondary products formed in the atmosphere. InMAP assumes atmospheric particle

diameter and density—which it only uses to calculate dry deposition rate—to be
constant at $0.3 \mu\text{m}$ and 1830 kg m^{-3} , respectively.

Spatial discretization

Air pollution model simulations with increased spatial resolution can potentially provide improved exposure predictions [33] and often yield higher overall health impact estimates [34, 35]. CTMs typically employ a regular (i.e., constant-resolution) horizontal grid; to increase spatial resolution over important areas they may use a small number of higher-resolution “nested” grids inside a lower resolution outer grid. InMAP instead employs a variable resolution rectangular grid where grid cell size varies throughout the domain. To focus computational resources on understanding exposures and health impacts, InMAP users can choose one of two grid cell size strategies. With the first option, grid cells are smaller in urban areas and larger in rural and remote areas. Horizontal resolution also varies with height: because horizontal variability in concentrations decreases with height above the ground, we employ a low-resolution horizontal grid for all cells above a specific height (here, set to approximately 1500 m). With the second option, grid cell size varies dynamically while the simulation is running based on gradients in population density and pollutant concentration. Fig 1 shows a result of applying the first option algorithm for grid cell sizes. In our simulations, we use a spatial domain that covers the contiguous US, southern Canada, and northern Mexico, with grid cell edge lengths ranging between 1 and 48 km. The results presented here use the second grid cell size algorithm as it tends to give shorter model run times, but both options yield very similar results. Both algorithms and sample run times are described in detail in S2 Appendix.

Temporal discretization

Instead of solving for pollutant concentrations at specific points in time using temporally explicit input data as CTMs do, InMAP directly estimates annual average pollutant concentrations using annual average input data and numerical integration. We selected this approach because, as mentioned above, the vast majority of monetized damages from air pollution are attributable to human mortality from chronic (annual or longer) exposure to PM_{2.5}.

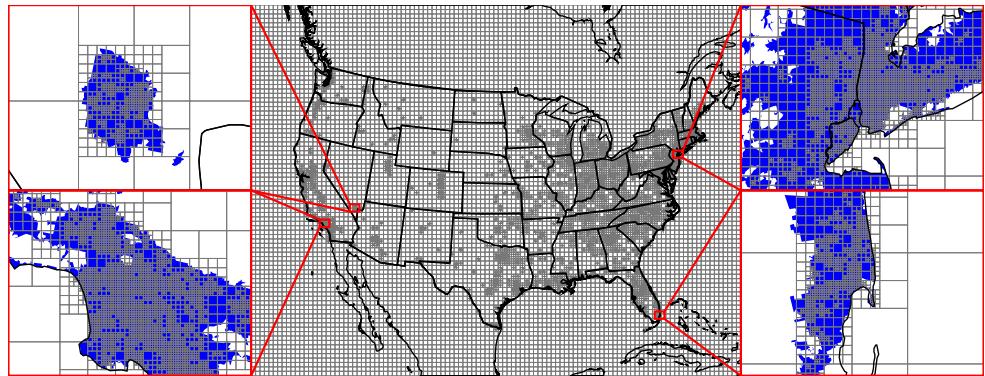


Fig 1. Spatial discretization of the model domain into variable resolution grid cells. The insets show the areas around the cities of Las Vegas, Los Angeles, New York, and Miami in detail. Blue shading represents urban areas as defined by the US Census.

To reach a steady-state solution, InMAP starts with an initial estimate of the changes in concentrations caused by an emissions scenario (the initial estimate is that there are no changes in concentrations) and iterates the model forward in time until the concentrations converge to a steady-state solution (i.e., until the predicted concentrations no longer change as the model continues to run). The integration time step Δt is chosen using the Courant–Friedrichs–Lewy condition [36] as in Eq. (2):

$$\Delta t = \frac{C_{\max}}{\sqrt{3}} \left(\max \left[\frac{|U_i| + |\tilde{U}_i|}{\Delta x_i}, \frac{|V_i| + |\tilde{V}_i|}{\Delta y_i}, \frac{|W_i|}{\Delta z_i} \right]; i = 1 \dots n \right)^{-1} \quad (2)$$

where C_{\max} is the maximum allowable Courant number (set to 1.0 for InMAP), the U , V , and W variables are annual average wind speeds in each grid cell i of n total grid cells as defined below, $|\tilde{U}_i|$ and $|\tilde{V}_i|$ are annual average absolute wind speed deviations as described below, and Δx , Δy , and Δz are the dimensions of each grid cell. With the model settings described here $\Delta t \sim 1$ min and is limited by the Courant number in the 1 km grid cells near ground level (typical annual average ground-level wind speed: 1 to 8 $m s^{-1}$). At the top of the model domain where wind speeds are relatively fast (up to 30 $m s^{-1}$ annual average), InMAP uses relatively large (48 km) grid cells to allow larger time steps. In contrast, in CTMs with constant-resolution grids, Δt is often limited by conditions in the top grid cells rather than at ground-level, so a 1 min time step typically corresponds to a horizontal resolution grid of 10 km. The net result is a similar Δt in InMAP as in a typical CTM (~ 1 min), but with smaller ground-level grid cells in InMAP relative to in a typical CTM.

During each time step in each grid cell, InMAP first adds the flux of new emissions, 125 accounting for plume rise from elevated sources [37] (as cited in [3]). The model then 126 calculates how changes in pollutant concentrations are affected by physical and chemical 127 processes including advection, turbulent mixing, atmospheric aerosol chemistry, dry 128 deposition, and wet deposition. Each process, with the exception of the instantaneous 129 gas- vs. particle-phase partitioning of organic, nitrate, and ammonia compounds, uses 130 an algorithm that calculates changes in concentrations based on the concentration at 131 the beginning of the time step rather than the concentration output by other process 132 algorithms during the same time step. Therefore, the concentrations resulting from 133 these steps do not depend on the order of process integration. The instantaneous 134 gas-particle partitioning, the result of which is theoretically influenced by the order of 135 integration, is performed last. 136

Input data

To reduce model complexity and runtime in the InMAP model itself, an InMAP 138 preprocessor uses the output of a more comprehensive model to extract emergent 139 atmospheric properties. Here, we use a previously published WRF-Chem model 140 simulation [8], but the preprocessor could also be adapted for use with other models and 141 configurations. The preprocessor makes it so that InMAP users do not need to access 142 the CTM results directly, only the results of the preprocessor are required to run the 143 model. InMAP uses WRF-Chem data in timesteps as output by WRF-Chem; for results 144 here the input data timestep is once per WRF-Chem simulation hour. 145

Many of the chemical and physical processes important to the fate and transport of 146 air pollution vary with the time of day and the season. A steady-state, annual-average 147 model risks being unable to represent the results of these temporally-explicit 148 phenomena. InMAP mitigates this potential limitation by using temporally explicit 149 information wherever possible when calculating annual average input properties. For 150 instance, the gas-phase oxidation of SO_2 to SO_4^{2-} is represented as the product of the 151 SO_2 concentration and a reaction rate constant, but the reaction rate constant has 152 a non-linear dependence on temperature and on the concentration of hydroxyl radical 153 (HO^*), both of which are temporally variable. To represent the formation of particulate 154 SO_4 ($p\text{SO}_4$), InMAP needs an annual average rate constant. To capture some of the 155

effects of temporal variability, instead of calculating the rate constant using annual average values for temperature and HO*, we instead use temporally explicit temperatures, solar radiation intensities, and HO* concentrations to then calculate rate constants for every hour during the year, and then take the average of these 8760 rate-constant values. Thus, the reaction rate InMAP uses for a given grid cell is an annual-average rate, not a rate calculated using annual-average values for input parameters.

In addition to SO₂ oxidation rates, information collected or inferred from the comprehensive model includes spatially explicit annual averages of wind vectors, eddy diffusivity and convective transport coefficients (annual average coefficients calculated using temporally explicit wind speed, temperature, pressure, friction velocity, boundary layer height, and heat flux information), dry and wet deposition rates of various pollutants (annual average rates calculated using temporally explicit wind speed, land cover, stability, and precipitation information), gas/particle phase partitioning for pollutants (described below), and parameters relevant to the calculation of emissions plume rise (annual averages of scalar windspeed; windspeed to the powers of -1, -1/3, and -1.4; temperature; and two parameters related to atmospheric stability). A full list of WRF-Chem variables used by the InMAP preprocessor is available in S1 Table.

Advection

The wind velocity that is responsible for advection ($\nabla \cdot (\vec{v}C)$ in Eq. 1) varies at time scales smaller than can be resolved by InMAP or by comprehensive CTMs. Therefore, variables \vec{v} and C in the advective transport term of Eq. (1) are commonly split up into resolved and unresolved components using Reynolds decomposition. CTMs typically split each variable x into two parts: one representing the average quantity of the variable during a model timestep (\bar{x}) and one representing the variability of the variable during the same timestep (x'). For InMAP to make predictions based on annual average information, it splits each variable into three parts instead of two: $\vec{v} = \bar{\vec{v}} + \tilde{\vec{v}} + \vec{v}'$ and $C = \bar{C} + \tilde{C} + C'$, where \bar{v} and \bar{C} represent annual average quantities, \tilde{v} and \tilde{C} represent deviations from the annual average that are temporally resolved by the underlying CTM (WRF-Chem in this case), and v' and C' represent deviations that are not temporally resolved by the underlying CTM. Substituting these decomposed variables into the

advection term of Eq. (1) and applying the rules of Reynolds averaging yields Eq. (3). 187

$$\nabla \cdot (\vec{v}C_i) = \nabla \cdot (\bar{v}\bar{C}_i) + \nabla \cdot (\tilde{\vec{v}}\tilde{C}_i) + \nabla \cdot (\vec{v}'\tilde{C}_i) + \nabla \cdot (\tilde{\vec{v}}C'_i) + \nabla \cdot (\vec{v}'C'_i) \quad (3)$$

InMAP discretizes $\nabla \cdot (\bar{v}\bar{C}_i)$ using the upwind advection scheme shown in Eq. (4): 188

$$\frac{\Delta C_i}{\Delta t} = \begin{cases} \frac{\sum_{w_j=1}^{n_{w,i}} U_i C_{w_j} f_{w_j}}{\Delta x}, & \text{if } U_i \geq 0 \\ \frac{\sum_{w_j=1}^{n_{w,i}} U_i C_i f_{w_j}}{\Delta x}, & \text{if } U_i < 0 \end{cases} \quad (4)$$

where ΔC_i is the change in volume-specific pollutant concentration in grid cell i caused by advection between cell i and each cell w_j of $n_{w,i}$ adjacent cells to the West during time step Δt . Because grid resolution varies, each cell may have more than one adjacent cell in each direction. U_i is the annual average wind velocity vector component in the East–West direction at the interface between cells i and w_i , C_i and C_{w_i} are concentrations in their respective grid cells at the beginning of the time step, f_{w_j} is the fraction of the edge of grid cell i that is touching neighbor w_j , and Δx_i is the length of the grid cell in the East–West direction. Eq. (4) is repeated for neighbors to the East, to the South, to the North, above, and below cell i . 189
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We chose the upwind advection scheme for its computational efficiency. A limitation of this scheme is that it is numerically diffusive, but this limitation is mitigated in InMAP because the variable resolution model grid uses smaller grid cells in high-population areas and thus limits numerical diffusion in the areas where accurate predictions are most important. 198
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InMAP parameterizes $\nabla \cdot (\tilde{\vec{v}}\tilde{C}_i)$ using the diffusion-like symmetrical advection scheme shown in Eq. (5): 203
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$$\frac{\Delta C_i}{\Delta t} = \frac{\sum_{w_j=1}^{n_{w,i}} |\tilde{U}_i| (C_{w_j} - C_i) f_{w_j}}{\Delta x} \quad (5)$$

where $|\tilde{U}_i|$ is the annual average absolute deviation of wind speed in the East–West direction, as calculated by WRF-Chem, at the interface between cells i and w_j . Eq. (5) is repeated for neighbors to the East, to the South, to the North, above, and below cell i . This scheme assumes that deviations from annual average wind velocity are 205
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symmetrical about each axis.

Finally, InMAP parameterizes $\nabla \cdot (\vec{v}' C'_i)$ using the combined local-nonlocal mixing scheme described below. We assume that the remaining two terms in Eq. (3), $\nabla \cdot (\vec{v}' \tilde{C}_i)$ and $\nabla \cdot (\tilde{\vec{v}} C'_i)$, account for a relatively small fraction of chemical transport. The results presented here – which show InMAP can perform reasonably without these two terms – support this assumption, but finding suitable parameterizations is an area for future research.

