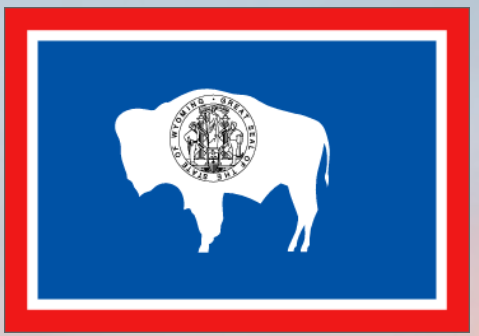
Three-State Air Quality Study (3SAQS)



Three-State Data Warehouse (3SDW)

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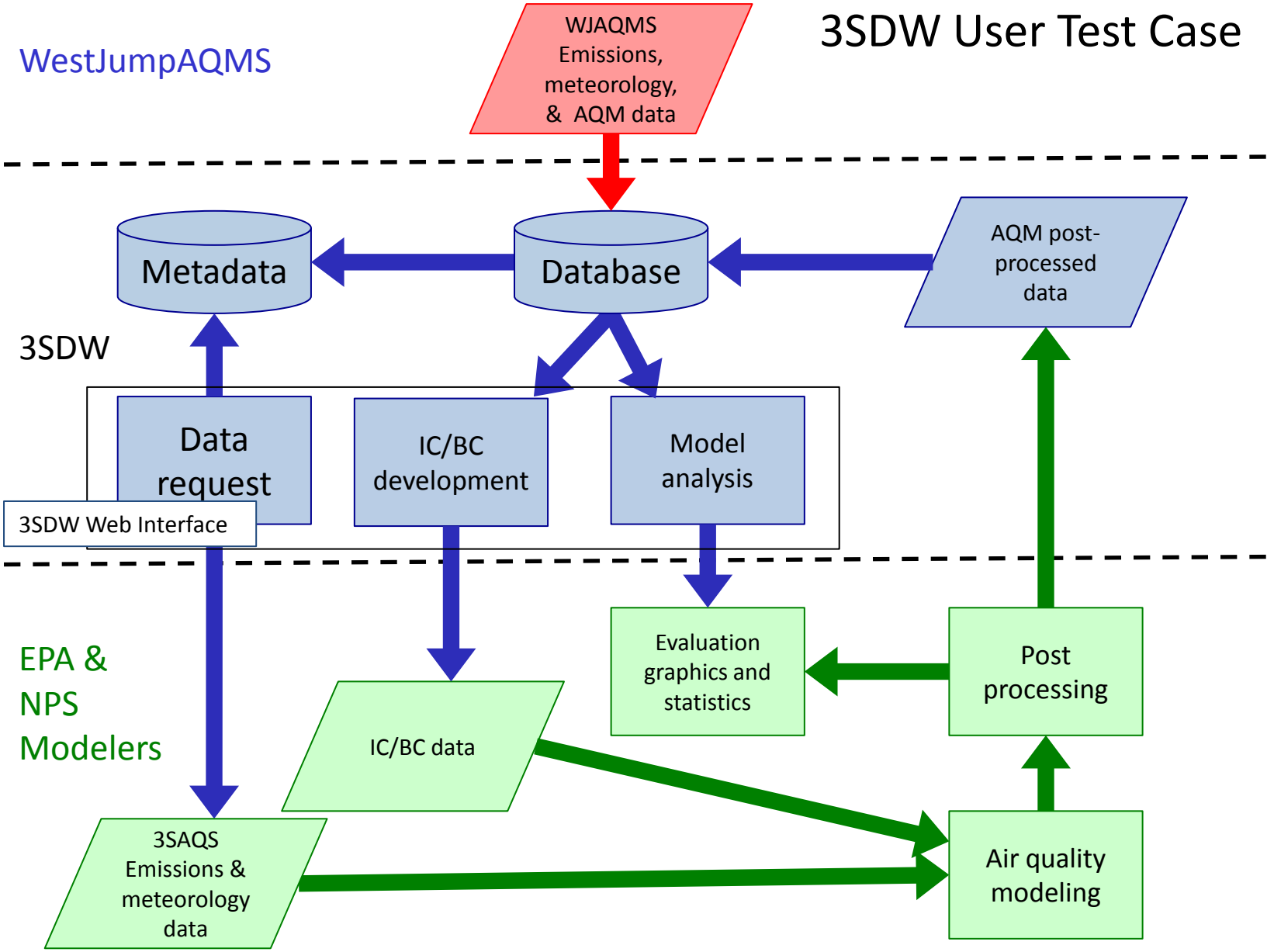
Three-State Air Quality Study

