

# DEVELOPMENT AND IMPLEMENTATION OF A FORMAL FRAMEWORK FOR BOTTOM-UP UNCERTAINTY ANALYSIS OF INPUT EMISSIONS: CASE STUDY OF RESIDENTIAL WOOD COMBUSTION

---

RABAB MASHAYEKHI, *ENVIRONMENT AND CLIMATE CHANGE CANADA*

SHUNLIU ZHAO, **Y. BURAK OZTANER**, SAHAR SAEEDNOORAN, AMIR HAKAMI  
*DEPARTMENT OF CIVIL AND ENVIRONMENTAL ENGINEERING, CARLETON UNIVERSITY, OTTAWA, CANADA*

MICHAEL MORAN, RICHARD MÉNARD,, AND JUNHUA ZHANG  
*AIR QUALITY RESEARCH DIVISION, ENVIRONMENT AND CLIMATE CHANGE CANADA*



# WHY IS EMISSIONS UNCERTAINTY QUANTIFICATION IMPORTANT?

---

- Impacts downstream applications of air quality models (AQMs), where costly decisions are made based on models' "best estimates"
- Identifies priorities for improving emissions estimates

# WHY A CASE STUDY FOR RESIDENTIAL WOOD COMBUSTION (RWC)?

---

- Provides proof of concept for emissions uncertainty framework
- Known to have a high level of uncertainty
- Important source of PM, VOCs in the U.S. and Canada during the cold months
- Create an Inventory of uncertainties consistent with the emission inventory

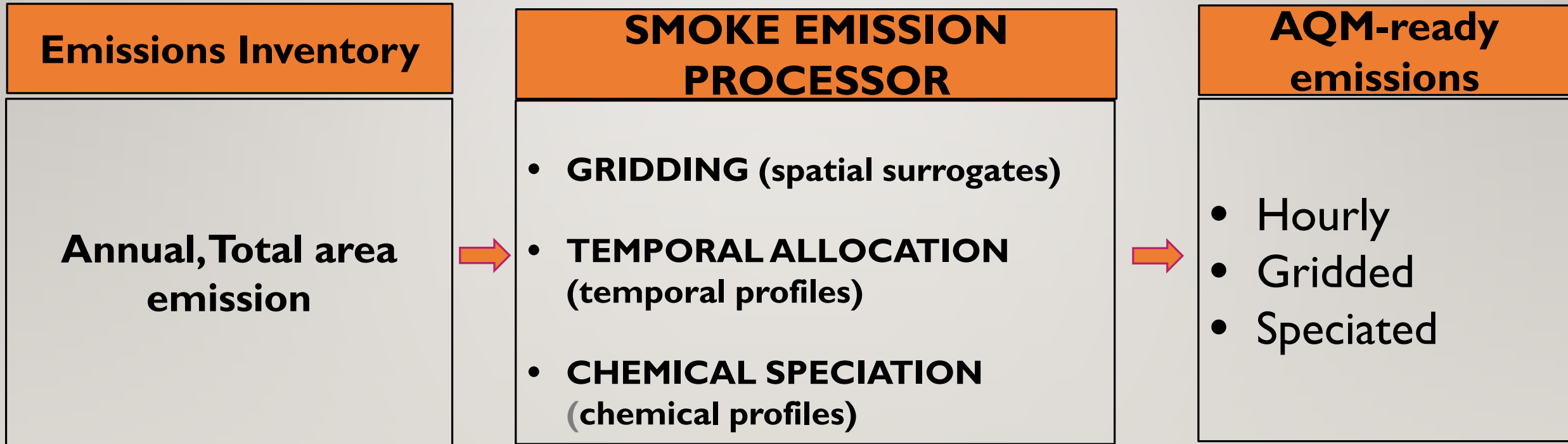


# HYPOTHESIS FOR UNCERTAINTY INVENTORY DEVELOPMENT

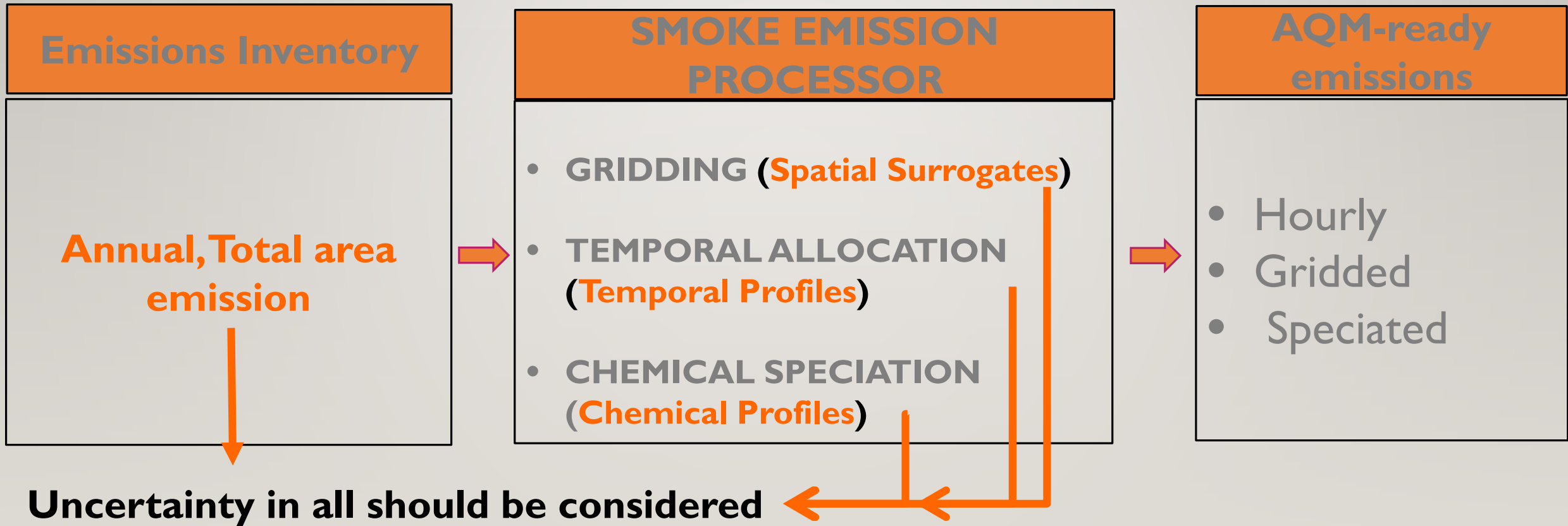
---

- It is easier and more accurate to quantify uncertainties in raw input into the emission model, than it is to estimate uncertainty in gridded emissions
- The purpose is to
  - I. develop an inventory of input uncertainties alongside the inventory of emissions,
  - II. Propagate these uncertainties through the emission model (SMOKE)
- The framework also allows to identify areas where we have less knowledge of uncertainties.

# BOTTOM-UP APPROACH FOR UNCERTAINTY ASSESSMENT



# BOTTOM-UP APPROACH FOR UNCERTAINTY ASSESSMENT



# RWC INVENTORY CALCULATION FOR U.S.

---

$$\text{Emission} = \text{ACTIVITY} \quad \times \quad \text{EMISSION FACTOR}$$

(Mass of wood) (Mass of pollutants/mass of wood)

$$\text{(Volume of wood)} \times \text{(Wood density)}$$

$$\text{(Number of appliances)} \times \text{(Burn Rate)} \times \text{(Climate adjustment)}$$

$$\text{(Occupied housing units)} \times \text{(Appliance Fraction)}$$

# SOURCES OF DATA FOR U.S

$$\text{Emission} = \text{ACTIVITY} \times \text{EMISSION FACTOR}$$

(Mass of wood) (Mass of pollutants/mass of wood)  
AP-42 documents

$$\text{(Volume of wood)} \times \text{(Wood density)} \leftrightarrow \text{U.S. Forest Service, Timber Products Output}$$