As shown above, to represent temporally-variable advection in an annual average modelling framework, InMAP splits advective transport into three steps, one of which is directional and two of which are symmetrical with respect to one or more axes. One result of this is that in some cases information regarding transport direction may be lost. For instance, an extreme case were wind travels from the Northwest half of the time at 2 m s^{-1} and from the Southeast the other half of the time at 2 m s^{-1} would be represented by InMAP as directional advection at 0 m s^{-1} and symmetrical advection in all horizontal directions at $\sqrt{2} \text{ m s}^{-1}$.

For advection and mixing, InMAP assumes zero concentration-change boundary conditions at the lateral and top edges of the model domain and an impermeable boundary at the bottom edge of the domain.

Mixing

For mixing (i.e., pollutant transport that is not resolved by WRF-Chem; $\nabla \cdot (\vec{v}' C'_i)$ in Eq. 3) within the planetary boundary layer, we use a combined local-nonlocal closure scheme [38]. For mixing above the boundary layer and for horizontal mixing, we only consider turbulent mixing [39]. We modify a previously published relationship [38] as shown in Eq. (6) to allow a variable number of adjacent cells and to include horizontal

and vertical mixing.

$$m_{g,i} = \sum_{g_j}^{1,n_{g,i}} (\text{M2u}_i C_{g_j} f_{g_j}) \quad (6)$$

$$m_{a,i} = \sum_{a_j}^{1,n_{a,i}} \left(\left[\text{M2d}_{a_j} C_{a_j} \frac{\Delta z_{a_j}}{\Delta z_i} - \text{M2d}_i C_i + \Delta z_i^{-1} K_{zz,a_j} \frac{2(C_{a_j} - C_i)}{\Delta z_i + \Delta z_{a_j}} \right] f_{a_j} \right) \quad (7)$$

$$m_{b,i} = \sum_{b_j}^{1,n_{b,i}} \left(\Delta z_i^{-1} K_{zz,b_j} \frac{2(C_{b_j} - C_i)}{\Delta z_i + \Delta z_{b_j}} f_{b_j} \right) \quad (8)$$

$$m_{w,i} = \sum_{w_j}^{1,n_{w,i}} \left(\Delta x_i^{-1} K_{xx,w_j} \frac{2(C_{w_j} - C_i)}{\Delta x_i + \Delta z_{w_j}} f_{w_j} \right) \quad (9)$$

$$m_{e,i} = \sum_{e_j}^{1,n_{e,i}} \left(\Delta x_i^{-1} K_{xx,e_j} \frac{2(C_{e_j} - C_i)}{\Delta x_i + \Delta x_{e_j}} f_{e_j} \right) \quad (10)$$

$$m_{s,i} = \sum_{s_j}^{1,n_{s,i}} \left(\Delta y_i^{-1} K_{yy,n_j} \frac{2(C_{s_j} - C_i)}{\Delta y_i + \Delta y_{s_j}} f_{s_j} \right) \quad (11)$$

$$m_{n,i} = \sum_{n_j}^{1,n_{n,i}} \left(\Delta y_i^{-1} K_{yy,n_j} \frac{2(C_{n_j} - C_i)}{\Delta y_i + \Delta y_{n_j}} f_{n_j} \right) \quad (12)$$

$$\Delta C_i = (m_{g,i} + m_{a,i} + m_{b,i} + m_{w,i} + m_{e,i} + m_{s,i} + m_{n,i}) \Delta t \quad (13)$$

In Eqs. (6–13), C_i refers to the pollutant concentration in grid cell i , g_j refers to one of 228
 $n_{g,i}$ cells at ground level directly below the cell of interest, and b_j , a_j , w_j , e_j , s_j , and n_j refer to cells directly below, above, west, east, south, and north of the cell of interest, 229
respectively. M2u and M2d are upward and downward convective mixing 230
coefficients [38]. K_{zz} is the turbulent mixing coefficient in the vertical direction, and 231
 K_{xx} and K_{yy} are horizontal mixing coefficients. We calculate mixing coefficients (both 232
local and nonlocal) for each time step in the WRF-Chem model output, using the 233
boundary layer height specific to that time step, and then use the average of these 234
values to represent mixing in InMAP. 235

Chemistry

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In InMAP, total $\text{PM}_{2.5}$ is comprised of primary $\text{PM}_{2.5}$, which is assumed to be 238
nonvolatile and nonreactive, and secondary $\text{PM}_{2.5}$ which can be formed from VOCs, 239
 SO_x , NO_x , or NH_3 . To model the secondary formation of $\text{PM}_{2.5}$ (R in Eq. 1), InMAP 240
estimates formation of particulate sulfate and ammonium using first-order chemical 241

reaction kinetics. Partitioning between the gas and aerosol phases for nitrogen oxide,
 242 ammonia, and organic compounds (VOCs and SOA) is done assuming instantaneous
 243 adjustment to match equilibrium partitioning coefficients. Because InMAP is designed
 244 to predict the impacts of marginal changes in emissions and because the chemical
 245 relationships are nonlinear, we calculate reaction rates and partitioning coefficients for
 246 marginal changes in concentrations.
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There are two main pathways from sulfur dioxide (SO_2) gas to sulfate (SO_4^{2-})
 particles: gas phase oxidation by hydroxyl radical (HO^*) and aqueous phase oxidation
 by hydrogen peroxide (H_2O_2) [3]. There are no major pathways for reaction of SO_4^{2-}
 back to SO_2 . After calculating an annual average overall reaction rate k_{S} for SO_2 to
 SO_4^{2-} using WRF-Chem output data and formulas for the gas phase and aqueous
 pathways from [3], we calculate the formation of SO_4^{2-} particles from SO_2 gas as in
 Eq. (14):

$$\Delta C_{\text{S,g2p},i} = k_{\text{S},i} C_{\text{S,g},i} \Delta t \quad (14)$$

where $\Delta C_{\text{S,g2p},i}$ is the transformation of sulfur from gas to particle phase during time
 248 step Δt in cell i and $C_{\text{S,g},i}$ is the gas phase concentration of sulfur at the beginning of
 249 the time step.
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For NO_x , NH_3 , and VOCs, the chemical reaction mechanisms governing partitioning
 between the gas and particle phase are more complex than the reactions driving sulfate
 formation. They are also reversible: gas-phase compounds can convert to aerosols and
 then back to gas-phase, and the direction of the reactions can vary according to the
 time of day and according to the season. It is not possible to directly represent these
 reactions in a steady-state, annual average model such as InMAP. For NO_x , NH_3 , and
 VOCs we instead calculate an annual average partitioning coefficient $f_{\text{p},i}$ in grid cell i
 for marginal changes in concentrations from the WRF-Chem output data as in Eq. (15):

$$f_{\text{p},i} = \sum_{j=1}^n \left(\frac{\Delta m_{\text{p},i,j}}{\Delta m_{\text{p},i,j} + \Delta m_{\text{g},i,j}} \right) / n \quad (15)$$

where $\Delta m_{\text{p},i,j}$ is change in mass in cell i the particle phase and $\Delta m_{\text{g},i}$ is change in mass
 in the gas phase from one WRF-Chem output time step j to the next, and n is the total

number of output time steps (8760). Then, we use this coefficient to calculate gas/particle partitioning in InMAP using Eqs. (16) and (17):

$$C_{p,i,f} = (C_{g,i,s} + C_{p,i,s}) f_{p,i} \quad (16)$$

$$C_{g,i,f} = (C_{g,i,s} + C_{p,i,s}) (1 - f_{p,i}) \quad (17)$$

where $C_{g,i,s}$, $C_{p,i,s}$, $C_{g,i,f}$ and $C_{p,i,f}$ are gas and particle phase concentrations in cell i at the start s and end f of the time step. The concentration at the end of one time step is used as the concentration at the beginning of the next time step. For partitioning between VOCs and secondary organic aerosol (SOA) we only consider those VOCs that are SOA precursors as defined by [40].

Wet and dry deposition

We assume that dry deposition $v_{dd,i}$ for gases in cell i can be represented as a function of resistances in series as in Eq. (18), where $r_{a,i}$ is aerodynamic resistance, $r_{b,i}$ is quasi-laminar boundary layer resistance, and $r_{c,i}$ is surface resistance [3]. For particles, this equation is slightly altered to account for settling velocity. We calculate an annual average dry deposition velocity for each ground-level grid cell using the output from WRF-Chem and previously published algorithms for $r_{c,i}$ for gases [41, 42]. To calculate $r_{c,i}$ for particles, and to calculate $r_{a,i}$ and $r_{b,i}$, we also use previously published algorithms [3]. We then calculate dry deposition within InMAP using Eqs. (18) and (19):

$$|v_{dd,i}| = (r_{a,i} + r_{b,i} + r_{c,i})^{-1} \quad (18)$$

$$\Delta C_i = -C_i v_{dd,i} \frac{\Delta t}{\Delta z_i} \quad (19)$$

where C_i is pollutant concentration in a grid cell in the lowest model layer.

We calculate an annual average wet deposition rate $r_{wd,i}$ for each grid cell i using output from WRF-Chem and a simple algorithm from the EMEP model [43] that estimates a rate of wet deposition from in-cloud and below-cloud scavenging rate as a function of cloud fraction, precipitation rate, and air density. The algorithm provides separate rate estimates for particles, SO_2 , and other gases. We then calculate wet

deposition within InMAP using Eq. (20):

$$\Delta C_i = -C_i r_{wd,i} \Delta t \quad (20)$$

Dry deposition is assumed to only occur in ground-level grid cells. Wet deposition is

calculated for every grid cell, with location-specific deposition rates.

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User inputs

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One goal for InMAP is ease of use. The only user-specified input required by running InMAP in its native layout is a shapefile or set of shapefiles [44] containing locations of changes in annual total emissions of VOCs, SO_x , NO_x , NH_3 , and primary fine particulate matter ($\text{PM}_{2.5}$). Locations can be specified as polygon, line, or point entities, and can include stack attributes which InMAP uses to calculate plume rise for elevated sources. InMAP allocates emissions from shapefiles to the corresponding model cells using area-weighting.

Performance evaluation

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InMAP provides a computationally inexpensive alternative to a CTM for calculating impacts of marginal emission changes. Therefore, its performance should be evaluated in terms of predicting marginal changes in concentrations rather than total ambient concentrations. Although the strongest evaluation would be to compare InMAP predictions to measured pollutant concentrations, long-term, nationwide measurements of the effects of marginal emissions changes on pollutant concentrations do not exist. Instead, we compare InMAP predictions for scenarios with changes in emissions to those from a CTM. It is common to evaluate air pollution sensitivity models against more complex models [21,25]. Specifically, for our model-model evaluation we employ WRF-Chem to model 11 scenarios of emission changes that would result from the hypothetical adoption of alternative light-duty transportation technologies. These scenarios include emissions from transportation, electric generation, agriculture, and various industrial sources in proportions that vary among scenarios – since these activities have different spatial distributions, the emissions scenarios are spatially heterogeneous – resulting in total $\text{PM}_{2.5}$ concentration changes on the order of 1%. A

brief description of each emissions scenario is provided in S1 Fig–S12 Fig. Additional information regarding the emission scenarios and the associated WRF-Chem modeling can be found elsewhere [34,45]. Below, we also compare InMAP results against an existing reduced-form model: the COBRA source-receptor matrix [26].

To explore how reliably InMAP can be expected to predict larger changes in concentrations, we separately evaluate InMAP performance in predicting measured year 2005 annual average PM_{2.5} concentrations [46]. As mentioned above, InMAP is designed to predict marginal changes in concentrations rather than total concentrations; comparing InMAP against observed values represents a use of the model that is beyond what that model was designed for. Nevertheless, we conduct and evaluate InMAP in that manner here (i.e., running it as though it were a conventional CTM rather than a model for marginal changes in emissions) to provide information on how widely applicable the model is, including its use in simulations of large changes in emissions. To compare InMAP predictions to observations, we use a previously described emissions inventory [8], with the exception that anthropogenic emissions are processed using the AEP model [47] to allow allocation of area source emissions to the InMAP spatial grid without the loss of spatial information.

