Applying CMAQ sensitivity analysis for the state of California: reduced order modeling, source attribution, and process analysis

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Abstract

We present results from our ongoing effort of investigating the potential of CMAQ sensitivity analysis in supporting air quality policy making and planning in the state of California. The model code for CMAQ-DDM-3D (v5.2) was adapted with the SAPRC07tic-AERO6i chemical mechanism, and then used for reduced order modeling (ROM), source attribution, and process analysis. A reduced order model (ROM) was constructed to establish first-order source-receptor relationships between emissions of NOx and VOCs from 58 counties in California and gridded surface concentrations for the full suite of CMAQ output species at a 12 km resolution. With nitrate as an example, the ROM is shown to allow efficient projections of changes in air quality due to emission perturbations at 58 counties as resulting from a future regulation, while its accuracy is illustrated by comparing against results from full CMAQ modeling. Source contributions from 58 counties to nitrate are estimated with the ROM, considering both transport and chemistry with a first-order approximation. These results also illustrate the potential of using sensitivity analysis to help understand chemical and transport processes (e.g., nitrate formation and its dependency on emissions of precursors).

CMAQ-DDM-3D testing

- ❑ **Adapted CMAQ-DDM-3D code to use SAPRC-07 mechanism**
  - Developed an R program to automatically generate the FORTRAN Jacobian subroutine for SAPRC07 mechanism (or any other mechanism)
- ❑ **Storage and computational cost largely scale with number of parameters (≈ 58 CMAQ runs in our case)**
  - Tested IOAPI-LARGE and adopted a combination of NetCDF-4 (small but slow), and NetCDF-3 (big but fast) formats for model outputs
  - Developed a relatively fast post-processing procedure in Python

Model setup & inputs

- ❑ CMAQ-DDM-3D v5.2 with SAPRC07tic and aero6i
- ❑ WRF meteorology for statewide 12 km domain with 30 vertical layers
- ❑ Boundary conditions from CAM-CHEM
- ❑ Emissions scenarios:

Emissions scenarios	Definition
GID610	2017 baseline (CMAQ and CMAQ-DDM-3D)
GID611	2032 baseline (CMAQ and CMAQ-DDM-3D)
GID612	2032 with Small Off-Road Engines (SORE) regulations (CMAQ)

- ❑ Shapefiles for 58 counties (TIGER) to develop a 12-km mask as part of the input for CMAQ-DDM-3D

Reduced order model and source attribution with first order sensitivities

❑ **Definition (first order, local)**

- Sensitivity $(\partial C_j/\partial E_i)$ = Δ concentration of pollutant *j* from unit Δ emission of precursor *i*

❑ **Application 1: Reduced order modeling**

Predict ΔConcentration given emission change ΔEmission for 58 counties

- $\Delta\text{Concentration} \approx \sum_{i=1}^{n=58\ CA\ counties} \frac{\partial C_j}{\partial E_i} \times \Delta E_i$
  - **Case 1:** (5%-10% ΔEmission) : 2032 baseline → Small Off-road Engine (SORE) regulations
  - **Case 2:** (25%-40% ΔEmission): 2017 baseline → 2032 baseline