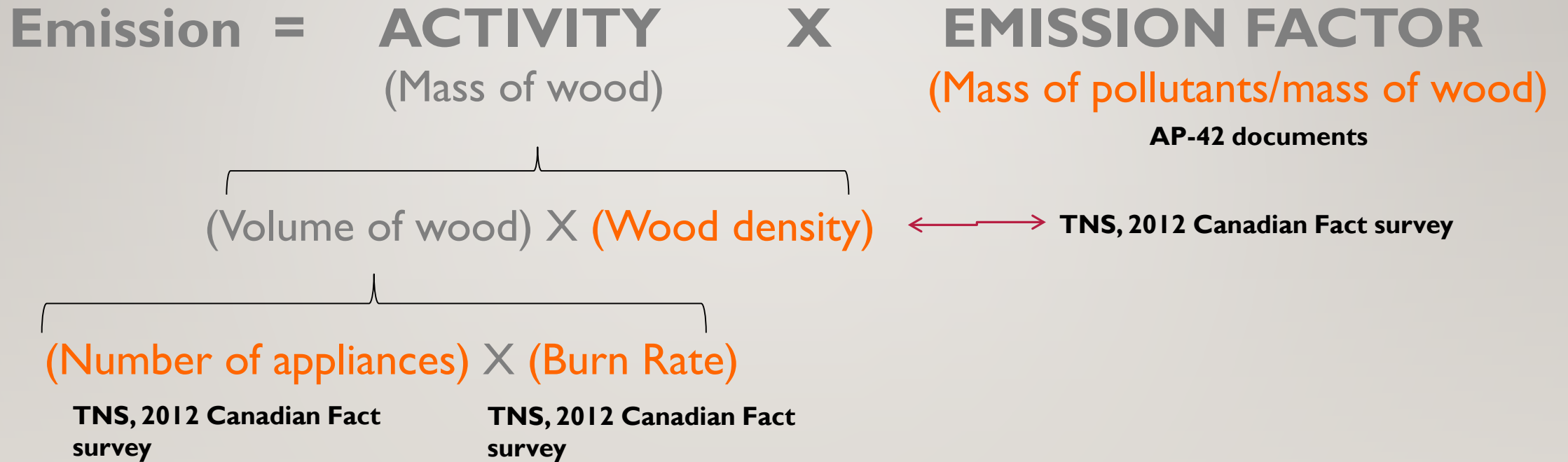
$$\text{(Number of appliances)} \times \text{(Burn Rate)} \times \text{(Climate adjustment)} \leftarrow \text{U.S. Department of Agriculture, Commercial Buildings Energy Consumption Survey}$$

$$\text{(Occupied housing units)} \times \text{(Appliance Fraction)} \leftarrow \text{2010 U.S. Census, American Housing Survey (U.S. Census Bureau)}$$



# SOURCES OF DATA FOR CANADA

---



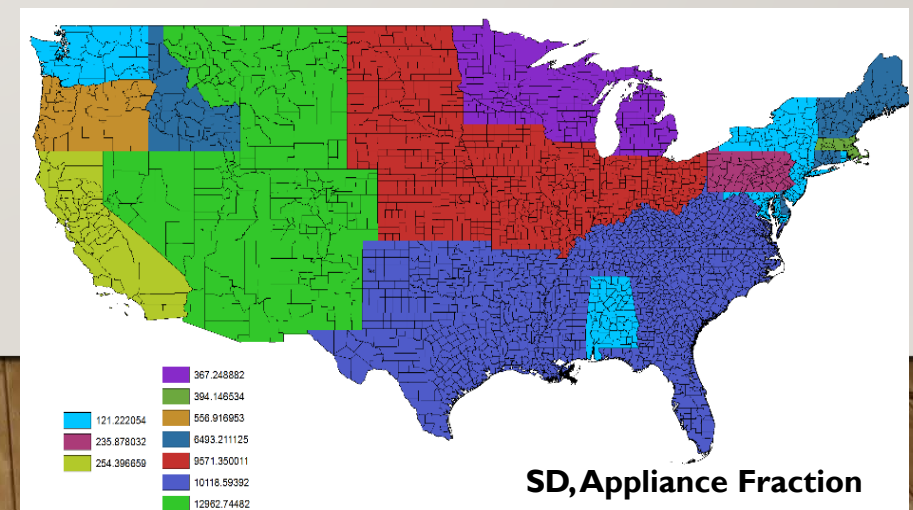
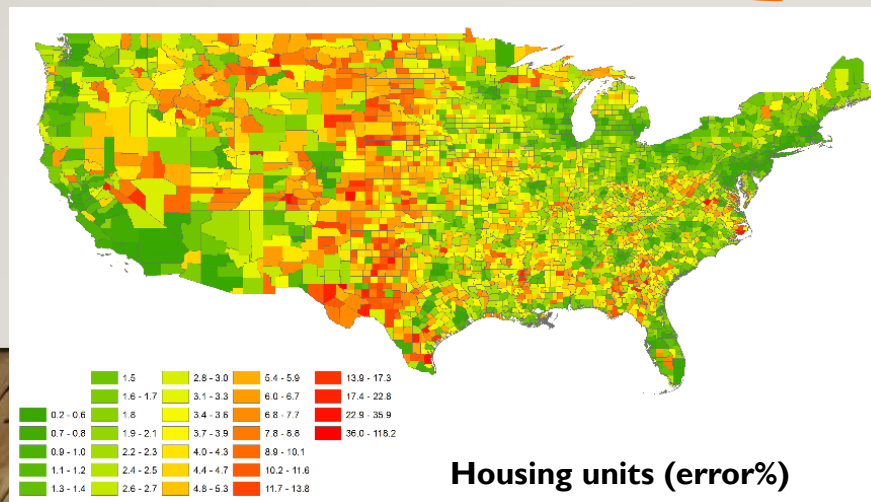
# CHARACTERIZING UNCERTAINTIES IN EACH INPUT

---

- Inventory parameters
- Spatial surrogates
- Temporal profiles
- Chemical speciation profiles

# CHARACTERIZING UNCERTAINTIES (INVENTORY PARAMETERS FOR THE U.S.)

- Inventory parameters
  - Spatial surrogates
  - Temporal profiles
  - Chemical speciation profiles
- Occupied housing: Marginal error at 95% confidence interval (CI)
  - Appliance fraction: Sampling error at 95% CI
  - Climate adjustment: Assumed certain
  - Burn rate: Sampling error at 68% CI
  - Wood density: Sampling error at 68% CI
  - Emission Factor: Quality rating (A-E)



# CHARACTERIZING UNCERTAINTIES (INVENTORY PARAMETERS FOR CANADA)

---

- Inventory parameters

- Spatial surrogates

- Temporal profiles

- Chemical speciation profiles

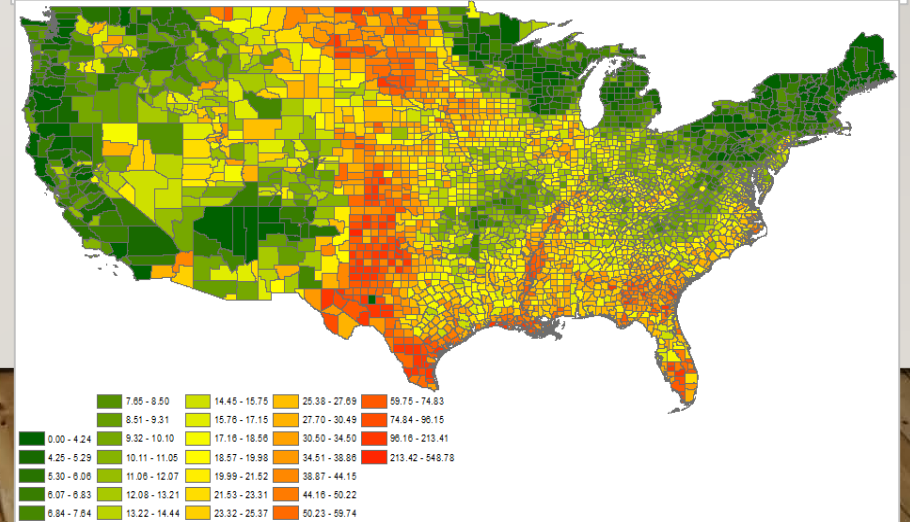
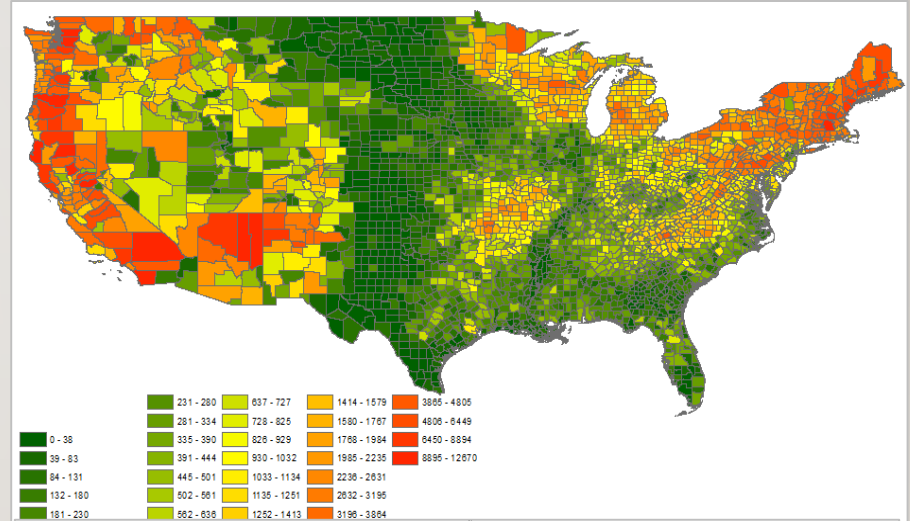
- Number of Appliance: Assumed 30%
- Burn rate: Sampling error at 68% CI
- Wood density: Sampling error at 95% CI
- Emission Factor: Quality rating (A-E)