Finally, to investigate InMAP's ability to predict temporally variable pollutant transport in a steady-state framework, and its ability to predict higher-resolution pollutant spatial patterns based on lower-resolution meteorology fields, we perform an additional independent comparison of InMAP vs. WRF-Chem. To perform this comparison, we first use WRF-Chem to simulate annual average transport and fate of 100 short tons per year of emissions from a single ground-level point source of non-reactive PM_{2.5} in downtown Los Angeles, California. We run the WRF-Chem simulation over a 9801×9801 km spatial domain with 9 km, 3 km, and 1 km nested grids. Each nested grid is comprised of 33×33 horizontal grid cells and 30 vertical layers centered over downtown Los Angeles. We split up year 2005 into 8 approximately 45 day periods and simulate approximately the first 15 days of each period with WRF-Chem to approximate annual average conditions. All other aspects of the WRF-Chem configuration have been previously described [8]. We use the results from the 9 km-resolution outer WRF-Chem domain to create two versions of InMAP: one with 9 km grid cells aligning with the native WRF-Chem grid cells ("InMAP LA-9km"),

and one with 1–27 km variable resolution grid cells ("InMAP LA-variable"). The 3 km-
 316
 and 1 km-resolution inner WRF-Chem domains are not used during the setup of InMAP.
 317
 We then compare InMAP LA-9km against the 9 km resolution WRF-Chem results and
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 we compare InMAP LA-variable against the 1 km resolution WRF-Chem results.
 319

We use several metrics to assess model-model and model-measurement agreement,
 including mean bias (MB, Eq. 21), mean error (ME, Eq. 22), mean fractional bias
 (MFB, Eq. 23), mean fractional error (MFE, Eq. 24), and model ratio (MR, Eq. 25), as
 well as linear regression slope (S), intercept (I), and squared Pearson correlation
 coefficient (R^2) values. In Eqs. (21)–(25), i corresponds to one of n comparisons, and X
 and Y are the annual average modeled or measured values we are comparing.

$$\text{MB} = \frac{1}{n} \sum_{i=1}^n (Y_i - X_i) \quad (21)$$

$$\text{ME} = \frac{1}{n} \sum_{i=1}^n |Y_i - X_i| \quad (22)$$

$$\text{MFB} = \frac{1}{n} \sum_{i=1}^n \frac{2(Y_i - X_i)}{(Y_i + X_i)} \quad (23)$$

$$\text{MFE} = \frac{1}{n} \sum_{i=1}^n \frac{2|Y_i - X_i|}{(Y_i + X_i)} \quad (24)$$

$$\text{MR} = \frac{1}{n} \sum_{i=1}^n \frac{Y_i}{X_i} \quad (25)$$

Results

The resulting InMAP computer model is comprised of \sim 2000 lines of code written in
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 the Go language [48] with an additional \sim 2900 lines of code for preprocessing
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 WRF-Chem output data into InMAP input data. Each InMAP model run takes
 323
 approximately two hours to complete on a desktop computer with an Intel Ivybridge
 324
 processor; S2 Appendix lists example simulation run times for different model settings.
 325
 The preprocessor takes approximately eight hours to run on a similar desktop computer,
 326
 but users will not need to run the preprocessor or obtain output from a CTM unless
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 they are interested in a spatial or temporal domain different than the continental U.S.
 328
 and year 2005. As recommended for scientific reproducibility [49], the model is freely
 329
 available at <http://inmap.spatialmodel.com> (doi:10.5281/zenodo.60671) and is licensed
 330

under the GNU General Public License (GPL). Results here are based on InMAP
version 1.2.0. Preprocessed input data and the data required to reproduce the results
shown here are also freely available (doi:10.5281/zenodo.166811).

Model to model comparison: full US

Fig 2 shows WRF-Chem, InMAP, and COBRA model results for an example emissions scenario where changes in vehicle tailpipe emissions are the largest emissions source. We show two InMAP configurations: the 12 km constant-resolution grid that mirrors the grid used for WRF-Chem simulations (“InMAP 12 km”) and a variable-resolution grid for which the smallest cells are 1 km² (“InMAP 1 km”). Overall, spatial patterns in concentration changes are similar in InMAP, COBRA, and WRF-Chem. In the specific example shown in Fig 2, differences in estimated concentrations are apparent in Southern California and the Gulf Coast. S1 Fig–S12 Fig show additional spatial detail comparing InMAP and WRF-Chem for this (S1 Fig) and other emissions scenarios. COBRA provides one prediction per county as can be discerned in Fig 2d where counties are large (e.g., in Southern California around Los Angeles). S1 Fig–S12 Fig contain information similar to Fig 2 for the remaining emissions scenarios investigated here, as well as corresponding performance statistics.

Fig 3 compares InMAP, WRF-Chem, and COBRA ground-level predictions for 12 emissions scenarios. Two sets of comparisons are shown: area-weighted (useful for understanding atmospheric processes such as mixing and removal) and population-weighted (useful for human exposures and health impacts).

InMAP 12 km reproduces the WRF-Chem predictions for changes in area-weighted concentrations with $R^2 = 0.92$ and MFB = -46 %) and in population-weighted concentrations with $R^2 = 0.90$ and MFB = -17 % (Fig 3a). InMAP 1 km performance (Fig 3b) is similar to that of InMAP 12 km. InMAP performance is not remarkably different from the existing COBRA model (Fig 3c). However, InMAP has capabilities not found in COBRA, such as predicting how pollutant concentrations vary within a county or a city and accounting for spatially variable aspects of secondary PM_{2.5} formation.

Fig 4 compares InMAP and WRF-Chem for PM_{2.5} subgroups: primary PM_{2.5},

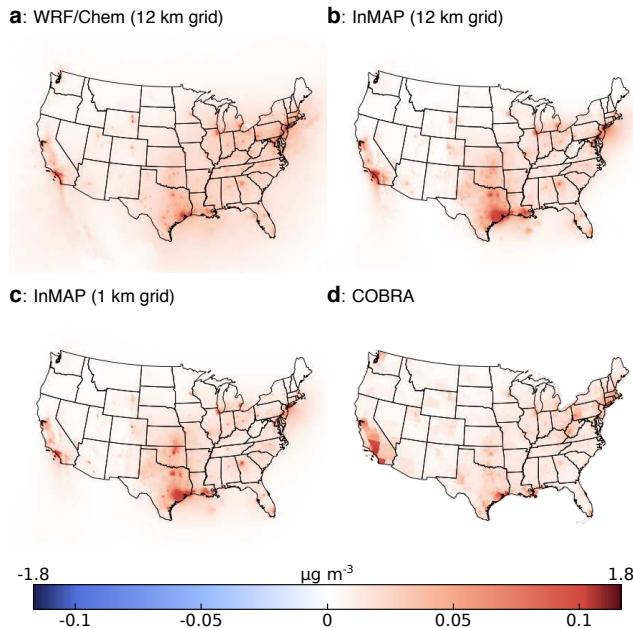


Fig 2. Changes in concentrations resulting from one emissions scenario as calculated by (a) WRF-Chem, (b) InMAP with a 12 km resolution grid, (c) InMAP with a 1 to 48 km variable resolution grid (i.e., a typical setup for InMAP), and (d) COBRA. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values. S1 Fig–S12 Fig provide similar information for the rest of the scenarios.

particulate nitrate ($p\text{NO}_3$), particulate ammonium ($p\text{NH}_4$), particulate sulfate ($p\text{SO}_4$), and secondary organic aerosol (SOA). InMAP primary PM_{2.5} predictions (Fig 4a and b) agree with WRF-Chem with R^2 values of 0.98 or greater (population-weighted MFE $\leq 26\%$; area-weighted MFE $\leq 68\%$). 361
362
363
364

InMAP agreement with WRF-Chem results for $p\text{NO}_3$ and $p\text{NH}_4$ is the poorest of 365 the species considered here ($R^2 = 0.42\text{--}0.78$). $p\text{NO}_3$ and $p\text{NH}_4$ formation rates have 366 large seasonal and diurnal variations, and so are more challenging to represent in 367 a steady-state, annual average model such as InMAP. 368

For $p\text{SO}_4$, InMAP predictions are well-correlated with WRF-Chem ($R^2 \geq 0.99$) but 369 tend to underpredict concentration changes (population-weighted MFB = -57%). $p\text{SO}_4$ 370 formation follows comparatively simple and slow-acting chemical mechanisms as 371 described above. 372

For secondary organic aerosol (SOA), InMAP predictions agree relatively well with 373 WRF-Chem for population-weighted concentration changes (MFB = -53%, $R^2 = 0.91$). 374 InMAP underpredicts area-weighted changes in concentrations relative to WRF-Chem 375 (MFB $\approx -110\%$). 376

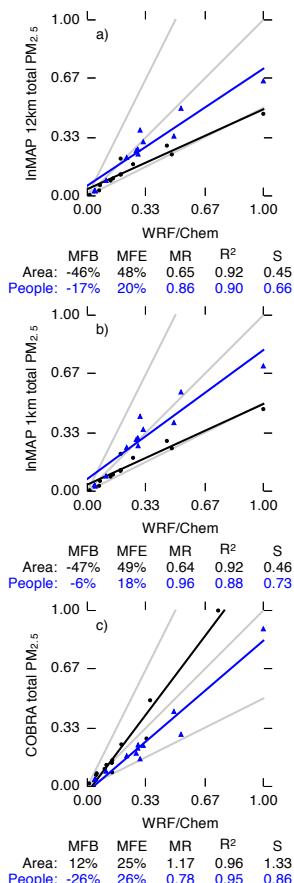


Fig 3. Comparison of total (primary plus secondary) area-weighted (black dots) and population-weighted (blue triangles) annual average predicted PM_{2.5} concentration change for WRF-Chem (x axis) and either InMAP or COBRA (y axis) for 11 emissions scenarios. To assist in comparison between area- and population-weighted predictions, concentrations shown here are normalized so that the largest value in each comparison equals one. The gray lines represent 1 : 1, 2 : 1, and 1 : 2 ratios between the models, and the black and blue lines represent least-squares regressions. Performance statistics for each comparison are listed below the plots. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MR = model ratio; R^2 = squared Pearson correlation coefficient; S = slope of regression line.

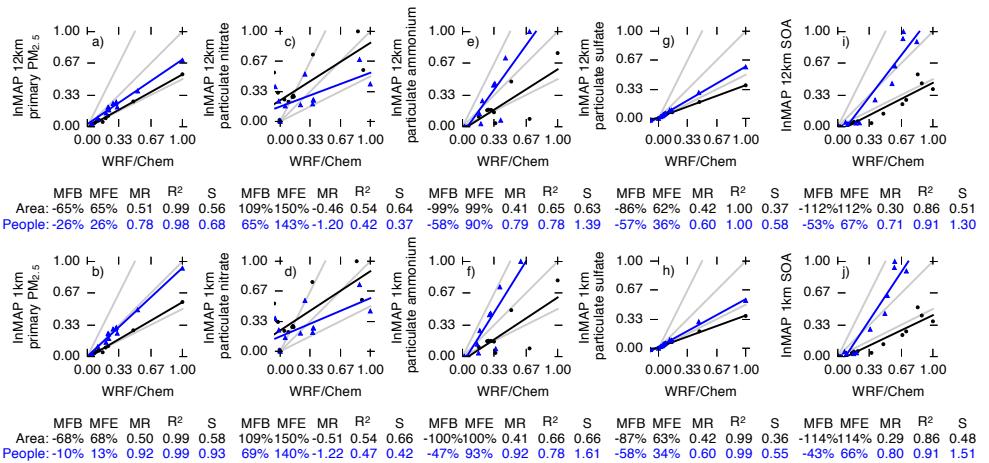


Fig 4. Comparison of area-weighted (black dots) and population-weighted (blue triangles) annual average predictions of changes in concentrations of PM_{2.5} subspecies between WRF-Chem (*x* axis) and InMAP (*y* axis) for 11 emissions scenarios. To assist in comparison between area- and population-weighted predictions, concentrations shown here are normalized so that the largest value in each comparison equals one. The gray lines represent InMAP : WRF-Chem ratios of 1 : 1, 2 : 1, and 1 : 2. The black and blue lines represent least-squares regressions. Performance statistics for each comparison are listed below the plots. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MR = model ratio; R^2 = squared Pearson correlation coefficient; S = slope of regression line.

Model to model comparison: regional

Fig 5 shows InMAP performance by US region. (Region boundaries are in S13 Fig.) Model performance is in general similar among regions. One exception is for particulate nitrate concentrations, where InMAP reproduces WRF-Chem predictions better in the Midwest (population-weighted $S = 0.67$) than elsewhere (population-weighted $S = 0.13\text{--}0.33$). This may be explained by the presence of negative WRF-Chem predictions of $p\text{NO}_3$ concentration changes in non-Midwest regions. These negative concentration changes are caused by interactions between PM_{2.5} subspecies that InMAP does not account for. As discussed below, these interactions are most important when changes in NO_x emissions are low, so their effect on total PM_{2.5} predictive performance is minor.

