How Does Regional Chemistry in Urban Wildfire Plumes Differ from Wildland Fires? *Insights from Chemical Transport Modeling*

Christine Wiedinmyer University of Colorado Boulder

Amara Holder and Kirk Baker (US EPA) Kelley Barsanti (Univ. of California-Riverside)

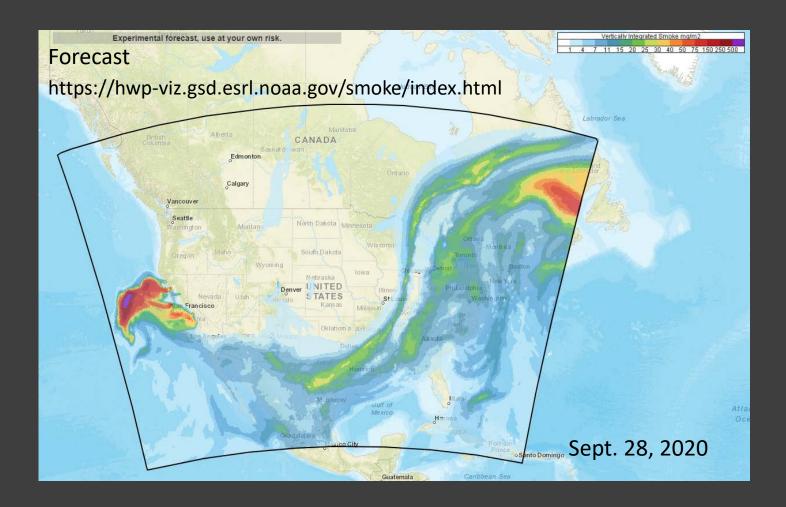


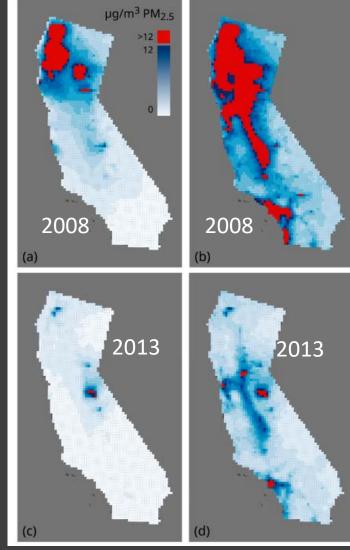
Regional Modeling of Wildland Fires

- Simulate where the smoke emissions go
- Predict plume chemistry and downwind chemical composition, air quality
- Forecast and hindsight applications