# CHARACTERIZING UNCERTAINTIES (RWC SURROGATES IN THE U.S)

- Inventory parameters
- Spatial surrogates (marginal error reported in U.S. Census American Community Survey (ACS))
- Temporal profiles
- Chemical speciation profiles

Number of houses burn wood as primary heating source

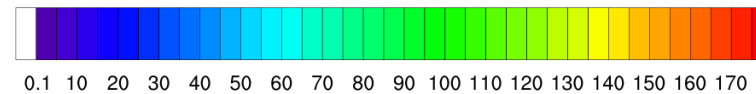
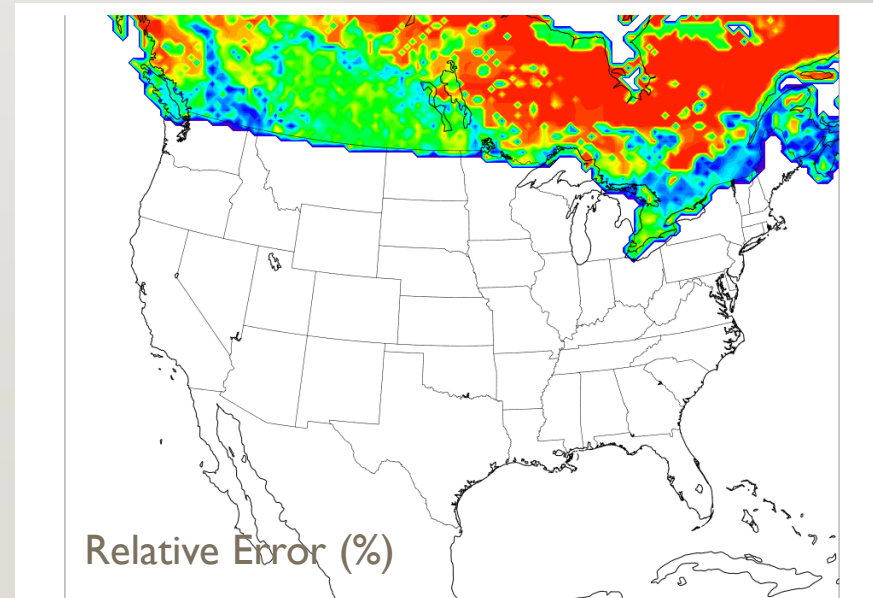
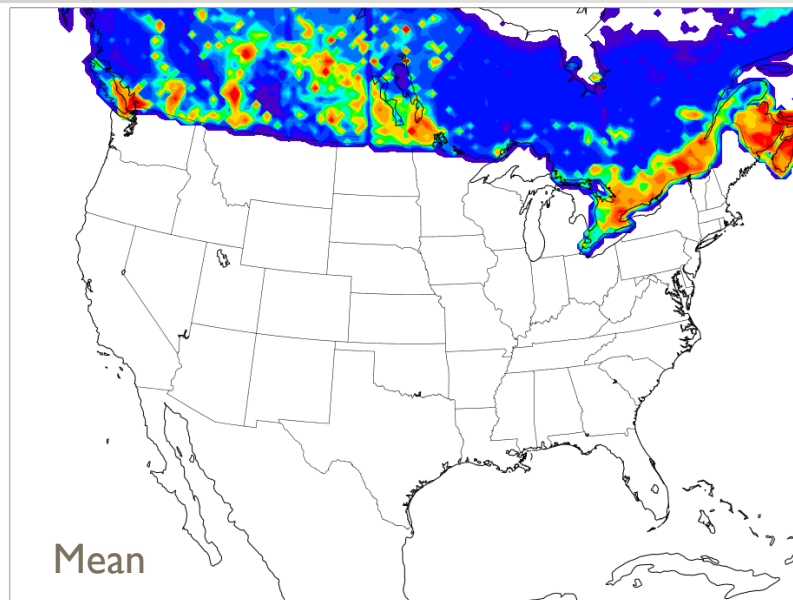
Relative Error (%)



# CHARACTERIZING UNCERTAINTIES (RWC SURROGATES IN CANADA)

- Inventory parameters
- Spatial surrogates (standard deviation using 3 different surrogates used to allocate Canadian RWC)

950A: combination of forest and dwellings  
950B: intersection of forest and dwellings  
951: RWC from HES and EUS surveys



# CHARACTERIZING UNCERTAINTIES IN EACH INPUT

---

- Inventory parameters
  - Spatial surrogates
  - Temporal profiles
  - Chemical speciation profiles
    - **We do not have any uncertainties reported in literature**
    - **For each temporal and speciation profile, each single coefficient is assigned a standard deviation assuming a 30% uncertainty with renormalization.**
- ***Suggestions are welcome!***