We additionally include grid-cell-specific comparisons between WRF-Chem and InMAP for the 12 emissions scenarios investigated here, as well as corresponding performance statistics, in S1 Fig–S12 Fig. Fractional performance statistics (e.g., MFB and MFE) can be highly influenced by concentrations in the lowest-concentration cells and absolute performance statistics (e.g., MB and ME) depend in part on the

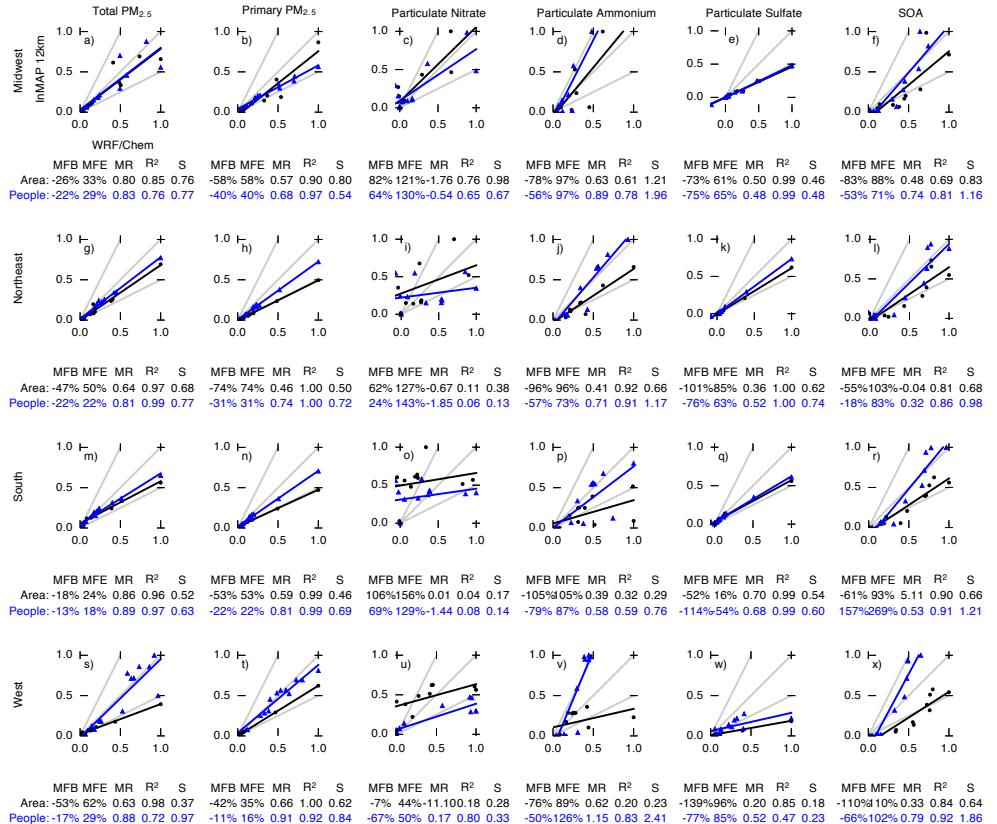


Fig 5. Region-specific comparisons of area-weighted (black dots) and population-weighted (blue triangles) annual average predictions of total PM_{2.5} and its subspecies between WRF-Chem (x axis) and InMAP (y axis) for 11 emissions scenarios. To assist in comparison between area- and population-weighted predictions, concentrations shown here are normalized so that the largest value in each comparison equals one. The gray lines represent InMAP : WRF-Chem ratios of 1 : 1, 2 : 1, and 1 : 2. The black and blue lines represent least-squares regressions. Performance statistics for each comparison are listed below the plots. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MR = model ratio; R² = squared Pearson correlation coefficient; S = slope of regression line.

magnitude of emissions in each emissions scenario. We therefore focus greatest attention
393 on population-weighted measures. Population-weighted R^2 values range between 0.00
394 and 0.99 among scenarios and pollutant types. The lowest R^2 values reflect an atypical
395 comparison and are not a strong indication of typical model performance, for the
396 following reason. The lowest R^2 values are observed for $p\text{NO}_3$ and $p\text{NH}_4$ predictions in
397 scenarios dominated by coal power plant emissions, where nonlinear effects related to
398 increased SO_2 concentrations, which are not represented in InMAP, outweigh $p\text{NO}_3$ and
399 $p\text{NH}_4$ formation from NO_x and NH_3 emissions. However, these nonlinear effects are
400 most important when changes in $p\text{NO}_3$ and $p\text{NH}_4$ concentrations are low, so in these
401 cases poor performance in predicting $p\text{NO}_3$ and $p\text{NH}_4$ concentrations does not
402 necessarily adversely impact InMAP performance in predicting total $\text{PM}_{2.5}$
403 concentrations.
404

Model to measurement comparison

405

InMAP is designed to model the changes in pollutant concentrations caused by marginal
406 changes in emissions, but there are no long-term, nationwide measurements of the
407 impacts of changes in emissions on changes in concentrations against which to evaluate
408 InMAP directly. Therefore, we use the model-to-model comparisons described above as
409 our main evaluation of InMAP performance. However, we also evaluate here InMAP
410 performance in predicting overall pollutant concentrations for the year 2005. One
411 purpose of this comparison is as a bounding estimate of how accurate InMAP would be
412 in predicting the impacts of large changes in emissions. Figs 6–9 show the results of this
413 comparison in terms of overall relationships between modeled and measured values and
414 the spatial patterns in those relationships for $\text{PM}_{2.5}$ and its subspecies. Corresponding
415 information for gas-phase pollutants is in S14 Fig–S16 Fig. Results in Figs 6–9 for
416 WRF-Chem refer to previously published WRF-Chem model results [8] that we use to
417 create InMAP inputs. In general, InMAP tends to underpredict observed total $\text{PM}_{2.5}$
418 concentrations ($\text{MFB} = -38\%$; WRF-Chem $\text{MFB} = 14\%$). However, even though
419 InMAP is designed to predict marginal changes in concentrations rather than total
420 concentrations, it still meets published air quality model $\text{PM}_{2.5}$ performance criteria of
421 $\text{MFB} \leq \pm 60\%$ and $\text{MFE} \leq 75\%$ [50] for predictions of all tested species except $p\text{SO}_4$.
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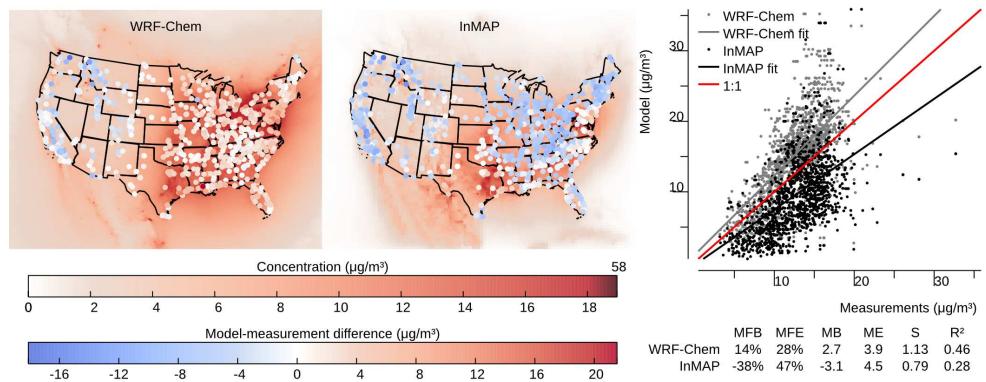


Fig 6. Comparison of WRF-Chem and InMAP performance in predicting annual average observed total $\text{PM}_{2.5}$ concentrations. The background colors in the maps represent predicted concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. For the comparison shown here, on average WRF-Chem overpredicts and InMAP underpredicts as compared to observations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

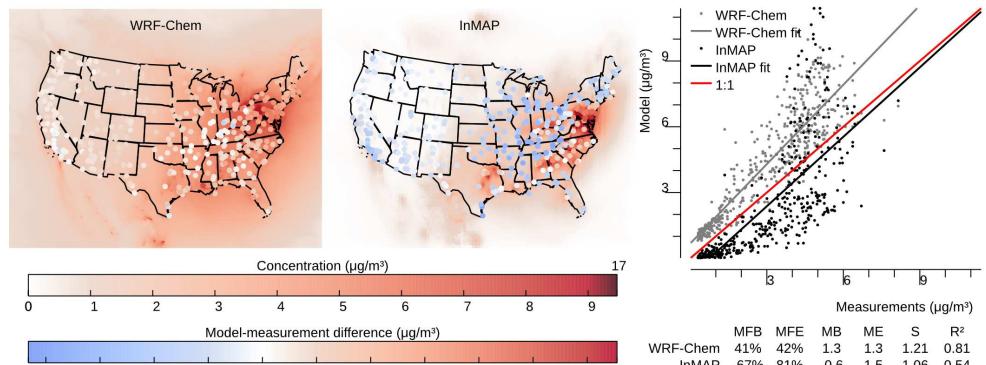


Fig 7. Comparison of WRF-Chem and InMAP performance in predicting annual average observed particulate SO_4 concentrations. The background colors in the maps represent predicted concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

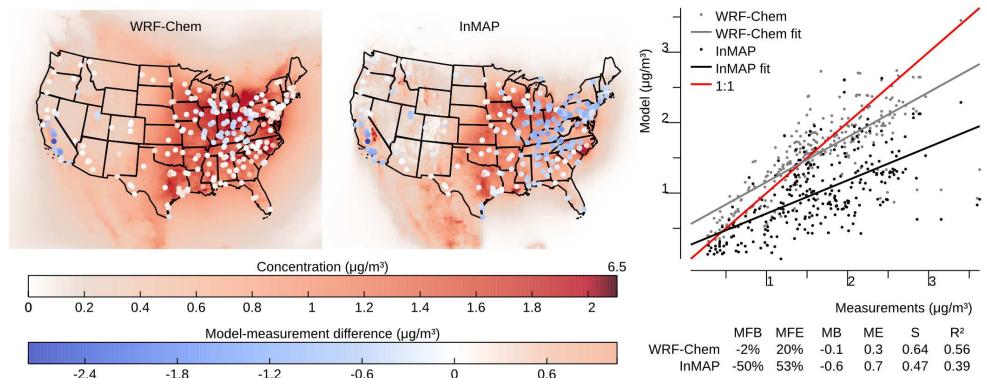


Fig 8. Comparison of WRF-Chem and InMAP performance in predicting annual average observed particulate NH_4 concentrations. The background colors in the maps represent modeled concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

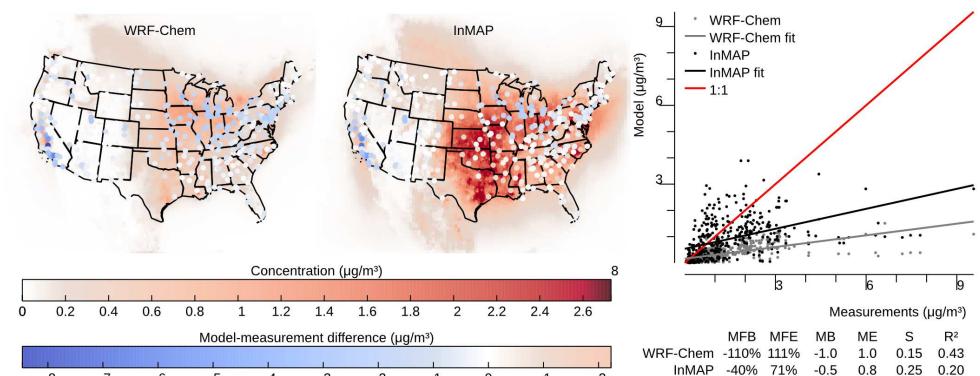


Fig 9. Comparison of WRF-Chem and InMAP performance in predicting annual average observed particulate NO_3 concentrations. The background colors in the maps represent modeled concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

Figs 6–9 show that much of the InMAP underpredictions of total PM_{2.5} concentrations relative to observations are caused by underpredictions in *pSO*₄. This inaccuracy in predicting observed *pSO*₄ concentrations is not unexpected because the chemical reactions that produce *pSO*₄ are nonlinear and InMAP is designed to predict marginal *pSO*₄ production rather total *pSO*₄ production. Future research could potentially re-parameterize InMAP to be a conventional (rather than marginal-change) model; that step is beyond the scope of the present article. There exist other criteria for determining model suitability [51] which could be explored in future research.