- Project team
  - Tom Moore (WRAP)
  - 3SAQS Cooperative Agreement between UNC and NPS
  - Shawn McClure (CIRA)
- Three-states: Colorado, Utah, Wyoming
- Objective is to develop consistent datasets (IC/BC, met, emissions) for use in NEPA air quality modeling studies in the three states
- Modeling work will develop base year air quality modeling inputs (2008 and 2011) and include some diagnostic and sensitivity studies (e.g. cumulative oil and gas impacts, source apportionment, transient methane)
- Additional data capabilities
  - Research, SIP modeling, economics/benefits analyses
- Data distribution and analysis infrastructure

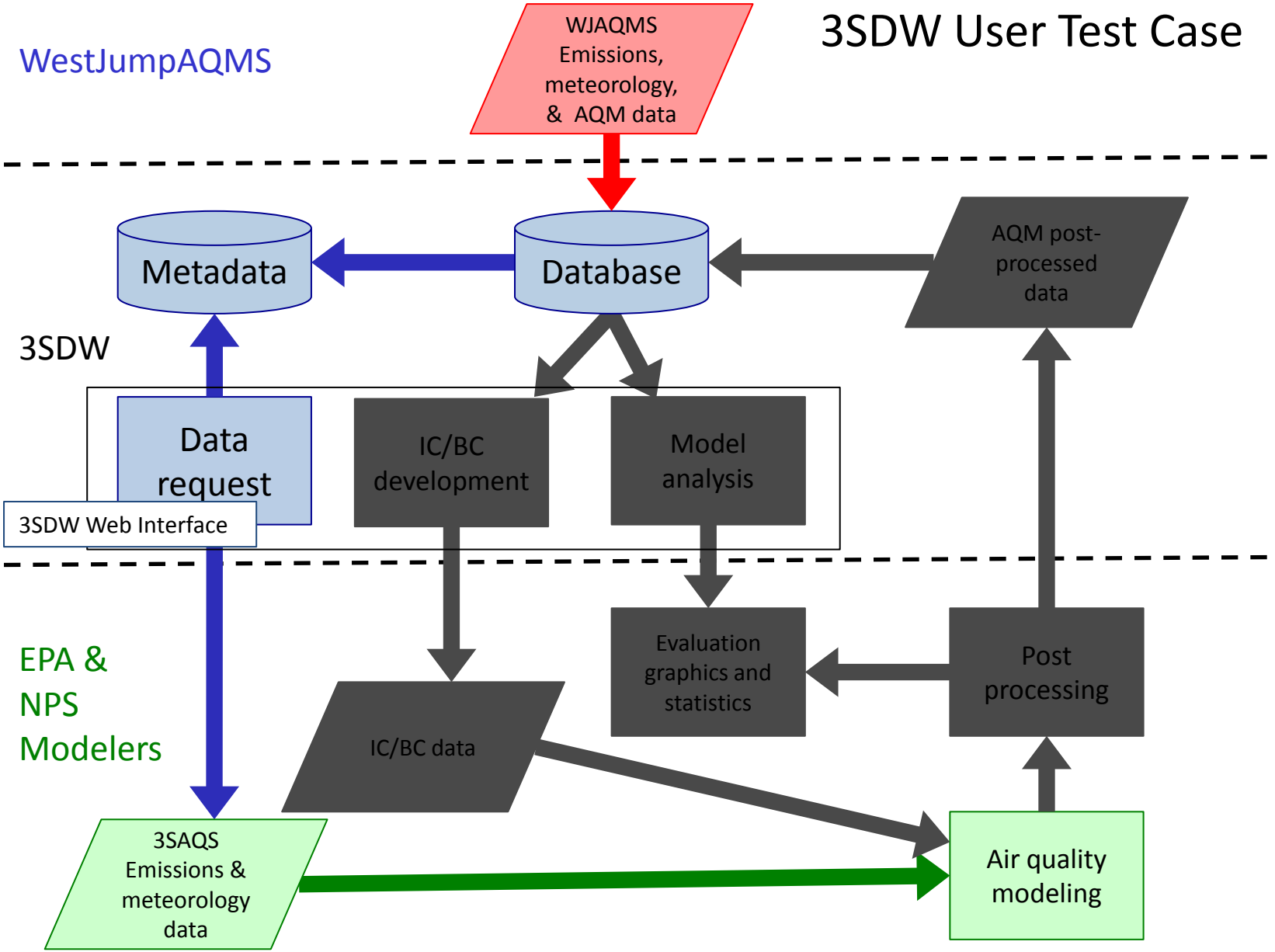
Three-State Data Warehouse

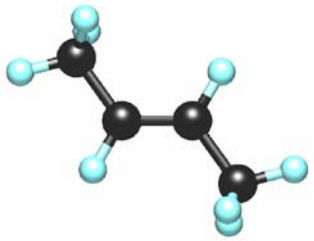
- Web-based data access to model-ready meteorology, emissions, and air quality data
  - Database of model data
  - Web front-end for access and analysis of these data
  - Data download and upload capabilities
- Standardized model performance and model-to-model comparison tools
- Initial focus on supporting NEPA modeling in the three states
  - Objective is to provide infrastructure for storing, distributing, and receiving modeling data for NEPA projects
  - Can evolve into a regional modeling resource for regulatory and research model applications