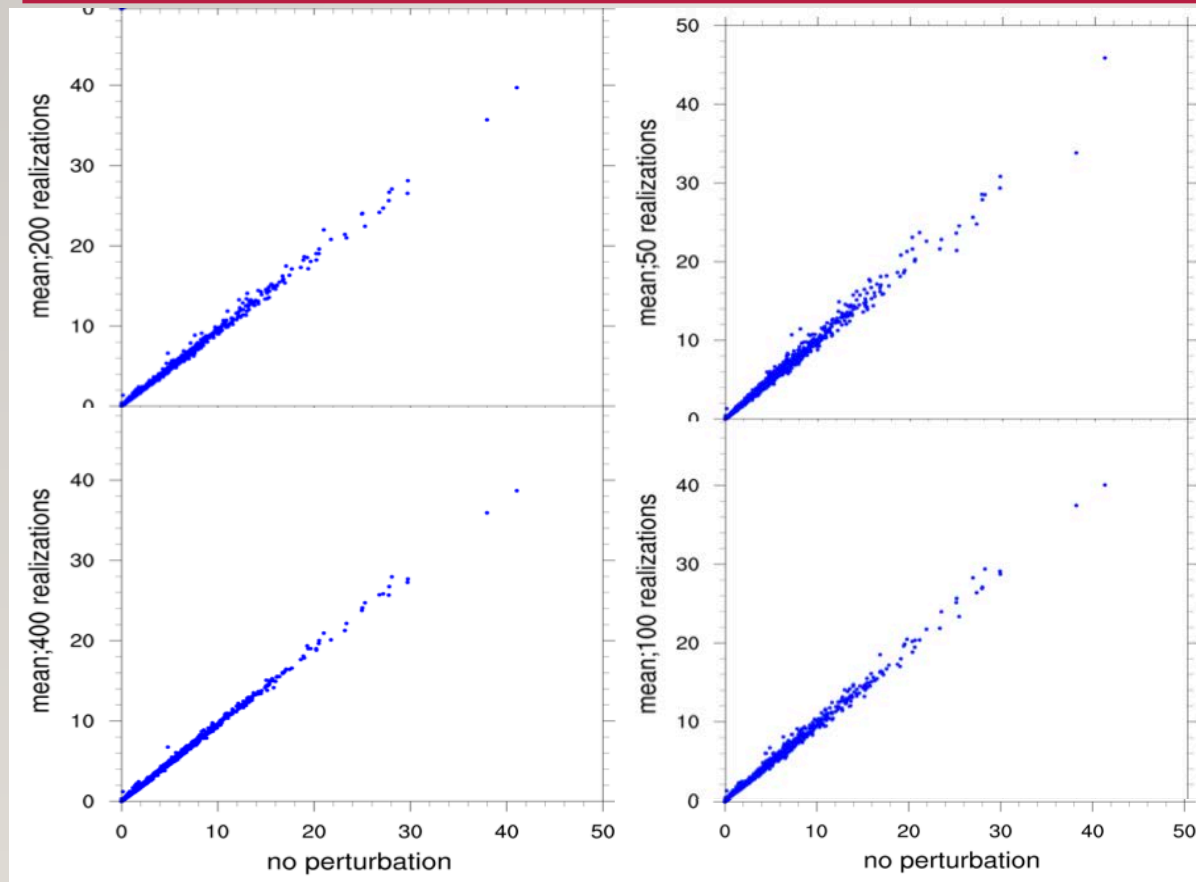
# PROPAGATING UNCERTAINTIES

---

- Monte Carlo simulations
- Sampling code is External to SMOKE
- Latin Hypercube Sampling (LHS) generates a set of 100 random realizations (other set sizes were also tested)
- Log-Normal distribution is assumed for inventory parameters and normal distribution is assumed for other processes



# THE SENSITIVITY OF OUTPUTS TO DIFFERENT SAMPLE SIZES (E.G. FOR CO)



The comparisons of several sample sizes suggest that a set of 100 samples (or even 50) provides an efficient and stable size for generating model-ready emission distributions.

# RESULTS

---

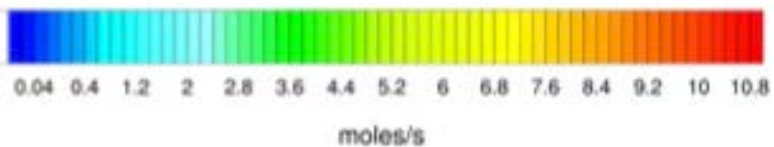
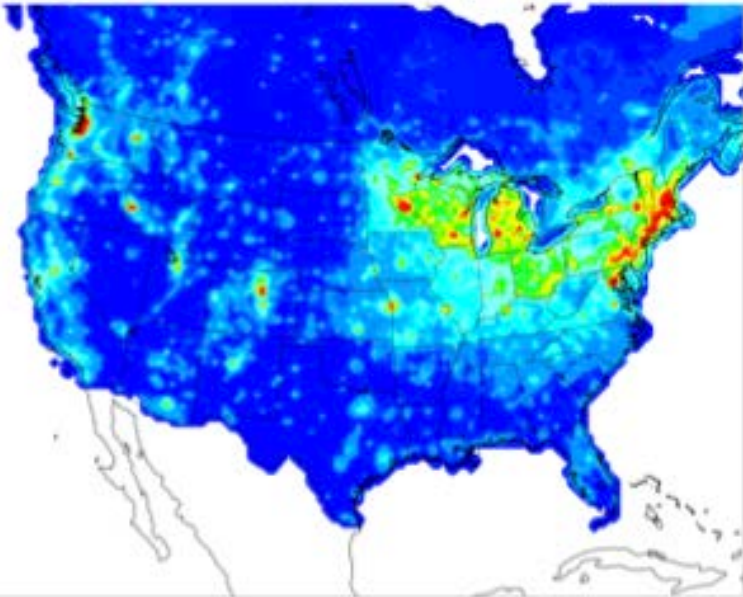
- THE CASE

- Resolution: CONUS, 36 km
- SMOKE version: v3.7
- Episode: February 1<sup>st</sup>, 2011
- Chemical speciation: ADOM gas-phase mechanism and 12-bin aerosol representation (GEM-MACH)

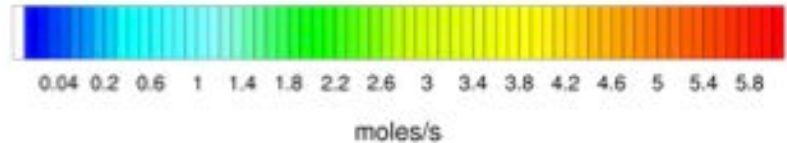
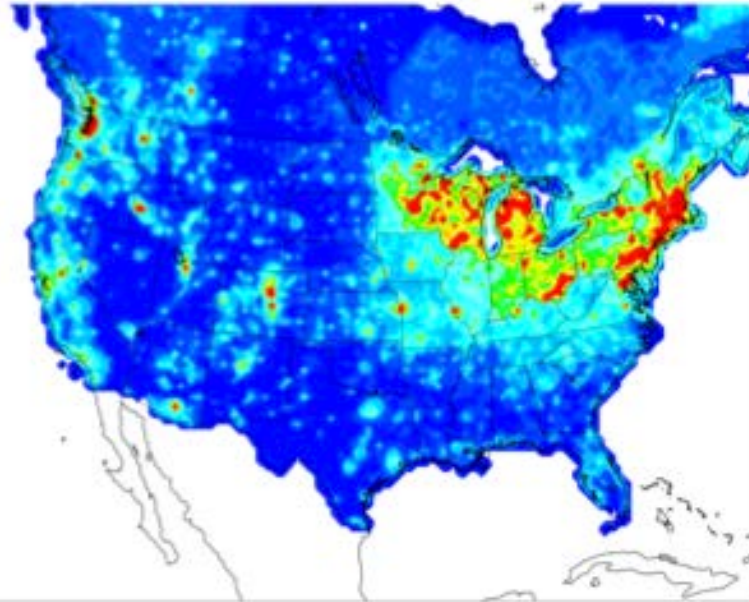
# RESULTS (ALL PROCESSES PERTURBED; 100 REALIZATIONS)

## PRIMARY ORGANIC CARBON (PC8) EMISSION, FEBRUARY 1<sup>ST</sup>, 18 UTC

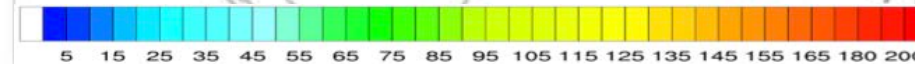
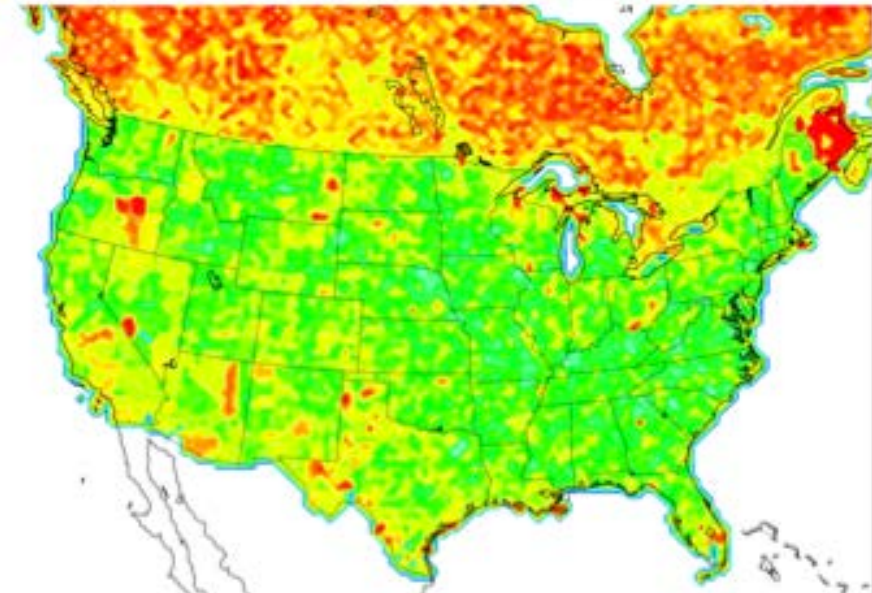
Primary Organic Carbon (PC8); mean, all processes perturbed