Single source model to model comparison

Fig 10 compares WRF-Chem and InMAP concentration predictions for a single ground-level point source of primary PM_{2.5} emissions. Comparisons are included for a 9 km-resolution WRF-Chem domain (Fig 10a) against a matching 9 km-resolution InMAP domain ("InMAP LA-9km"; Fig 10b), and for a nested 1 km-resolution WRF-Chem domain (Fig 10d) against a 1–27 km variable-resolution InMAP domain ("InMAP LA-variable"; Fig 10e) that was created based on the 9 km WRF-Chem results. The main difference between the two models for the 9 km domain is that WRF-Chem predicts higher concentrations in the grid cell where the emissions are located than InMAP does. One reason for this is InMAP's use of a numerically diffusive advection scheme. The same effect can be seen in the 1 km resolution results, although these results also show that the advection solver used by WRF-Chem also creates numerical artifacts in the form of a much higher rate of transport in the exact Northward, Southward, and Westward directions from the emissions source than would generally be expected. InMAP LA-variable reproduces the spatial pattern predicted by the 1 km WRF-Chem results with MFB and MFE ≈ 100% and $R^2 = 0.69 - 0.79$. When interpreting these results, it is important to consider that the InMAP predictions are based on lower (9 km) resolution meteorological information from WRF-Chem and should not be expected to match the WRF-Chem predictions exactly.

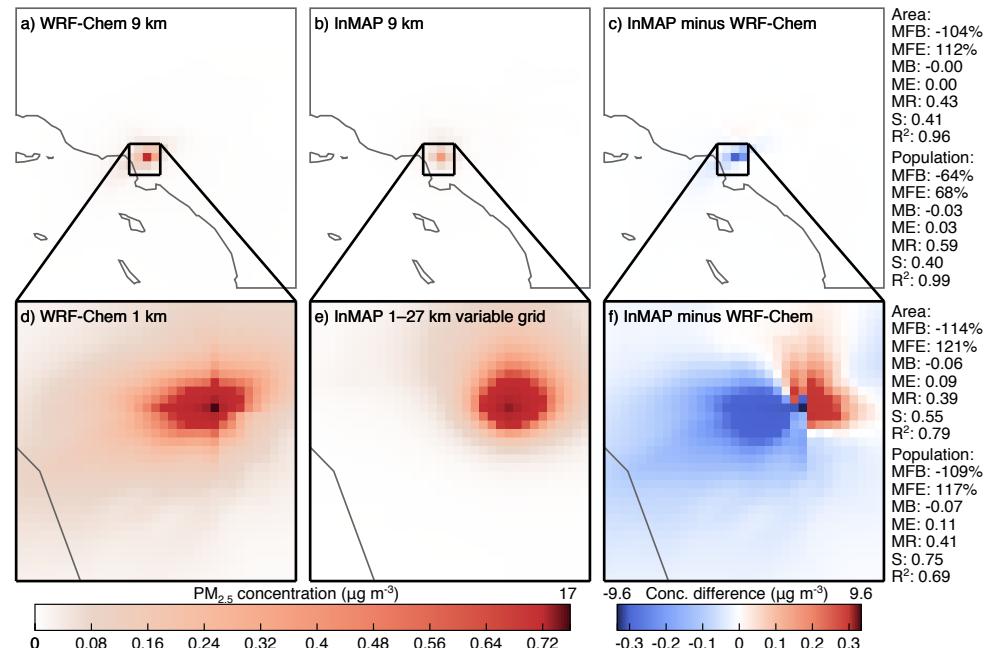


Fig 10. Comparison of WRF-Chem and InMAP performance in predicting the impacts of 100 tons per year of primary nonreactive PM_{2.5} emissions in Los Angeles at 9 km (panels a and b), 1 km (panel d), and 1–27 km variable (panel f) grid resolutions. InMAP predictions in panel e are based on meteorology from the 9 km-resolution WRF-Chem simulation (panel a) rather than the 1 km-resolution simulation (panel d). Panels c and f show the differences between the panels to their left. Area- and population-weighted statistics are shown on the right. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

Discussion

We have presented here a new air quality model for determining the human health impacts of marginal changes in pollutant emissions. InMAP is a reduced complexity model with the goal of reducing computational intensity and required user effort while minimizing losses in predictive performance. In comparisons run here, InMAP recreates WRF-Chem predictions of changes in total PM_{2.5} concentrations with population-weighted MFE and MFB < 18% and $R^2 \approx 0.9$. Among individual PM_{2.5} species, the best predictive performance is for primary PM_{2.5} (MFE: 26%; MFB: -26%) and the worst predictive performance is for particulate nitrate (MFE: 143%; MFB: 65%). InMAP is reduced in complexity compared to comprehensive chemical transport models but more accessible to non-specialists and more spatially detailed than other reduced-complexity national-scale air quality models. One of these existing models is the COBRA model, which we show performs similarly to the InMAP model presented here in terms of reproducing WRF-Chem changes in population-weighted average concentrations. InMAP, however, has features and capabilities that make it better suited than COBRA or other existing models for certain use cases (e.g., for simulations where it is desirable to estimate within-city, or even within-county, differences in PM_{2.5} concentrations, while also estimating long range transport of PM_{2.5} in the same simulation).

Fig 11 shows a small area of the maps in Fig 2, centered on one example urban area (Las Vegas, Nevada). COBRA represents all of the county that contains Las Vegas as having the same PM_{2.5} concentration, so most of the map is only one color. WRF-Chem, as configured here, is able to resolve differences in pollutant levels at a 12 km scale for the contiguous US (If the size of the total spatial domain were decreased to only include the area surrounding Las Vegas, WRF-Chem could resolve differences at a $\sim 1\text{--}4$ km scale.) InMAP is unique among existing models in that it can model changes in pollutant concentrations across the entire contiguous US with 1 km spatial resolution in all high-population areas, all in a single model run.

The ability to resolve differences in pollution concentrations within urban areas is important for certain types of analyses, such as those that seek to determine how pollution exposure differs among demographic groups (environmental justice) or

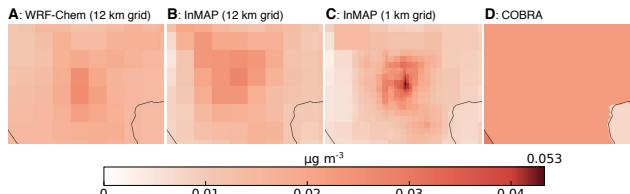


Fig 11. A detail view of Fig 2 centered on the city of Las Vegas. Changes in concentrations resulting from one of the emissions scenarios as calculated by (a) WRF-Chem, (b) InMAP with a 12 km resolution grid, (c) InMAP with a 1 to 48 km variable resolution grid, and (d) COBRA, which has county-level outputs. InMAP 1 km (panel c) provides the highest spatial resolution, which is important for calculating health impacts in areas with high spatial gradients in pollutant concentration and in population.

neighborhoods.

InMAP is much less computationally intensive than are CTMs. For example, 481
InMAP 1 km produces the results for each of the scenarios shown here in ~ 2 hr on 482
a current desktop computer, requiring a factor of ~ 15 000 less computational power 483
than was required to produce the WRF-Chem results shown here. S2 Appendix lists 484
example simulation run times for different model settings. This computational speed-up 485
makes possible uncertainty, sensitivity, and scenario analyses that could not be 486
attempted with WRF-Chem or other comprehensive chemical transport models. 487

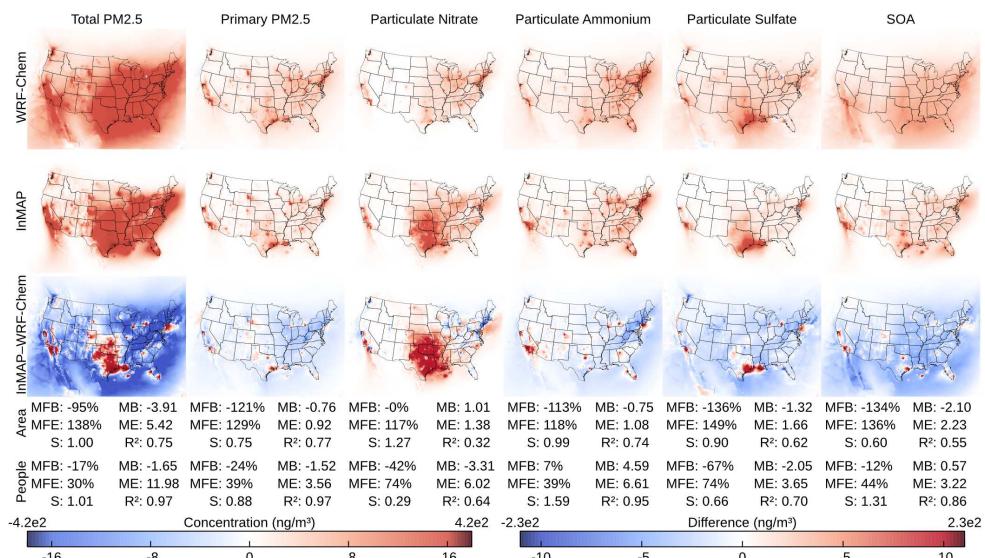
Limitations of InMAP include the following. Model performance is better for 488
population-weighted primary PM_{2.5}, pSO₄, and SOA concentrations ($R^2 \geq 0.9$) than for 489
changes in pNO₃ and pNH₄ concentrations ($R^2 \sim 0.4\text{--}0.8$). The setup and testing of 490
InMAP has mainly considered SOA formed from anthropogenic sources; further testing 491
is needed to determine InMAP performance in predicting impacts of biogenic VOC 492
emissions. Additional testing could be useful to further evaluate the accuracy of 493
InMAP's high-resolution urban area predictions against other high-resolution model 494
simulations or measurements. At present, InMAP does not predict concentrations of 495
ground-level ozone (O₃), which is considered the distant-second largest source of human 496
health burden from air pollution after PM_{2.5} [1,2]. Additionally, InMAP performance is 497
better for population-weighted metrics (e.g., for health studies, exposure, or 498
environmental justice) than for area-weighted metrics (e.g., for understanding “average 499
atmospheric” processes). 500

A future version of InMAP, including more comprehensive mechanisms for gas- and 502
aerosol-phase chemistry and iterating through diurnal cycles representative of each 503

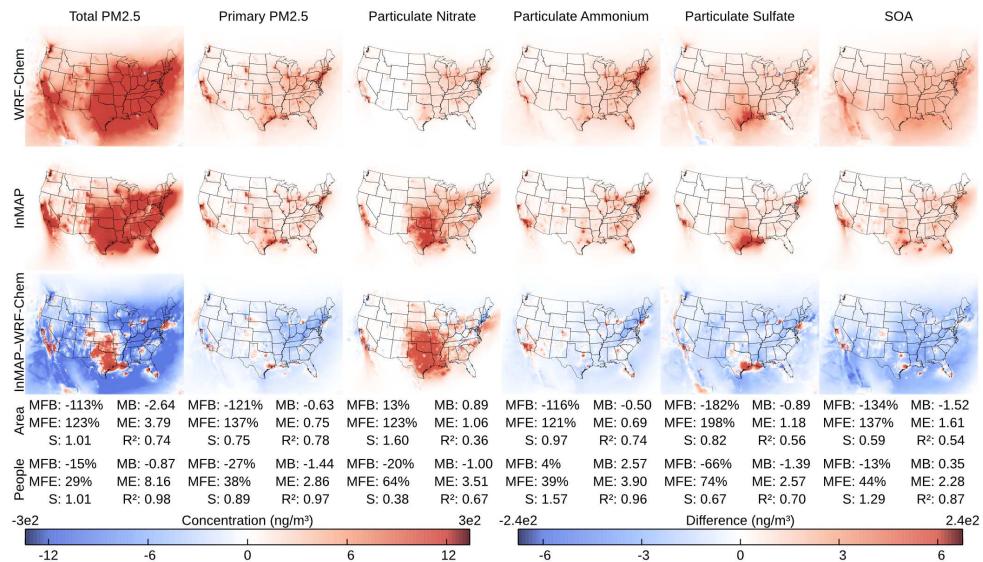
season of the year instead of using annual average information, could potentially
 ameliorate many of these limitations, and would have the added benefit of allowing the
 prediction of concentrations of a larger number of pollutants. This approach would by
 necessity be more computationally intensive than the current version and require more
 user input information, so increased predictive power may come at the expense of ease,
 speed, and flexibility. A future version of InMAP could use distributed-memory
 parallelization or cloud computing to minimize the impact to users of any increased
 computational intensity. Future development is also planned to allow the preprocessor
 to accept output from models other than WRF-Chem, such as GEOS-Chem and CAMx.