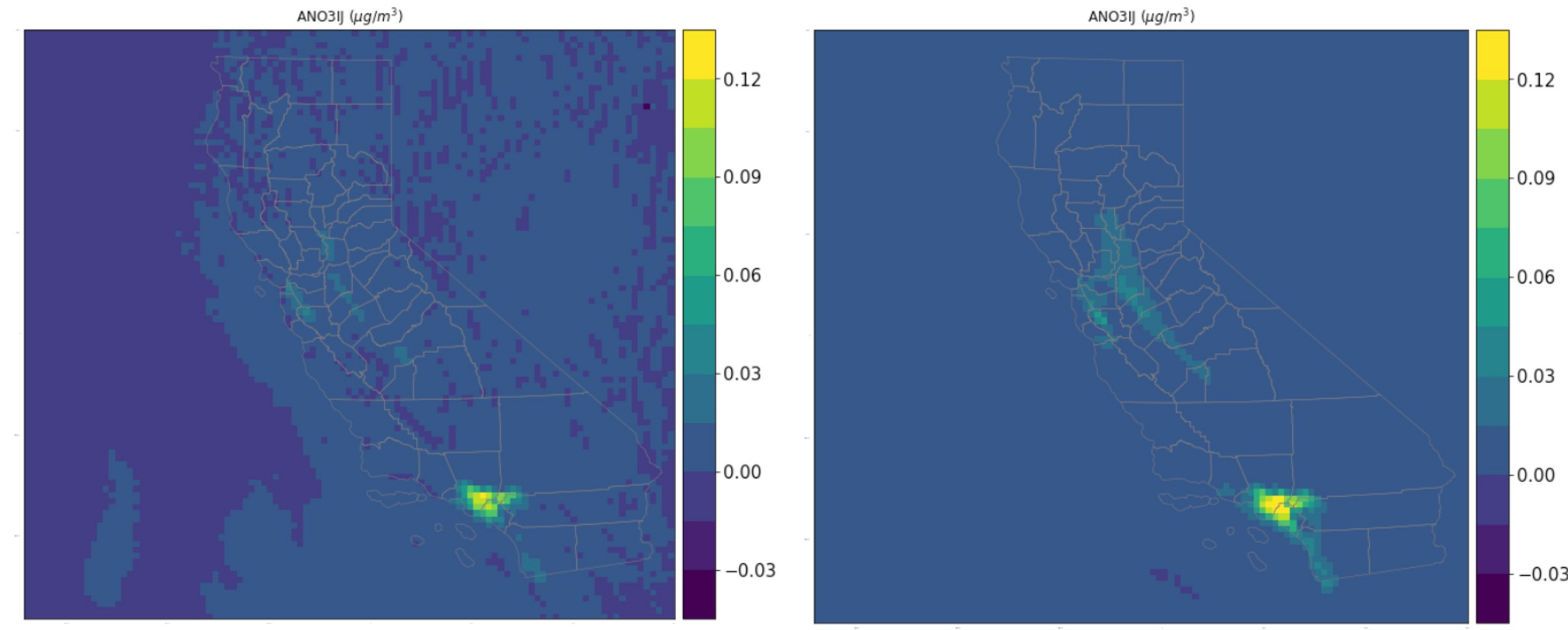
❑ **Application 2: Source attribution**

Break down of ΔConcentration to