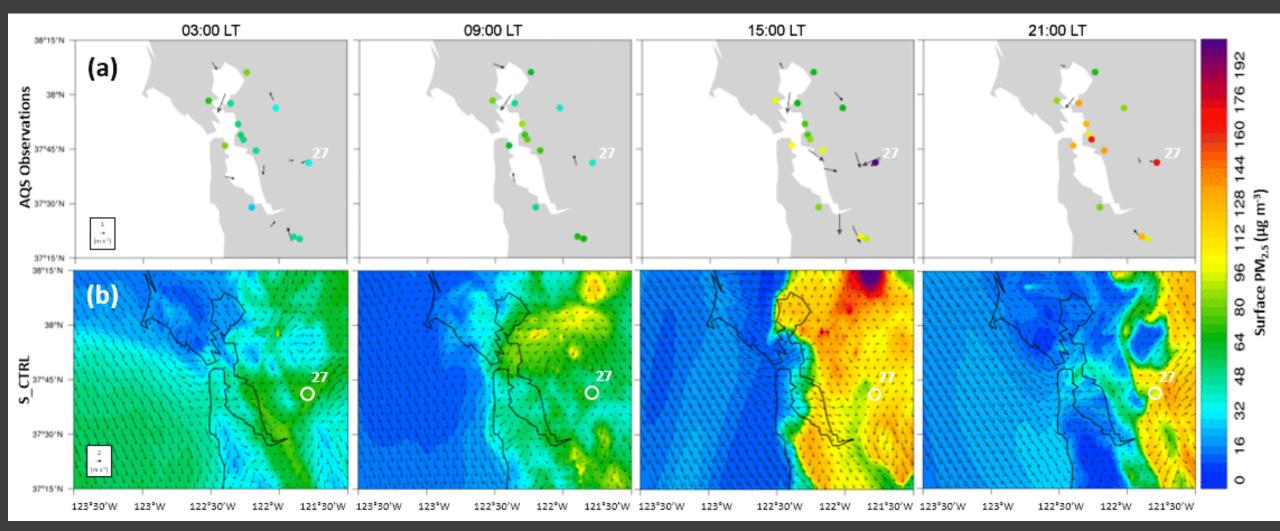


Christine Wiedinmyer, 21 October 2020, ~4pm MT



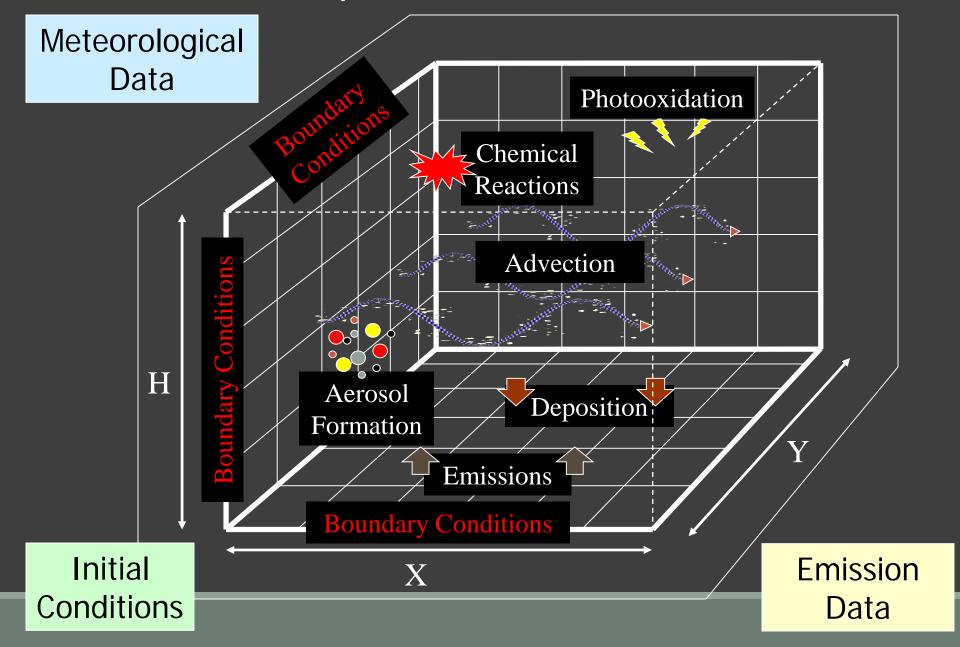


Annual PM_{2.5} from CMAQ (12km) a, c – Only fire emissions b, d – All emission sources [Koman et al, Mapping Modeled exposure of wildland fire smoke for human health studies in California, *Atmosphere*, 2019]



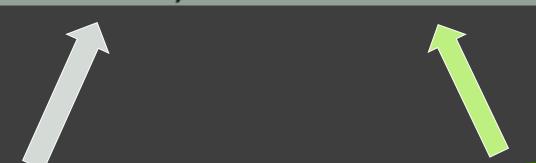
Surface observations (a) and Modeled (b) PM_{2.5} in San Francisco Bay area on 14 November 2018 during Camp fire [Rooney et al, Air quality impact of the Northern California Camp Fire of November 2018, *Atmos. Chem & Physics*, 2020]