PC8; sigma, all perturbations



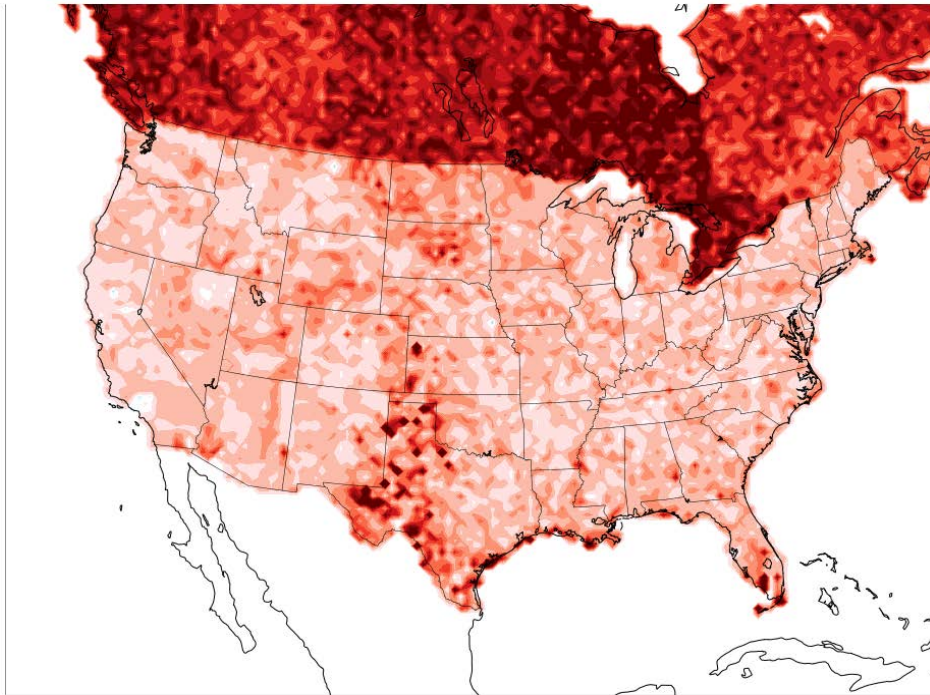
PC8 relative error (%); all perturbations



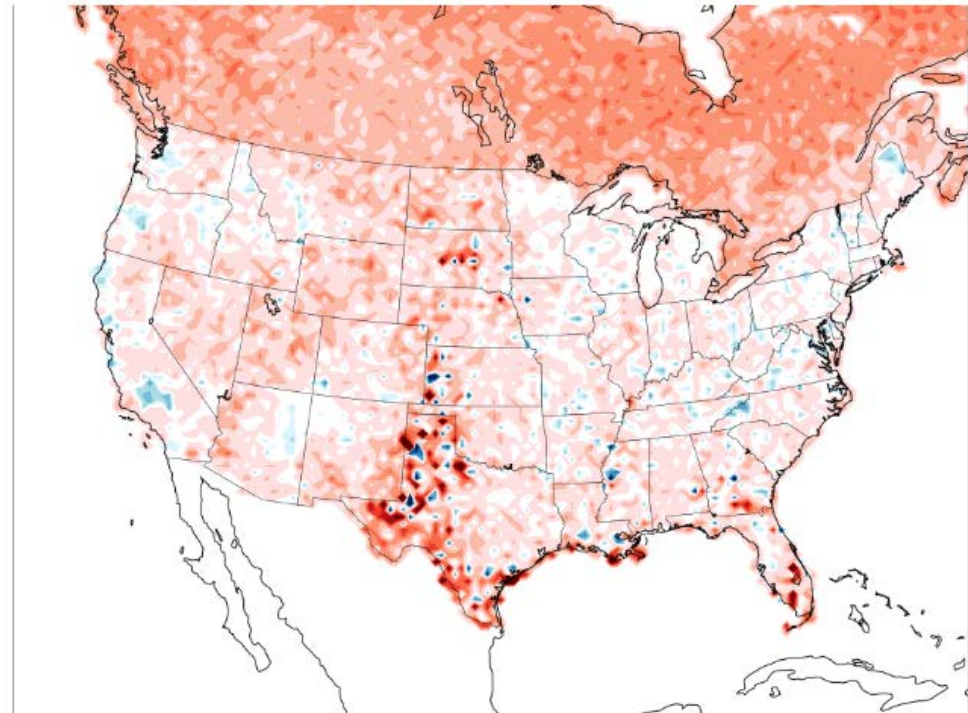
- Higher uncertainty over Canada
- Indication of high values over central U.S.

**CONTRIBUTION OF INVENTORY UNCERTAINTY IN SHAPE OF DISTRIBUTION (SKEWNESS; MEASURE OF SYMMETRY)  
PRIMARY ORGANIC CARBON (PC8) EMISSION, ON FEBRUARY 1<sup>ST</sup> AT, 18 UTC**