individual sources/regions

Δ Nitrate

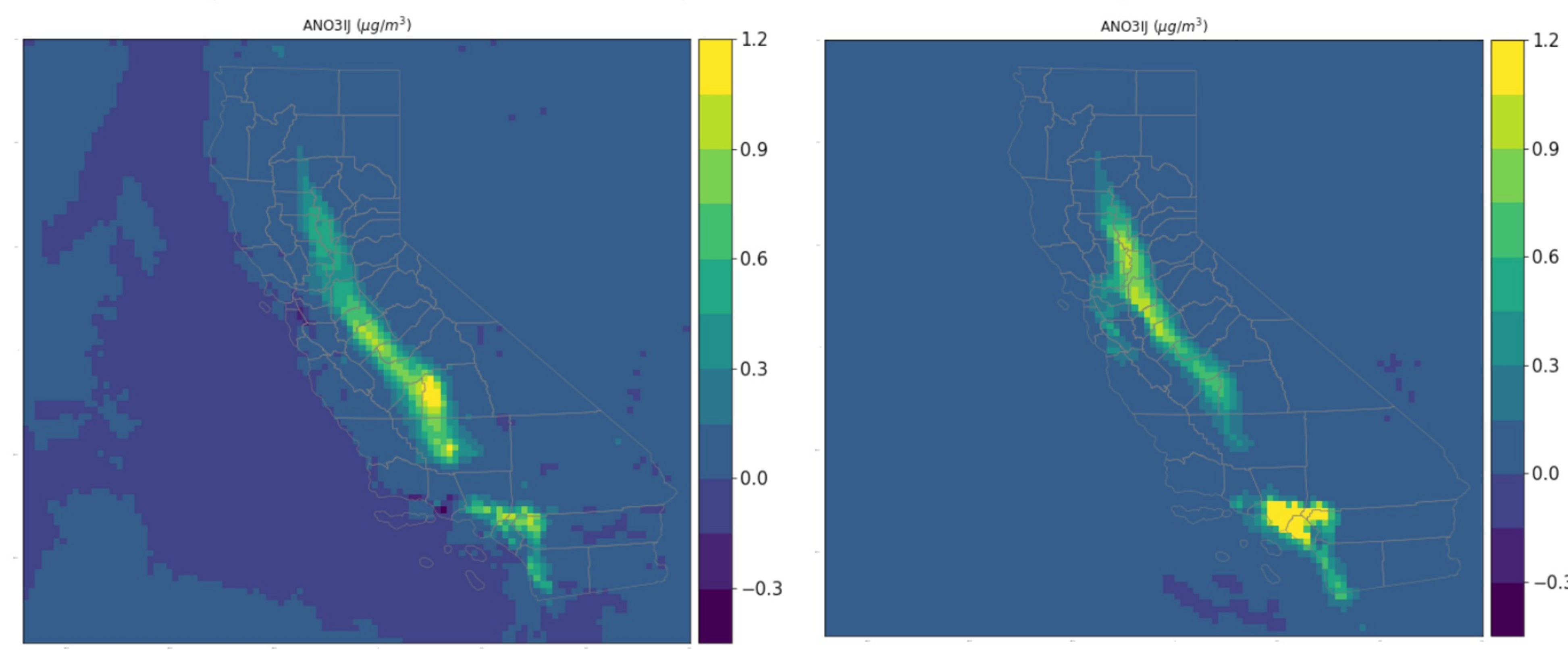
(Case 1: 2032 baseline → 2032 SORE)