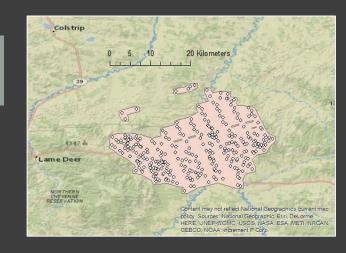
3D Chemical Transport Models



Modeling Wildland Fires: Emissions

Emission_i= $f(ef_{i}, Biomass Burned)$





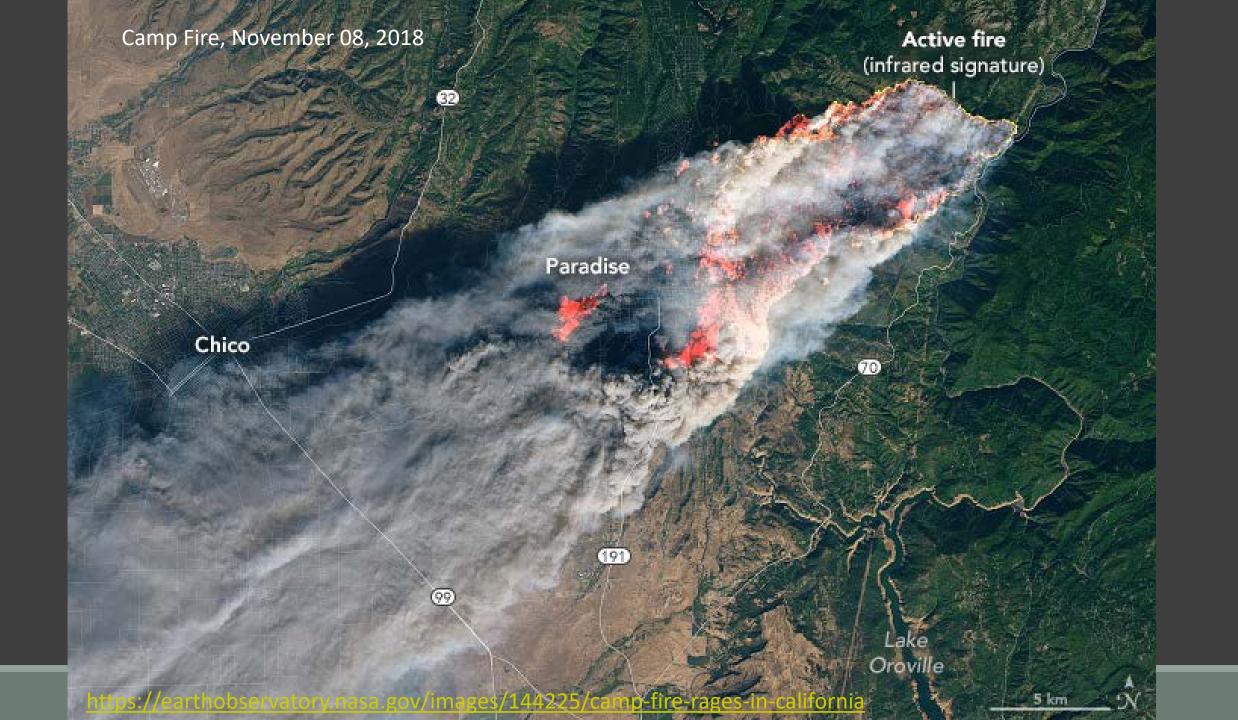
Emission Factor

- Vegetation
 - o Type
 - o Condition
- Fire
 - Intensity
 - o Stage



Biomass Burned

- Vegetation
 - o Type
 - Condition
 - o Density
 - Loading
- Fire
 - o Intensity
 - Duration



Emissions from urban fires

Emission Factors – What is released? How much?

Activity – What is burning? When? How much?





Emissions from Urban Fires

Emission_x = EF_x * Material Burned



- * Criteria Pollutants (PM, CO, NO2, SO2)
- * Metals
- * Organic Compounds
- * Toxics
- * Reactive compounds
- * Chlorinated compounds

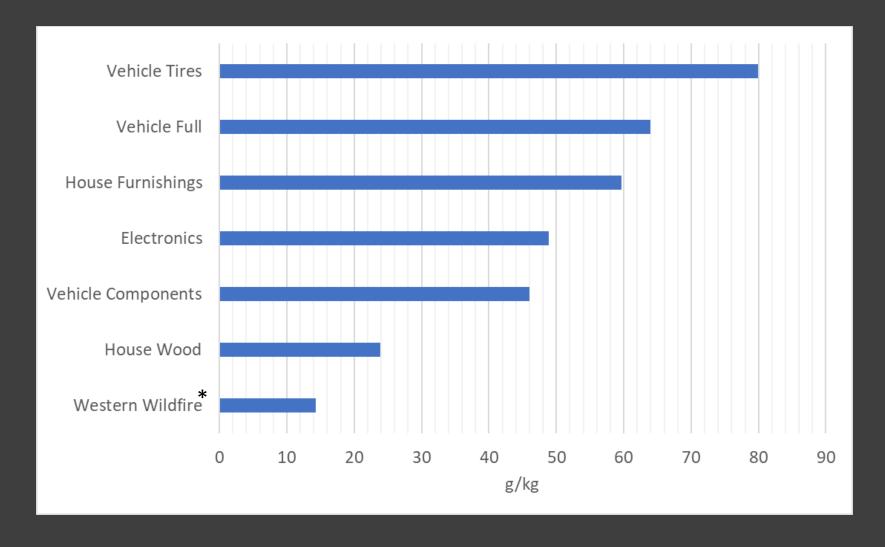
WHAT IS BURNED?