**All processes perturbed**

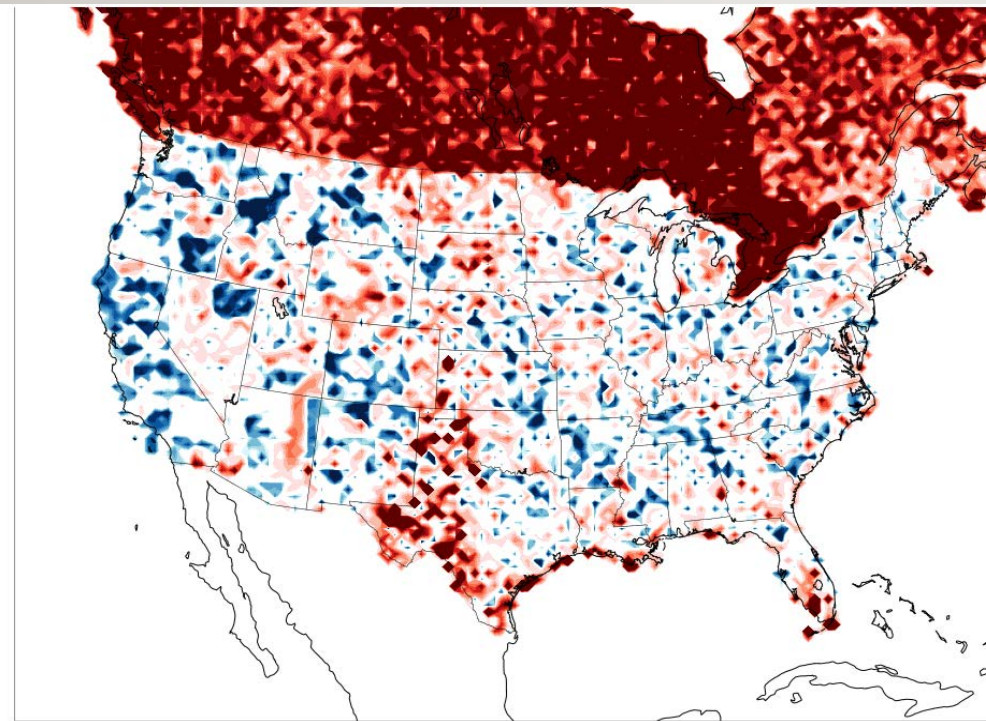


**All processes perturbed except inventory**

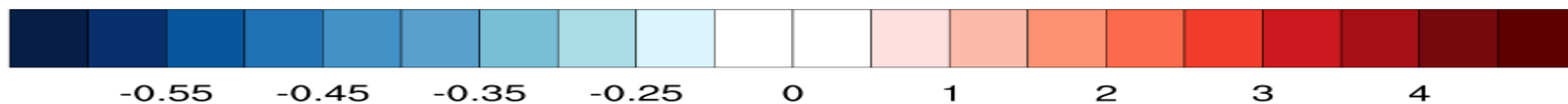
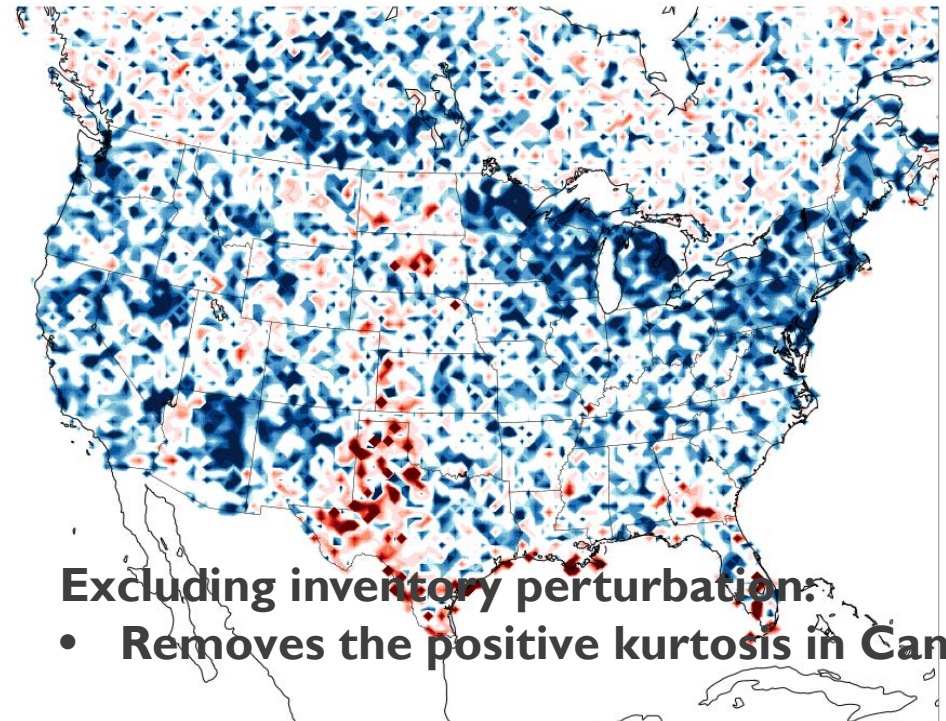


# CONTRIBUTION OF INVENTORY UNCERTAINTY IN SHAPE OF DISTRIBUTION (KURTOSIS; MEASURE OF THE SHARPNESS OF THE PEAK OF DISTRIBUTION) PRIMARY ORGANIC CARBON (PC8) EMISSION, ON FEBRUARY 1<sup>ST</sup> AT, 18 UTC

All processes perturbed

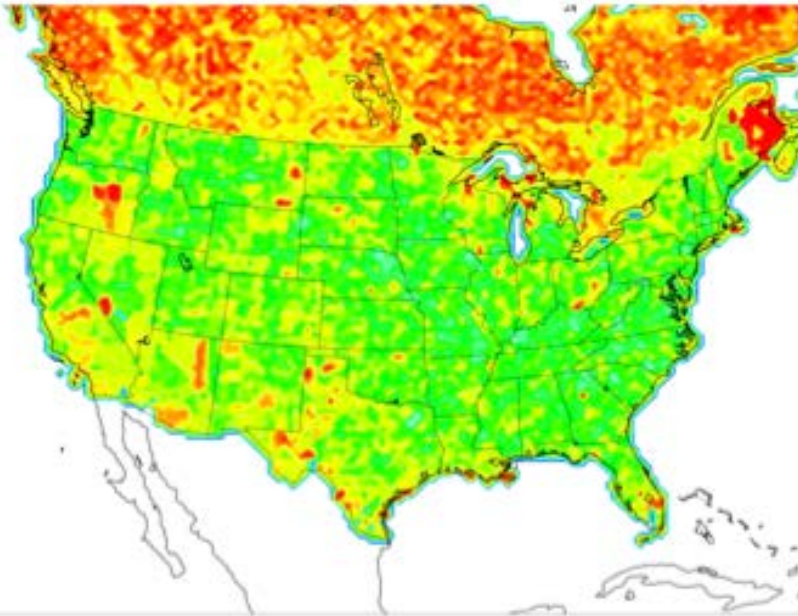


All processes perturbed except inventory

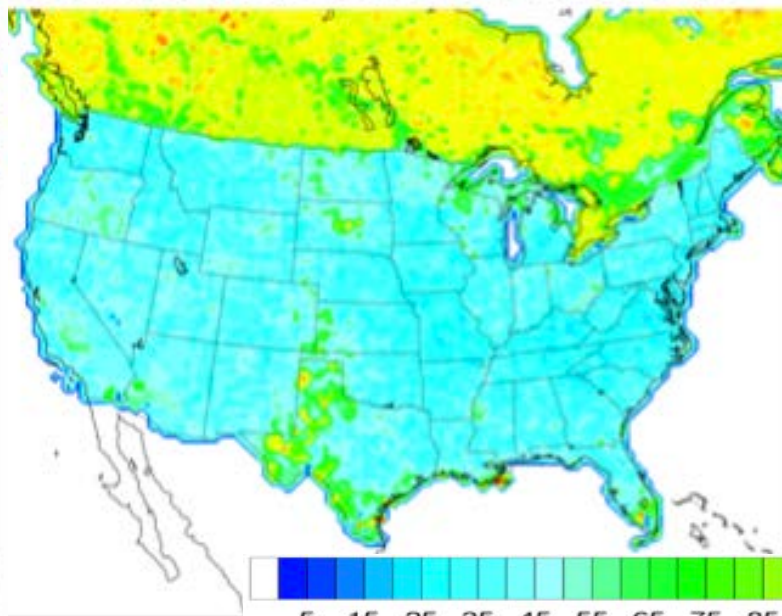


## RELATIVE ERROR FOR DIFFERENT PERTURBATION PRIMARY ORGANIC CARBON (PC8) EMISSION, ON FEBRUARY 1<sup>ST</sup> AT, 18 UTC

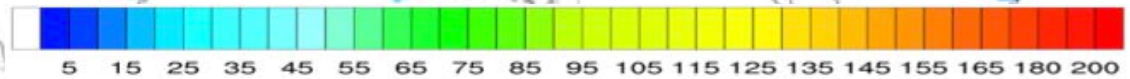
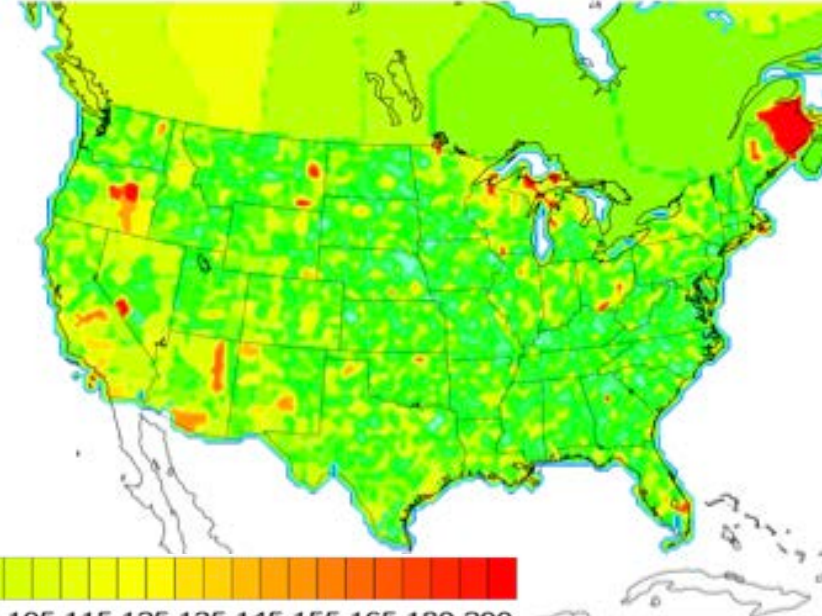
PC8 relative error (%);all perturbations



PC8 relative error (%);all perturbations except inventory



PC8 relative error (%);all perturbations except surrogates



Excluding temporal perturbation:

Excluding surrogate perturbation:

- Reduces relative error by 50%
- Reduces the uncertainty in Canada
- removes the high uncertainty in central U.S.