InMAP is designed to be readily adapted to different spatial and temporal domains.
 This can be done by obtaining output from a CTM for the desired domain and
 processing it with the InMAP preprocessor. (An evaluation of model accuracy in the
 new domain would also be recommended.) By producing an air quality model that is
 computationally inexpensive to operate, relatively easily adaptable to new geographical
 regions, able to be operated with a moderate level of specialist knowledge, we hope to
 make air quality modeling more widespread, easier, and more accessible to scientists,
 policymakers, and concerned citizens worldwide.

Supporting Information



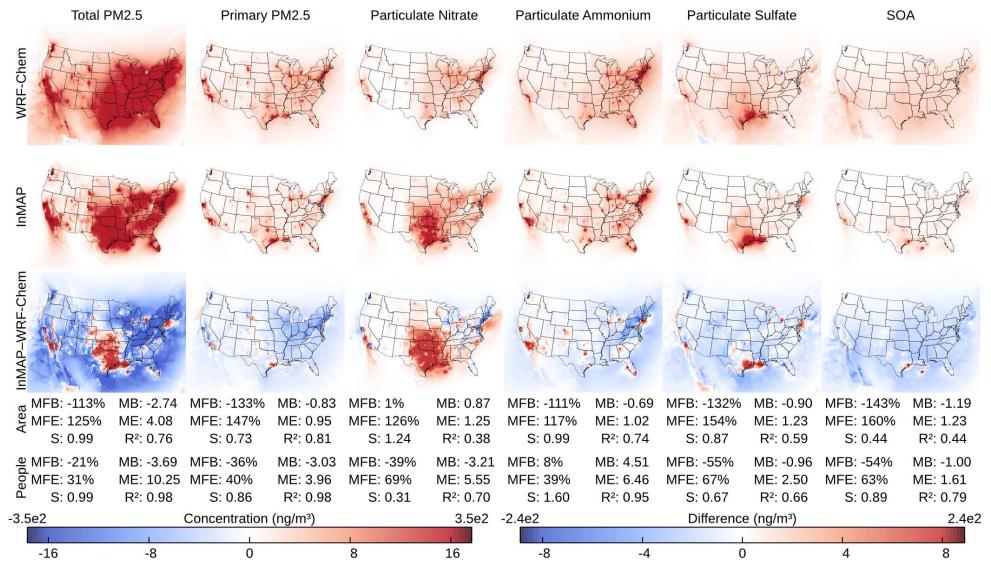
S1 Fig Annual average increases in pollutant concentrations caused by an emission scenario with on-road emissions from gasoline powered vehicles as the largest emissions source, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



S2 Fig Annual average increases in pollutant concentrations caused by an emission scenario with on-road emissions from hybrid gasoline-electric powered vehicles as the largest emissions source, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error;

S = slope of regression line; R^2 = squared Pearson correlation coefficient.

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S3 Fig Annual average increases in pollutant concentrations caused by an emission scenario with on-road emissions from diesel powered vehicles as the largest emissions source, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

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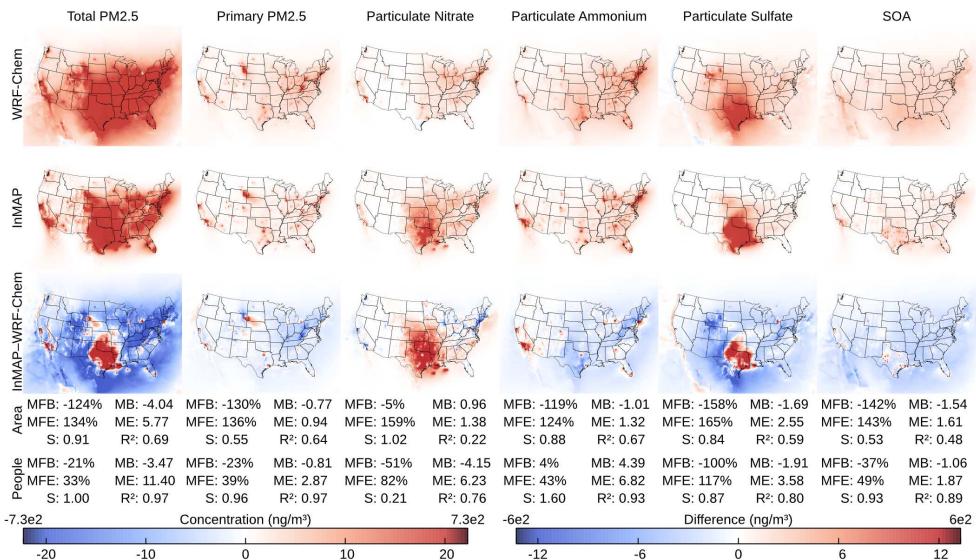
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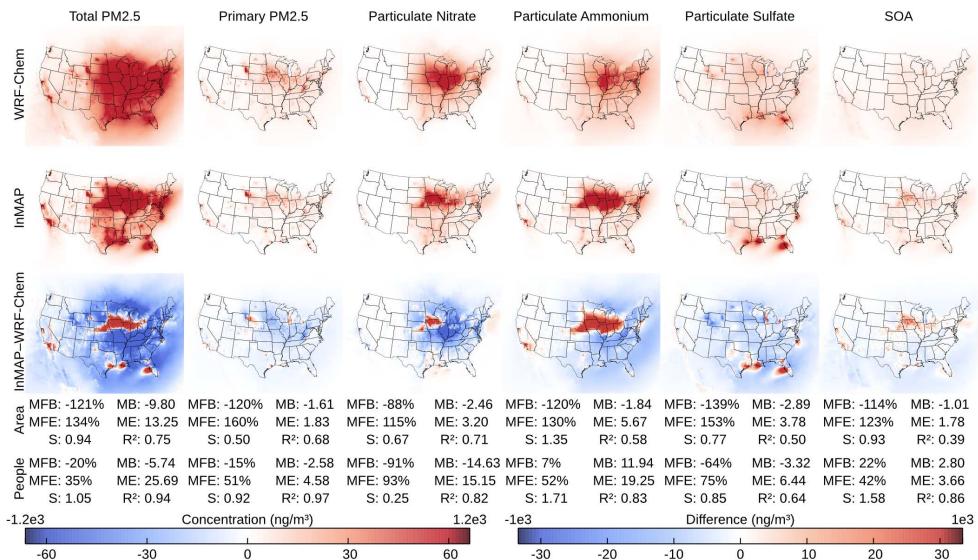
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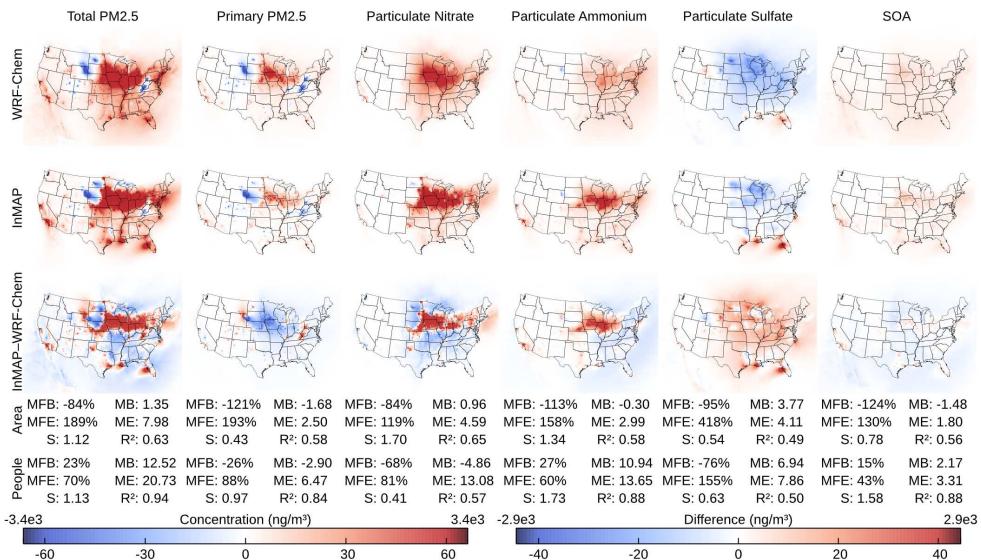
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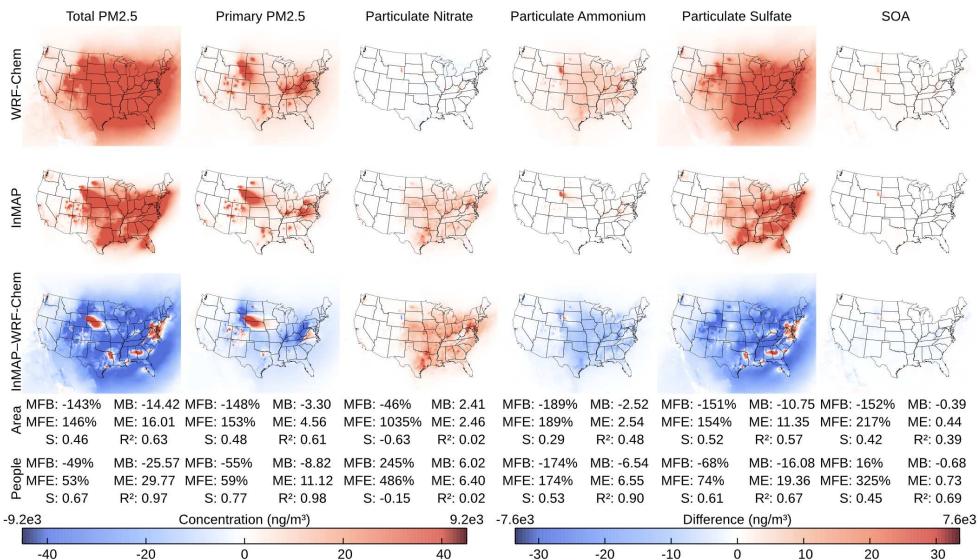
S4 Fig Annual average increases in pollutant concentrations caused by an emission scenario with on-road emissions from compressed natural gas (CNG) powered vehicles as the largest emissions source, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



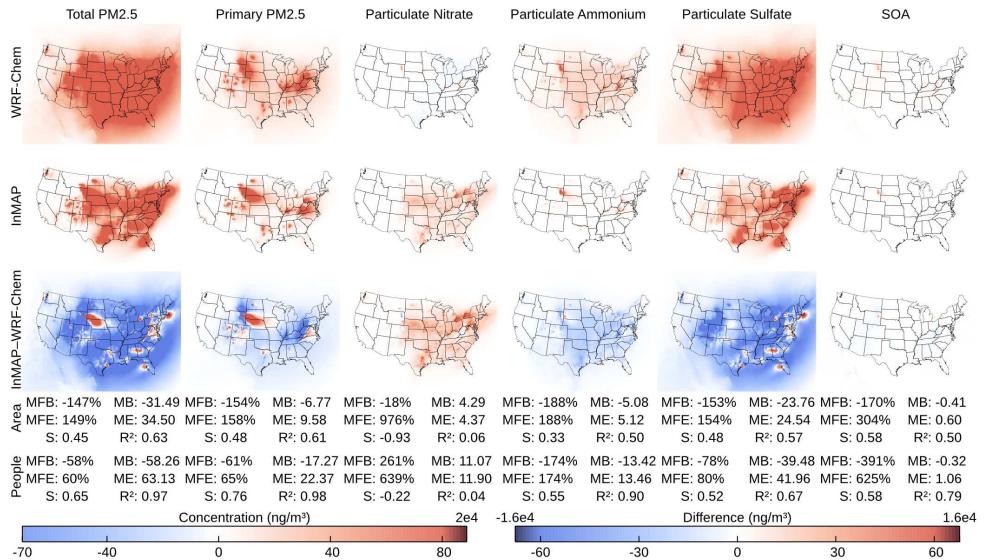
S5 Fig Annual average increases in pollutant concentrations caused by an emission scenario with industrial emissions, agricultural emissions, and on-road emissions from ethanol powered vehicles as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