- * Building Materials
- * Cars
- * Electrical
- * PVC
- * Carpet
- * Furnishings
- * Electronics

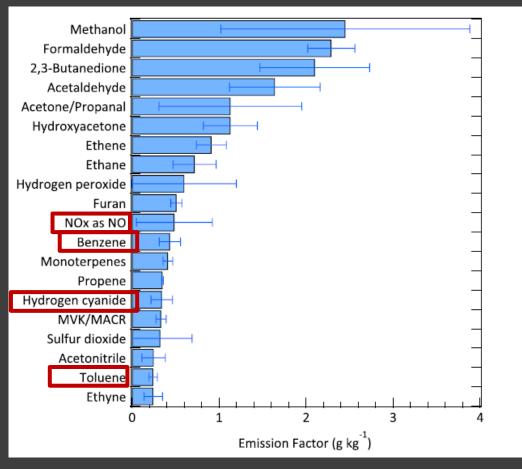


- * How many or How much
- * Fraction of material burned

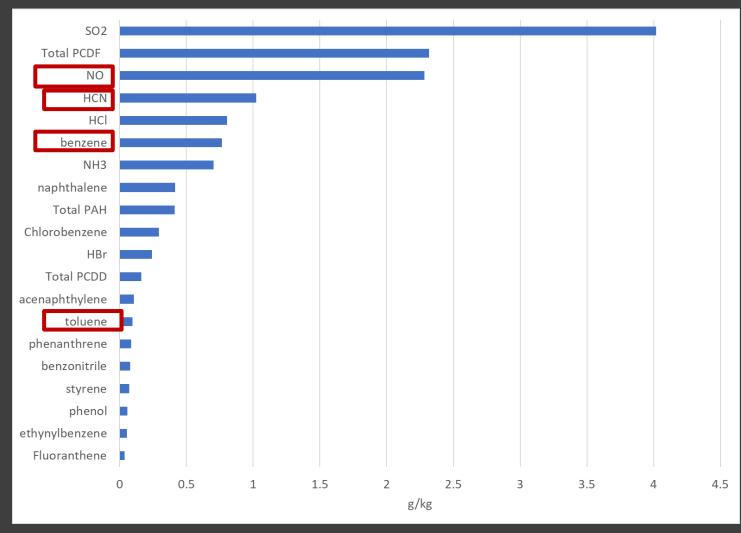
Particulate Matter Emission Factors



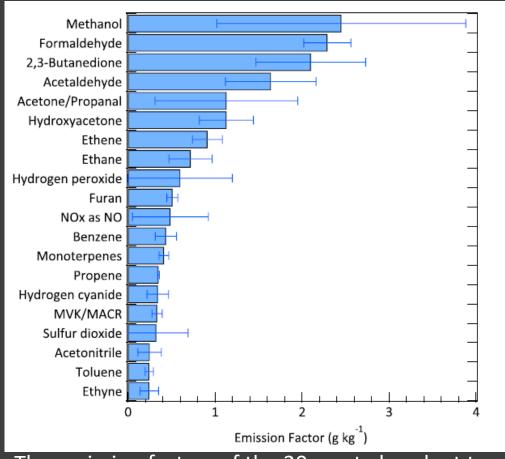
* EF from Western Evergreen Forest (Prichard et al, 2020)



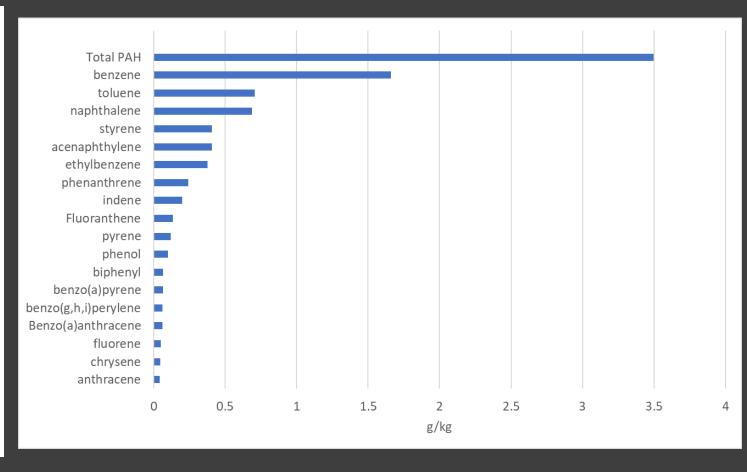
The emission factors of the 20 most abundant trace gases (except CO2, CO and CH4) in three western wildfires (Liu et al, *JGR-Atm*, 2017)