- Excluding the inventory perturbation decreases the relative error

# BOX PLOTS FOR CO (100 REALIZATIONS)

All perturbations



All perturbations except speciation



All perturbations except Inventory



All perturbations except surrogates



All perturbations except temporal



Box plots show the range, median, and 25 – 75 percentiles for select locations

Particularly in the U.S. the inventory has important contributions to the overall uncertainty, while for Canadian locations surrogates show up prominently

# MAIN FINDINGS:

---

- **Emission Inventory is a significant contributor to overall RWC uncertainty**
- **Uncertainty in inventory has also important impact on shape of distribution (both symmetry and sharpness of distribution)**
- **Higher uncertainty in Canada is due to more uncertain input data, especially for inventory parameters, and larger reporting jurisdictions**



# BY APPLYING THIS FRAMEWORK WE CAN:

---

- **Generate a set of random realizations of model-ready emission input files, propagate through CTMs**
- **Provide an effective means for formal quantification of uncertainties in emissions from other source sectors**
- **Identify gaps in available information for raw emission uncertainty**

# ACKNOWLEDGEMENT

---

Thanks to Environment Canada for providing  
funding for this project

---

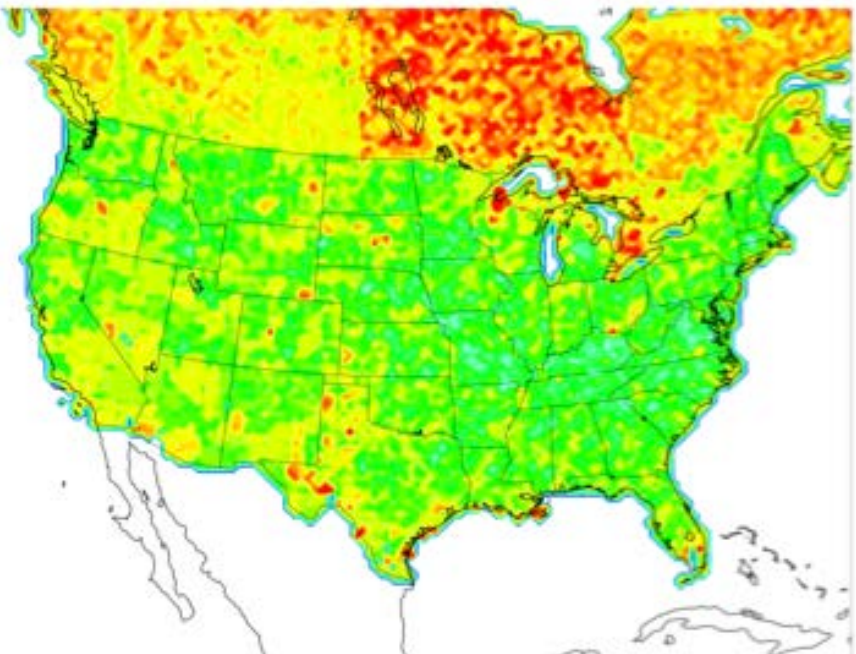
**THANK YOU**



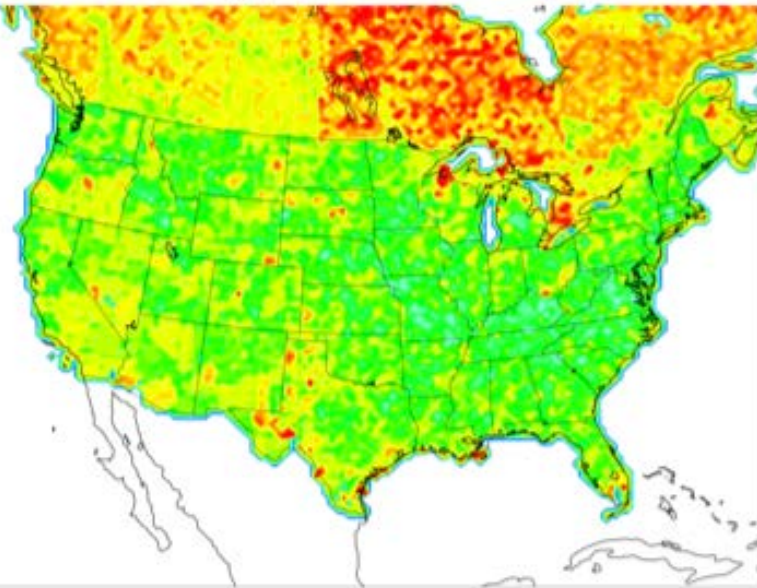
# EXTRA SLIDES

---

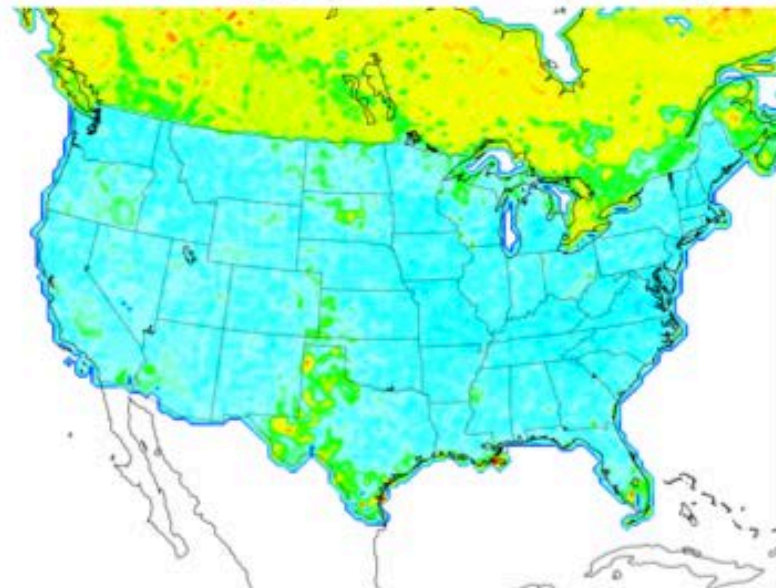
CO relative error (%);all perturbations



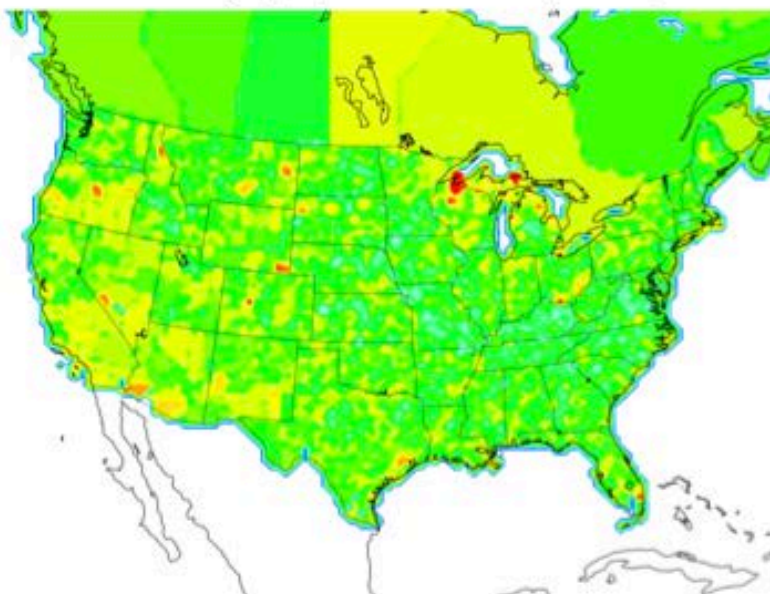
CO relative error (%);all perturbations except speciation