CMAQ (2032 baseline minus **2032 SORE)** | **CMAQ-DDM-ROM**

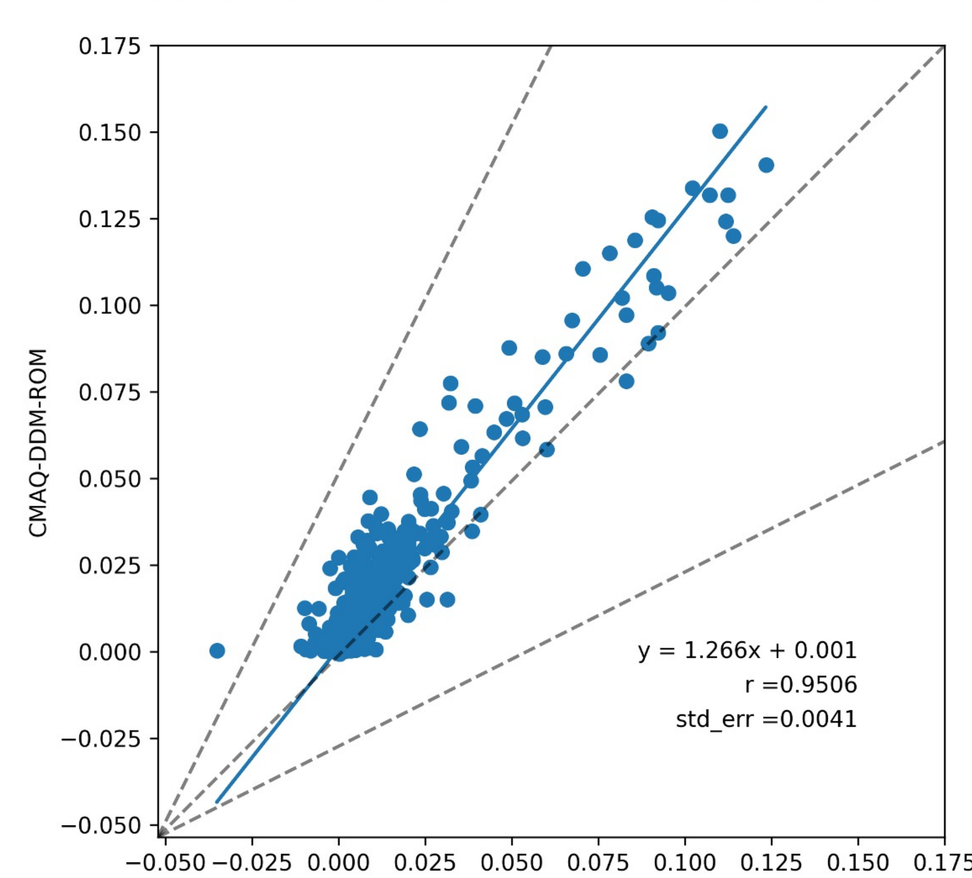


(Case 2: 2017 baseline → 2032 baseline)

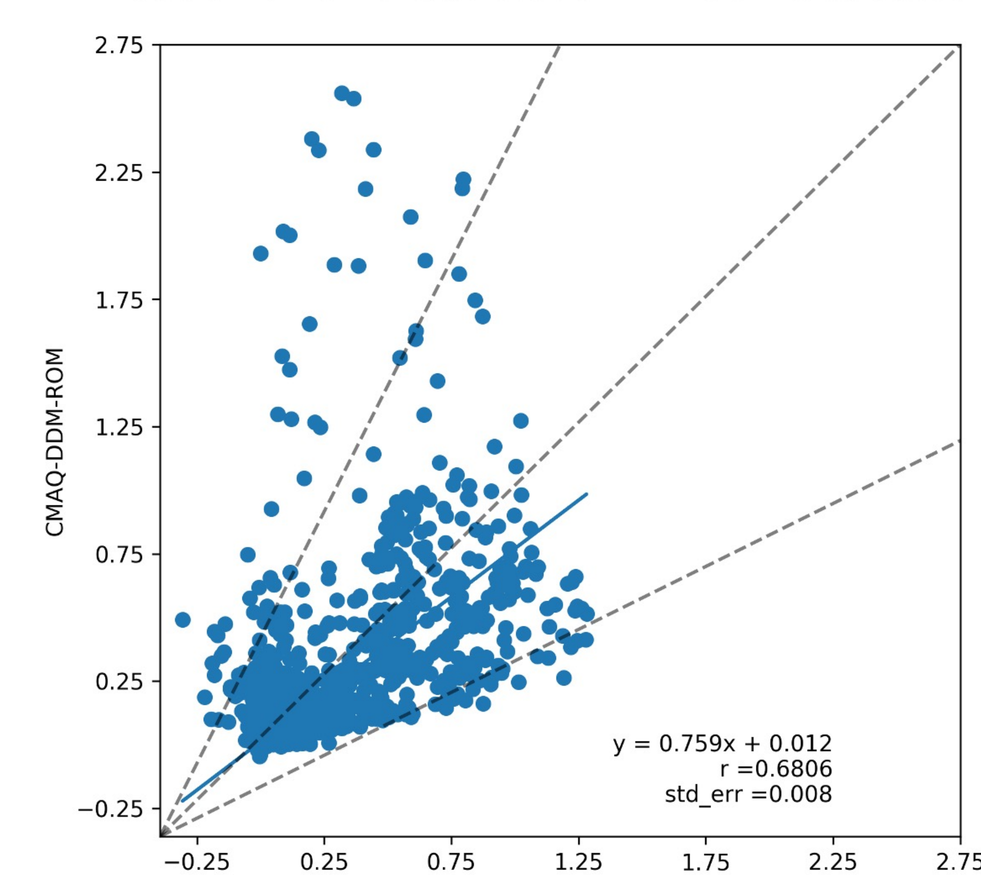
CMAQ (2017 baseline minus **2032 baseline)** | **CMAQ-DDM-ROM**