The emission factors of the 20 most abundant trace gases (except CO2, CO) for total house burning (Total PCDF = Polychlorinated dibenzodioxins, dibenzofurans)



The emission factors of the 20 most abundant trace gases (except CO2, CO and CH4) in three western wildfires (Liu et al, *JGR-Atm*, 2017)



The emission factors of the 19 most abundant trace gases (except CO2, CO) for Tire burning (SO_2 EF = 24 g/kg)

Emissions from Urban Fires

Emission_x= EF_x * Material Burned



WHAT IS EMITTED?

- * Criteria Pollutants (PM, CO, NO2, SO2)
- * Metals
- * Organic Compounds
- * Toxics
- * Reactive compounds
- * Chlorinated compounds

WHAT IS BURNED?

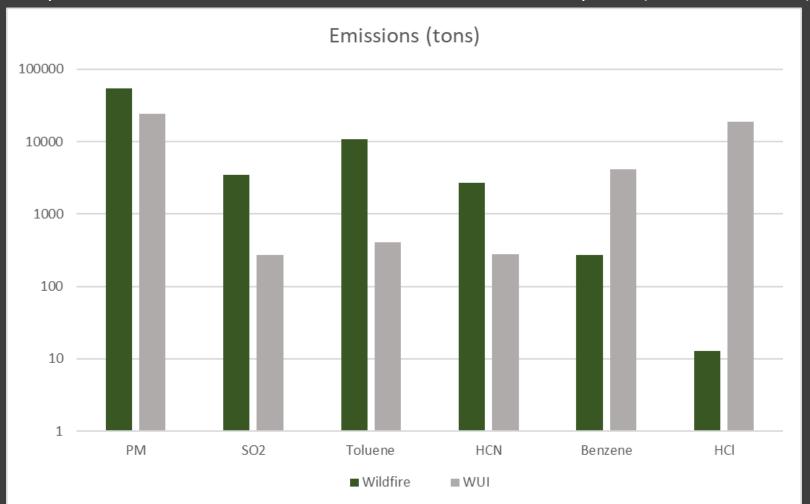
- * Building Materials
- * Cars
- * Electrical
- * PVC
- * Carpet
- * Furnishings
- * Electronics



- * How many or How much
- * Fraction of material burned

Emission Estimates

Comparison of wildland fire and urban emissions from Camp Fire (November 2018)



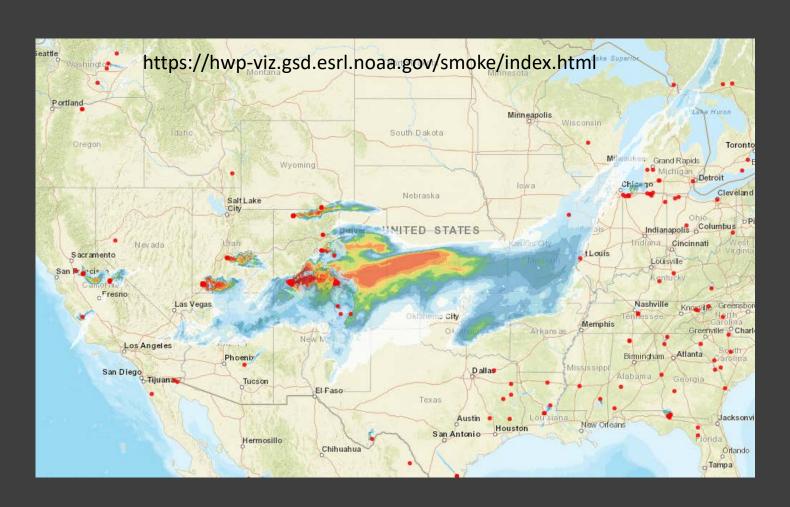


Wildland fire emissions estimates from FINNv2.2 (MODIS+VIIRS)