CO relative error (%);all perturbations except inventory



CO relative error (%);all perturbations except surrogates



CO relative error (%);all perturbations except temporal

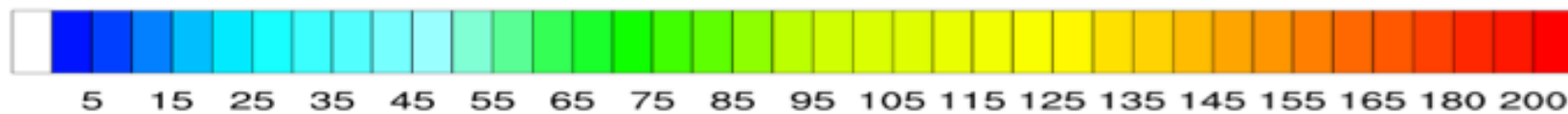
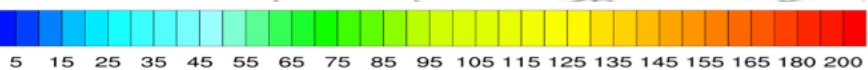
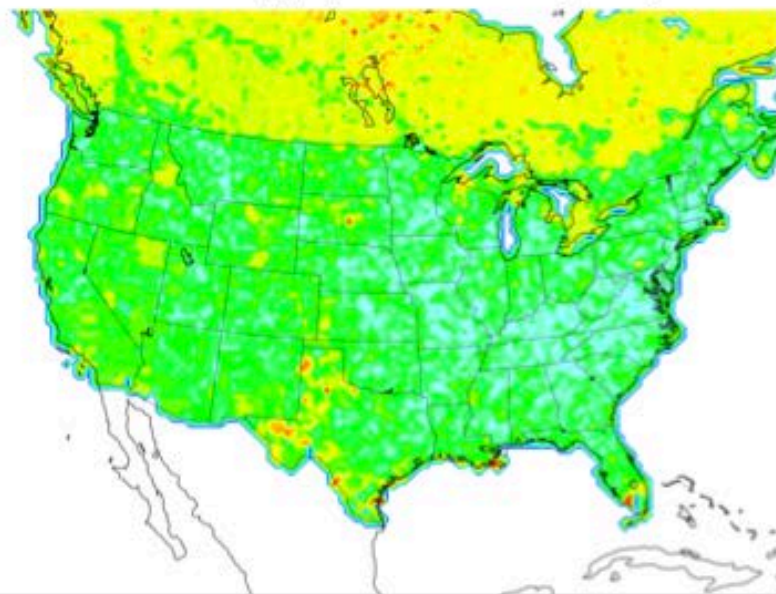


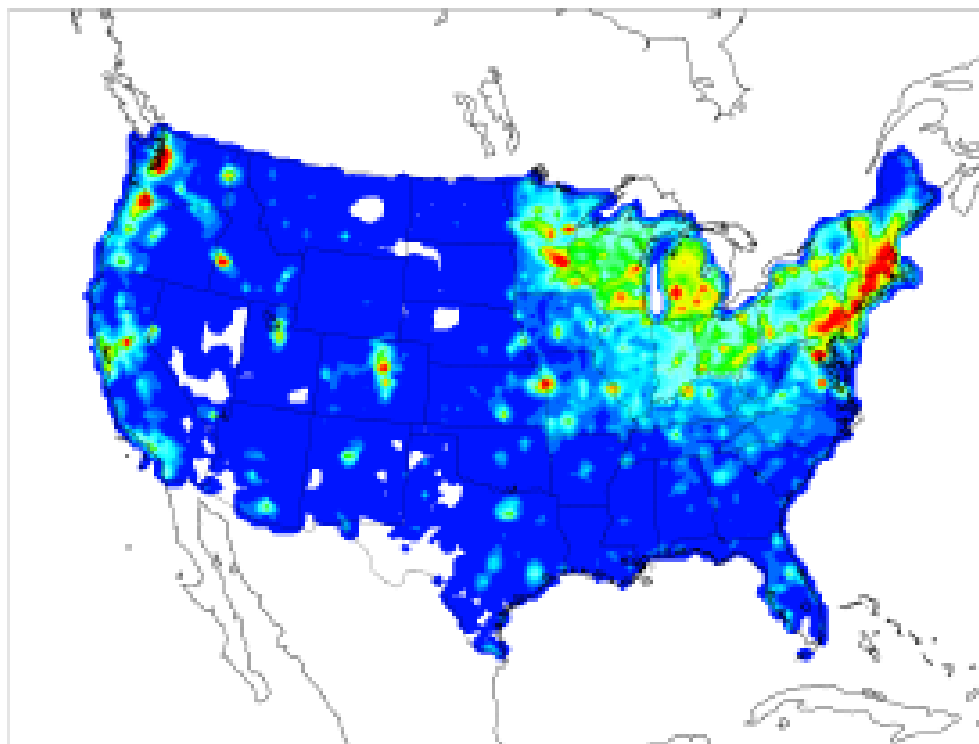
Table 3. list of Canadian RWC appliance and SCCs

<b>Canadian Appliance type</b>	<b>SCC</b>
Woodstove advance tech	2104008030
Woodstove conventional-no air tight	2104008051
Woodstove conventional-air tight	2104008051
Fireplace conventional- no door	2104008001
Fireplace conventional-door	2104008001
Fireplace conventional- insert	2104008001
Fireplace conventional-insert-advance tech	2104008001
Fireplace conventional- any cat	2104008001
Furnace boiler	2104008060
Wood other equipment	2104008070

Table 1. list of U.S. RWC appliance and SCCs

<b>Appliance type</b>	<b>SCC</b>
Woodstove: free standing; EPA certified, catalytic	2104008330
Woodstove: free standing; EPA certified, non-catalytic	2104008320
Woodstove: free standing; non-certified	2104008310
Fireplace: inserts; EPA certified, catalytic	2104008230
Fireplace: inserts; EPA certified, non-catalytic	2104008220
Fireplace: inserts; non-certified	2104008210
Fireplace: without inserts	2104008100

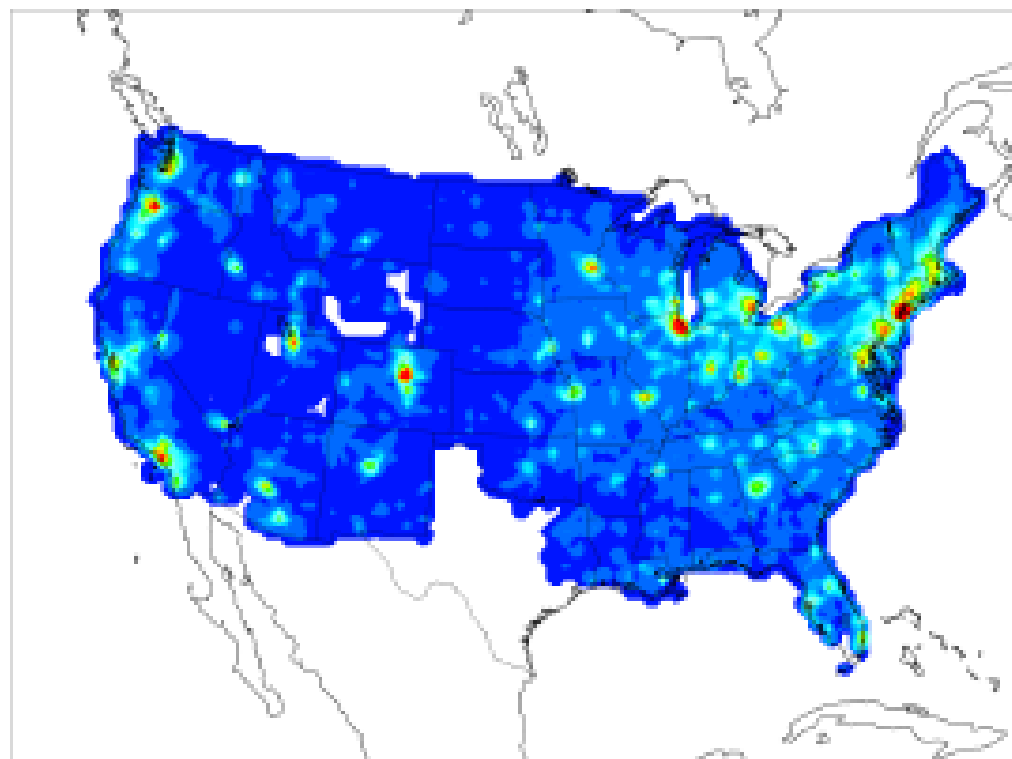
CO (from default SMOKE inventory)



0.01 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

moles/s

CO (SMOKE output from uncertain raw emission data)



0.1 0.9 1.7 2.5 3.3 4.1 4.9 5.7 6.7 7.5 8.3 9.1 9.9 10.7 11.5

moles/s