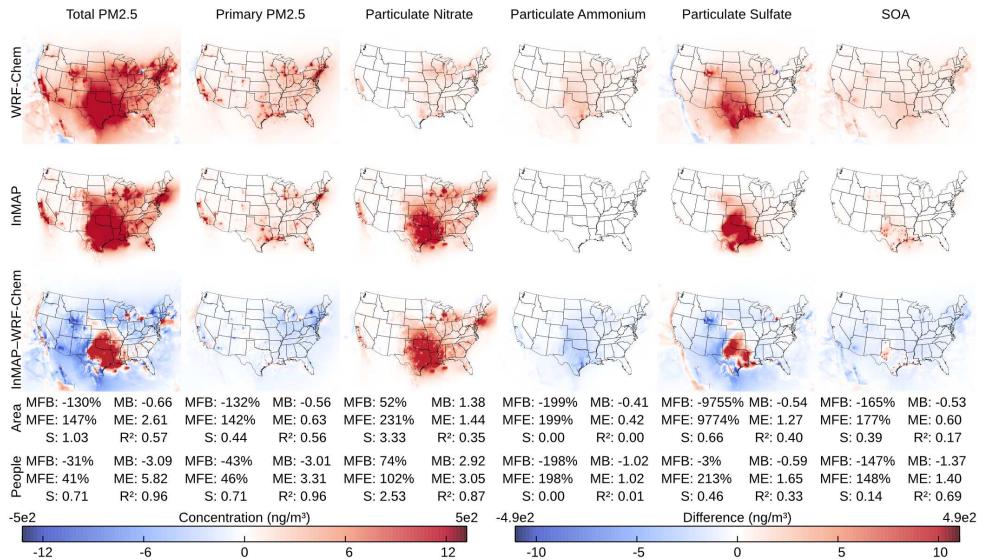
S6 Fig Annual average increases in pollutant concentrations caused by an emission scenario with industrial emissions, agricultural emissions, and on-road emissions from ethanol powered vehicles as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



S7 Fig Annual average increases in pollutant concentrations caused by an emission scenario with emissions from coal- and natural gas-powered electric generation and from coal mining as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

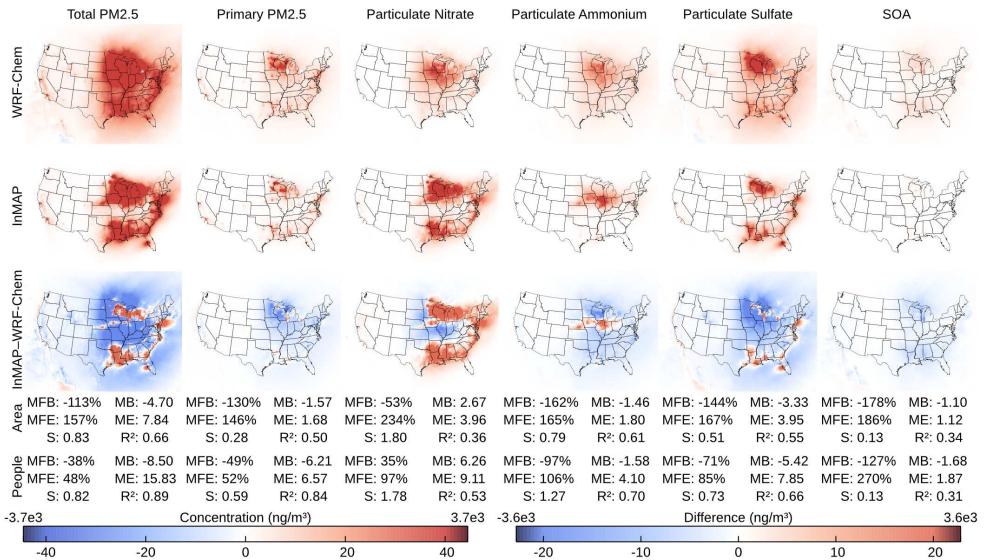


S8 Fig Annual average pollutant concentrations caused by an emission scenario with emissions from coal-powered electric generation and from coal mining as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



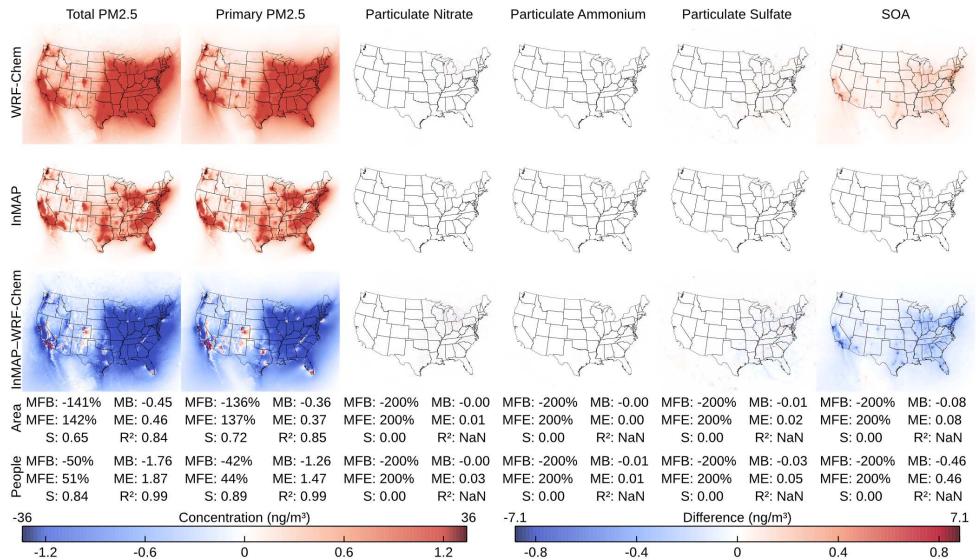
S9 Fig Annual average pollutant concentrations caused by an emission scenario with emissions from natural-gas powered electric generation and natural gas extraction and processing as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale.

Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

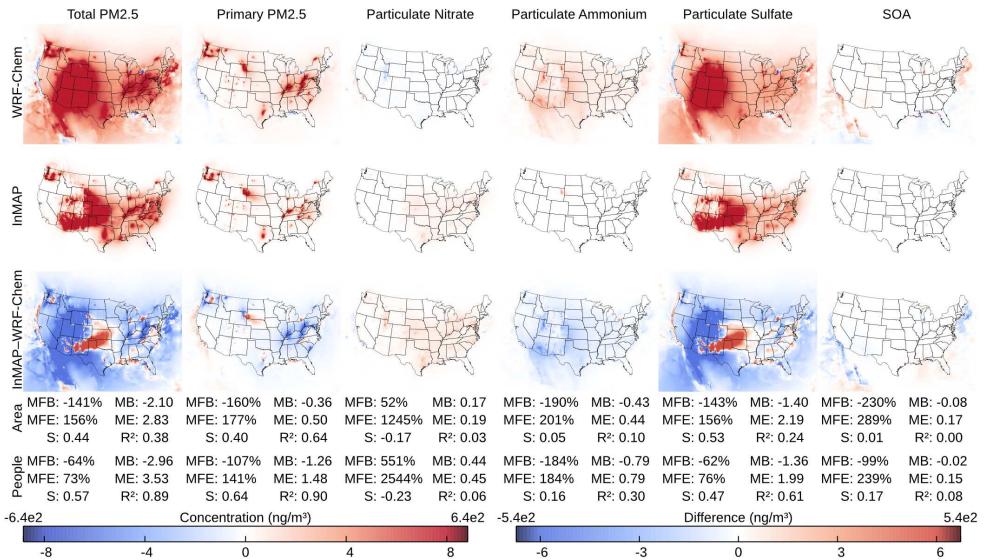


S10 Fig Annual average pollutant concentrations caused by an emission scenario with emissions from agricultural sources and from biomass-powered electric generation as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale.

Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



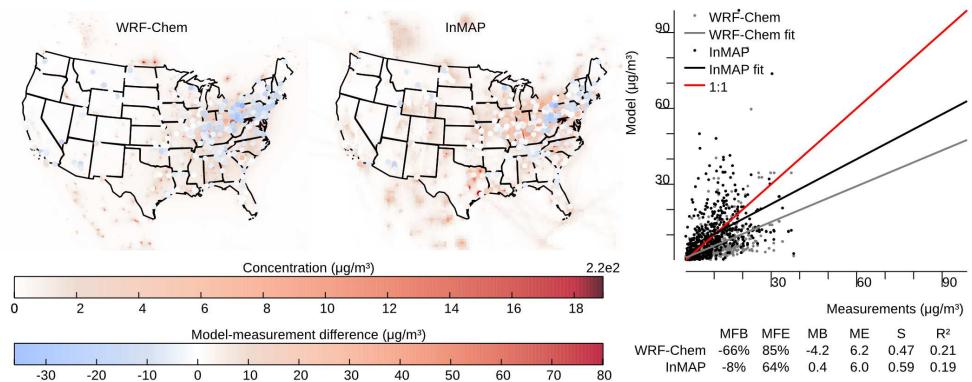
S11 Fig Annual average pollutant concentrations caused by an emission scenario with on-road emissions from vehicle brake and tire wear as the only emissions source, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



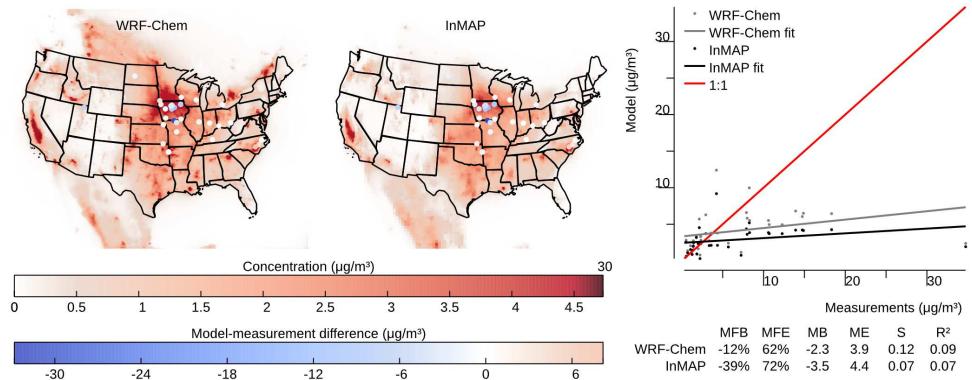
S12 Fig Annual average pollutant concentrations caused by an emission scenario with emissions from mineral extraction and electricity production as the largest emissions sources, as predicted by WRF-Chem (first row) and InMAP with a 12 km resolution grid (second row), as well as the difference between the two models (third row). Colors in the first two rows correspond to the legend on the left and colors in the third row correspond to the legend on the right. For ease of viewing, there is a discontinuity at the 99th percentile of concentration values in each color scale. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



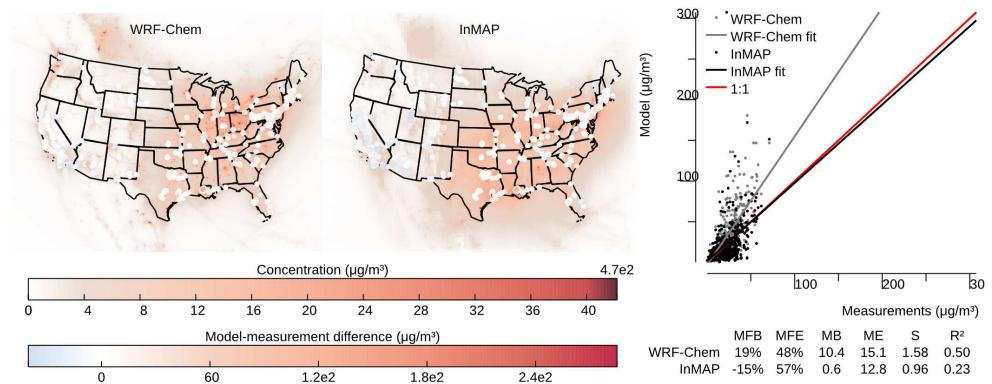
S13 Fig Boundaries of US regions used in this article.



S14 Fig Comparison of WRF-Chem and InMAP performance in predicting annual average observed SO_x concentrations. The background colors in the maps represent predicted concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



S15 Fig Comparison of WRF-Chem and InMAP performance in predicting annual average observed NH_3 concentrations. The background colors in the maps represent modeled concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.