Δ Nitrate
Case 1: 2032 baseline → 2032 SORE

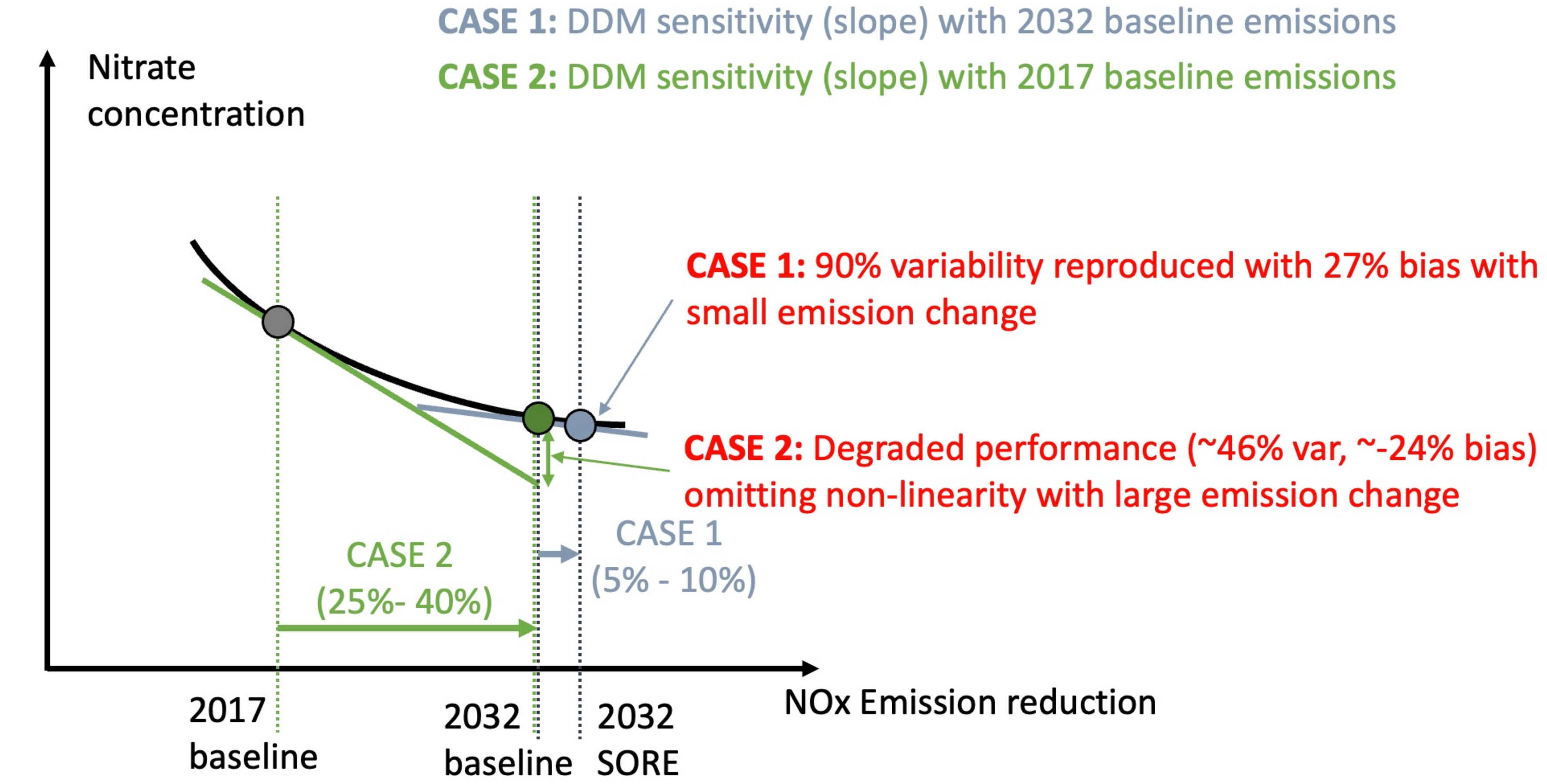


Δ Nitrate
Case 2: 2017 baseline → 2032 baseline

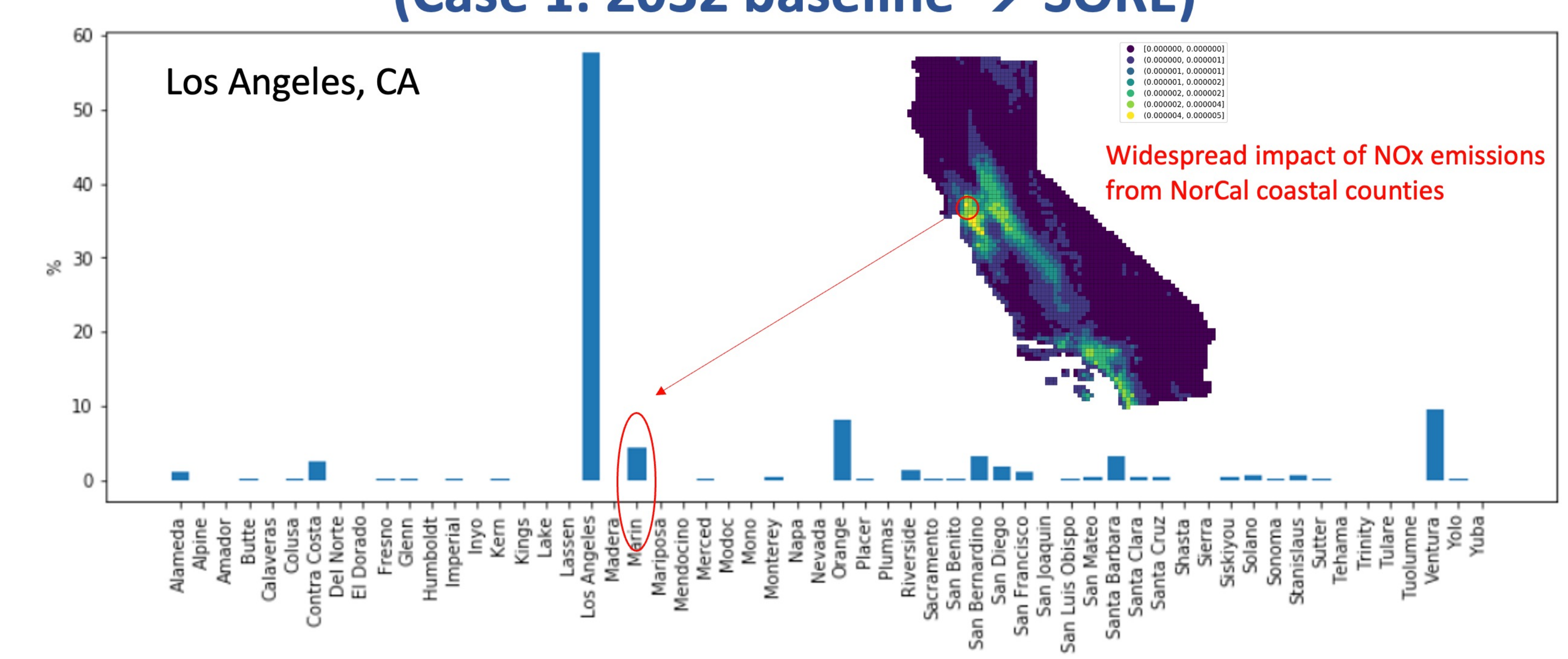


Non-linear response of nitrate to NOx emission reduction

Black line (CMAQ): True response of concentration to emission change
CASE 1: DDM sensitivity (slope) with 2032 baseline emissions
CASE 2: DDM sensitivity (slope) with 2017 baseline emissions



Source attribution of Δnitrate (Case 1: 2032 baseline → SORE)



Summary of findings

- ❑ Computational cost of CMAQ-DDM-3D largely scales with number of parameters
- ❑ CMAQ-DDM-ROM (first order, local) can reproduce 90% of nitrate spatial variability with a mean bias of 27% with 5% - 10% emission change
- ❑ CMAQ-DDM-ROM can be useful in understanding sources of secondary pollutant such as nitrate

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