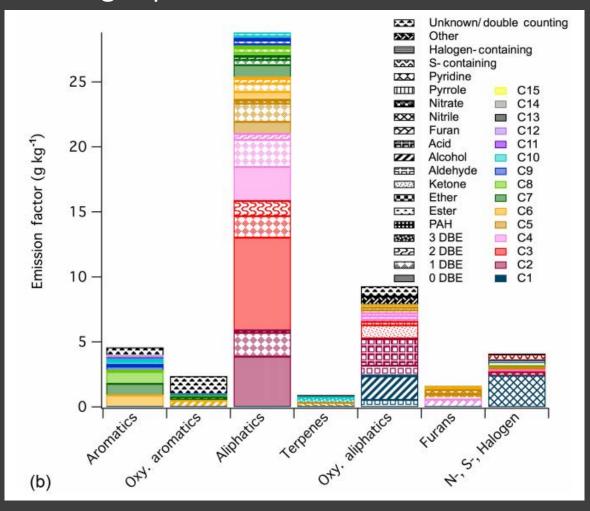
Urban emission estimates developed by A. Holder (US EPA)

Regional chemical transport modeling

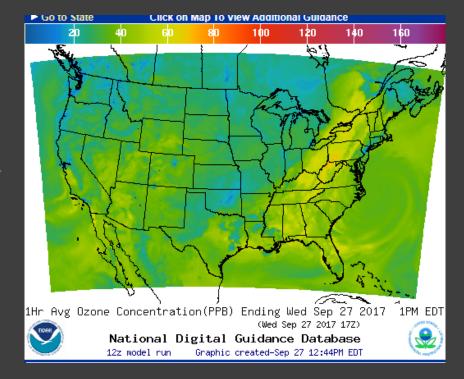
What is the impact of different sources on chemistry, air quality, exposures?



100's of NMOCs measured from Biomass Burning experiments



How do we represent these compounds and their chemistry?



Simulating Chemistry

Multiple mechanisms are available to simulate chemistry in chemical transport models

For example: SAPRC18

- 11 inorganic species (e.g., NO, NO₂, O₃)
- 42 explicit organic species (e.g., benzene, isoprene, methanol)
- 65 lumped organic surrogates (e.g., lumped alkanes, alkenes, aromatics of different reactivity)
- 8 non-reactive species (e.g., CO₂)
- Furans (Jiang et al., 2020)

(SAPRC18, Carter, W. P. L., 2020, https://intra.engr.ucr.edu/~carter/SAPRC/18/)

Modeling Hazardous Air Pollutants

Gas-Phase Hazardous Air Pollutants Represented in the Current CMAQ Model.

HAP Name	HAP Name
acetaldehyde - total and emitted	ethylene oxide
acetonitrile	formaldehyde - total and emitted
acrolein - total and emitted	Hexamethylene 1-6-diisocyanate
acrylic acid	n-hexane
acrylonitrile (propenenitrile)	Hydrazine
benzene	hydrochloric acid
1,3-butadiene	Mercury - elemental and gas
carbon tetrachloride	methanol
carbonyl sulfide	methyl chloride
chlorine	Maleic anhydride
chloroethene (vinyl chloride)	naphthalene
chloroform	quinoline
chloroprene	styrene (ethenylbenzene)
1,2-dibromoethane	1,1,2,2-tetrachloroethane
p-dichlorobenzene	tetrachloroethylene (perchloroethylene)
1,2-dichloroethane	toluene
dichloromethane	2,4-Toluene Diisocyanate
1,2-dichloropropane	trichloroethylene
1,3-dichloropropene	Triethylamine
ethylbenzene	xylene - sum of o-, m- and p- isomers

Aerosol-Phase Hazardous Air Pollutants Represented in the Current CMAQ Model.

HAP name
Arsenic - fine and coarse modes
Beryllium - fine and coarse modes
Cadmium - fine and coarse modes
Chromium 3 - fine and coarse modes
Chromium 6 - fine and coarse modes
Diesel PM elemental carbon - fine modes
Diesel PM organic carbon - fine modes
Diesel PM sulfate - accumulation mode
Diesel PM nitrate - accumulation mode
Diesel PM other components - fine modes
Diesel PM - coarse mode
Lead - fine and coarse modes
Manganese - fin and coarse modes
Mercury - fine and coarse modes
Nickel - fine and coarse modes

Regional modeling of wildland and WUI fires

How to get the best estimates of emissions?

- * Activity data needed!
- * Timing of emissions is important to downwind estimates
- * What is emitted?

Are we simulating what is important for fires in the WUI?

- * What chemical mechanisms should be used?
- * What pollutants and chemistries are missing?
- * Are the compounds of interest reactive or inert?

When and where are urban fires important?