S16 Fig Comparison of WRF-Chem and InMAP performance in predicting annual average observed NO_x concentrations. The background colors in the maps represent modeled concentrations, and the colors of the circles on the maps represent the difference between modeled and measured values at measurement locations. Abbreviations: MFB = mean fractional bias; MFE = mean fractional error; MB = mean bias; ME = mean error; MR = model ratio; S = slope of regression line; R^2 = squared Pearson correlation coefficient.

S1 Appendix A review of existing reduced-complexity air quality models.

S2 Appendix A description of the spatial discretization algorithm and the computational time required to run the model with different spatial grid settings.

S1 Table The names of WRF-Chem variables used by the InMAP preprocessor and their descriptions.

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InMAP: a model for air pollution interventions: supporting information appendix 1

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1 Existing reduced-complexity air quality models

1.1 CTM-based sensitivity models

Several CTM-based tools can reduce the computational requirements of determining how changes in emissions would impact air pollution concentrations. The direct decoupled method (DDM, Zhang et al., 2012; Foley et al., 2014), can, for example, calculate spatially explicit changes in health impacts attributable to changes in overall emissions. The adjoint method (Hakami et al., 2007; Dedoussi and Barrett, 2014), can, for example, calculate how spatially explicit changes in emissions cause changes in overall health impacts. Source apportionment attributes pollutant concentrations or concentration sensitivities among different sources. One example of a source apportionment tool is the Particle Source Apportionment Tool (PSAT) (Wagstrom et al., 2008). All three of these approaches can be computationally inexpensive to use once the original sensitivities are calculated and are likely more accurate than the approach we present here. However, the calculated sensitivities are often not widely adaptable to different use-cases. For instance, changing the spatial distribution of emissions in the case of DDM, the spatial distribution of the human population in the case of the adjoint method, or the sources of interest in the case of source apportionment would require re-running the CTM to create a new set of sensitivities. For this reason, these methods generally are not amenable to use by non-experts.

There additionally exist statistical models based on the results of many CTM runs (e.g., the Response Surface Model, US EPA, 2006; Foley et al., 2014; models based on neural networks or neuro-fuzzy systems, Carnevale et al., 2009; EASIUR, Heo et al., 2016; or the model by Buonocore et al. (2014)); the requirement of many CTM runs renders these models computationally expensive to create and update.

1.2 Gaussian

Gaussian plume models (e.g., AERMOD, Cimorelli et al., 2005) and models that are derived from them (e.g., COBRA, US EPA, 2012; APEEP, Muller and Mendelsohn, 2006; SIM-air, Guttikunda, 2009; or the model developed for the US EPA National Air Toxics Assessment (NATA), Logue et al., 2011) analytically estimate the downwind impact of individual sources or source groups. These models are computationally inexpensive and useful for predicting near-source impacts but are not recommended for predictions of pollution transport over long distances (> 50 km, US EPA, 2015). Additionally, Gaussian plume models generally cannot robustly represent nonlinear or spatially variable rates of formation and evaporation of secondary PM_{2.5} (Seinfeld and Pandis, 2006).

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1.3 Lagrangian

Lagrangian models such as CALPUFF (Scire et al., 2000) and HYSPLIT (Draxler and Hess, 1997) track long range transport from individual sources by tracking a packet of air as it interacts with its surroundings. These models typically are less computationally intensive than CTMs if the number of sources is small, but simulating many individual sources over a broad area can be computationally prohibitive.

1.4 Chemical mass balance

Chemical mass balance models (e.g., CMB: US EPA, 2004) estimate the contribution of different emissions source types to ambient pollution concentrations by analyzing the relative contributions of different chemical tracers and matching them to tracer profiles of known sources. This method is useful for estimating the contribution specific source types, but requires detailed location-specific measurements and can only track contributions from sources with known tracer profiles. Additionally, chemical mass balance models cannot directly predict how changes in emissions would impact concentrations.

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InMAP: a model for air pollution interventions: supporting information appendix 2

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1 Spatial discretization algorithm

To use numerical integration to solve the chemical and physical equations that describe the processes relevant to air pollution, a model must break up the spatial and temporal domains of interest into finite elements. InMAP spatially discretizes the model domain using a variable resolution rectangular grid, where individual grid cells can nest and telescope between lower and higher resolution based on human population density or other attributes. Grid cell resolution is determined by one of the two algorithms described here. In both algorithms, given a list of possible grid cell sizes, the model domain is first filled with the lowest resolution grid cells (48 km). We will refer to grids produced by the first algorithm as "static variable resolution", as grid cell size does not change during the simulation, and we will refer to grids produced by the second algorithm as "dynamic variable resolution", as grid cell size does change during the simulation.

In the first algorithm, the program next iterates through the grid cells, determining if the population in each grid cell is above a certain threshold level. If the population in the grid cell is above the threshold level, the grid cell is split into grid cells of the next smallest size. The algorithm recurses through this process until either all of the cells are below the population threshold or the smallest specified grid cell size has been reached. The algorithm also has a second constraint, where any of the smallest-size grid cells having a maximum population density greater than a certain threshold level are kept at the finest resolution. This constraint is important where high population density areas are directly adjacent to low population density areas, such as in coastal cities. Because variability in pollutant concentrations decreases with increased height above the ground, all grid cells above a given height cutoff are kept at the lowest model resolution. As shown in Fig. 1 of the main manuscript, we use here a spatial domain which covers the contiguous US, southern Canada, and northern Mexico, with grid cell edge lengths of 48, 24, 12, 4, 2, and 1 km, a population threshold of 40 000 people per grid cell, a population density threshold of 5500 people km^{-1} , and a height cutoff of the eighth model layer (approximately 1500 m, chosen because this height is usually above the planetary boundary layer). These settings are chosen to achieve a balance between the spatial detail and model runtime. Other spatial domains are possible: the spatial extent of the modeling domain is only limited by the availability of meteorological and chemical input data. Meteorological and chemical properties in InMAP cells that do not exactly coincide with grid cells in the input data set are taken as the average of all input grid cells that they overlap with.

The second algorithm runs occasionally during the simulation to create a dynamically varying grid rather than before the simulation starts as the first algorithm does. When the second algorithm runs, it first calculates the total human population P_t and the total mass of all pollutants M_t in the simulation domain.

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Then for each grid cell, it iterates through each neighboring grid cell, calculating the difference between the population in the grid cell and the population in the neighbor ΔP . Then it iterates through each pollutant species, calculating the sum of concentration differences ΔC_t as in Eq 1:

$$\Delta C_t = \sum_{i=1}^n (|C_i - C_{n,i}|) \quad (1)$$

where C is concentration, i is one of n pollutant species, and C_n is the concentration in the neighboring grid cell. Then, whether the grid cell should be split into smaller grid cells is decided by the criteria in Eq 2:

$$\Delta C_t (V + V_n) \Delta P (M_t P_t)^{-1} > t \quad (2)$$

where V and V_n are the volume of the grid cell and the neighbor, respectively, and t is a threshold value. If Eq 2 is true for the relationship between the grid cell and any of its neighbors, then the grid cell is split into smaller grid cells.

As the model simulation runs, it first starts out with $t = 1$ to ensure no grid cell division and runs until the simulation converges. Then, it sets t to a user-specified value ($t = 1 \times 10^{-11}$ in simulations performed here) and continues to run the simulation until it converges again. This reduces overall model runtime compared with initially setting t to the user-specified value.

2 Model computational requirements

Table 1 shows the time required to run InMAP simulations with different emissions scenarios and different grid types and parameters using the computer hardware described in Table 2. Simulation results presented in the main text use a dynamic variable resolution grid with a threshold of 1e-11, which for the National Emissions Inventory scenario has a runtime of approximately two hours.

This computational intensity can be compared to the computational intensity of the WRF-Chem simulation that we used to create preprocessed InMAP inputs, as both the InMAP and WRF-Chem simulations cover the same spatial domain and time period. That simulation was split into eight segments, each of which ran approximately 20 hours on 96 nodes on a high-performance computing (HPC) cluster, with each node consisting of two quad-core 2.8 GHz Intel Xeon X5560 "Nehalem EP" processors sharing 24 gigabytes of memory. This adds up to approximately 122,880 core-hours for the WRF-Chem simulation, compared to 8 core-hours for an InMAP simulation (2 hours on a 4-core computer), for a speedup factor of approximately 15,000. The hardware used for the WRF-Chem simulations is not identical to the hardware used for the InMAP simulations (shown in Table 2), but it is of similar vintage.

Table 1: InMAP Simulation Run Time for NEI Emissions with a Static and Dynamic Variable Resolution Spatial Grids

Grid type	Threshold	Cell size ^b	Number of Grid cells	Elapsed time (Hours)
static	4e4; 5.5e3 ^a	11	6.0E+05	10.1
dynamic	1e-06	48	9.3E+03	0.4
dynamic	1e-08	36	1.0E+04	0.6
dynamic	1e-10	12	3.2E+04	0.8
dynamic	1e-11	7	8.0E+04	1.9
dynamic	1e-12	4	2.0E+05	8.1

^a Static variable grid simulations require two parameters for population and population density, respectively.

^b Cell size is the population-weighted average grid cell horizontal edge length.

Table 2: Computational Hardware Used in Simulations Described in Table 1

Component	Specification
Processor	Intel Core I7-6700 3.40 GHz 8 M Processor Cache 4 LGA 1151
Memory	Kingston HyperX FURY Black 32GB (4x8GB) 2133MHz DDR4 NonECC
Motherboard	MSI Intel Skylake H170 LGA 1151 DDR4 USB 3.1 Micro ATX
Hard drive	Samsung 850 EVO 1 TB 2.5Inch SATA III Internal SSD

InMAP: a model for air pollution interventions: supporting information table 1

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Table 1: Names of WRF-Chem Variables used by the InMAP Preprocessor and their Descriptions

Name(s)	Description and use in InMAP preprocessor
hc5, hc8, olt, oli, tol, xyl, csl, cvasoa1, cvasoa2, cvasoa3, cvasoa4	Anthropogenic VOCs that are SOA precursors; used to determine VOA/SOA partitioning
asoal1, asoa1j, asoa2i, asoa2j, asoa3i, asoa3j, asoa4i, asoa4j	Anthropogenic SOA; used to determine VOA/SOA partitioning
iso, api, sesq, lim, cvbsoa1, cvbsoa2, cvbsoa3, cvbsoa4	Biogenic VOCs that are SOA precursors; used for model evaluation
bsoal1, bsoa1j, bsoa2i, bsoa2j, bsoa3i, bsoa3j, bsoa4i, bsoa4j	Biogenic SOA; used for model evaluation
no, no2	Components of NO_x ; used to determine $\text{NO}_x/p\text{NO}_3$ partitioning
no3ai, no3aj	Components of $p\text{NO}_3$; used to determine $\text{NO}_x/p\text{NO}_3$ partitioning
so2, sulf	Gaseous SO_2 and sulfate; used to determine $\text{SO}_x/p\text{SO}_4$ partitioning
so4ai, so4aj	Particulate SO_4 ; used to determine $\text{SO}_x/p\text{SO}_4$ partitioning
nh3	Ammonia; used to determine $\text{NH}_3/p\text{NH}_4$ partitioning
nh4ai, nh4aj	Particulate Ammonium; used to determine $\text{NH}_3/p\text{NH}_4$ partitioning
PM2_5_DRY	Total PM _{2.5} concentration in the baseline simulation; used for model evaluation
U, V, W	Wind fields; used to determine advection and mixing coefficients
PBLH	Planetary boundary layer height; used to determine mixing coefficients
PHB, PH	Base state geopotential and perturbation geopotential; used to calculate layer heights
HFX	Surface heat flux; used to determine mixing and dry deposition
UST	Friction velocity; used to determine mixing and dry deposition
T	Temperature; used to calculate chemical reaction rates and plume rise
PB, P	Base state pressure plus perturbation pressure; used to calculate chemical reaction rates and plume rise
ho, h2o2	Hydroxyl radical and hydrogen peroxide concentrations; used to calculate chemical reaction rates
LU_INDEX	Land use type; used to calculate mixing
QRAIN	Mixing ratio of rain; used to calculate wet deposition
CLDFRA	Fraction of grid cell covered by clouds; used to calculate wet deposition
QCLOUD	Cloud mixing ratio; used to calculate aqueous-phase chemical reaction rates
ALT	Inverse air density; used to calculate mixing and to convert between mixing ratio and mass concentration
SWDOWN, GLW	Downward shortwave and longwave radiative flux at ground level; used to calculate dry deposition

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