3SDW User Test Case



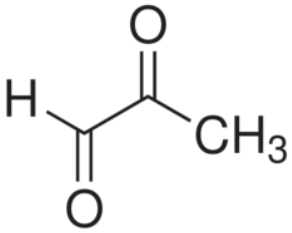
3SDW User Test Case



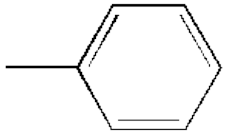


3-State Air Quality Study
VOC Analysis

Reactivity Analysis of Air Pollutant Emission Inventories



Western Air Quality Workshop
Boulder, CO
July 9-11, 2013



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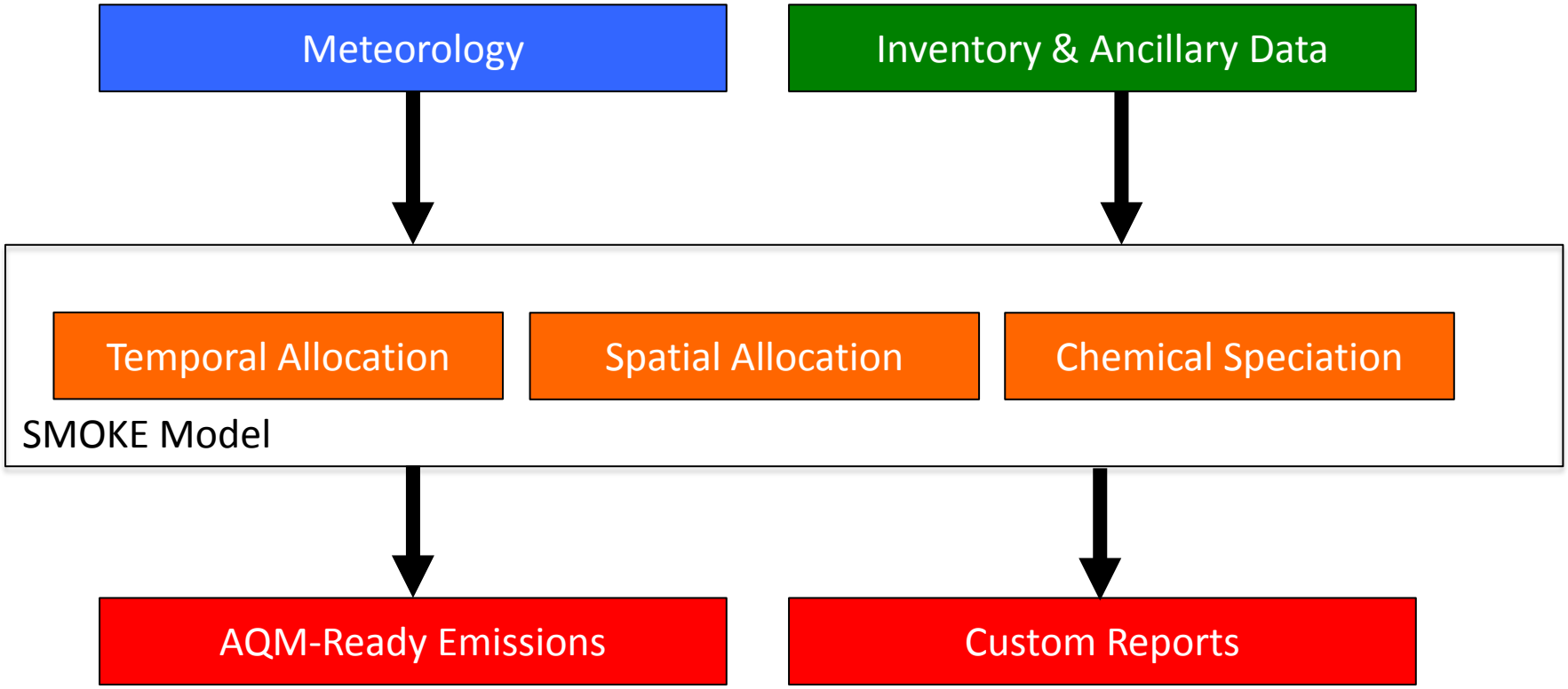
Reactivity Analysis of Air Pollutant Emission Inventories

- Bill Carter, UC-Riverside
- Gail Tonnesen, US EPA Region 8
- Michele Jimenez and Ralph Morris, ENVIRON
- Tom Moore, WESTAR

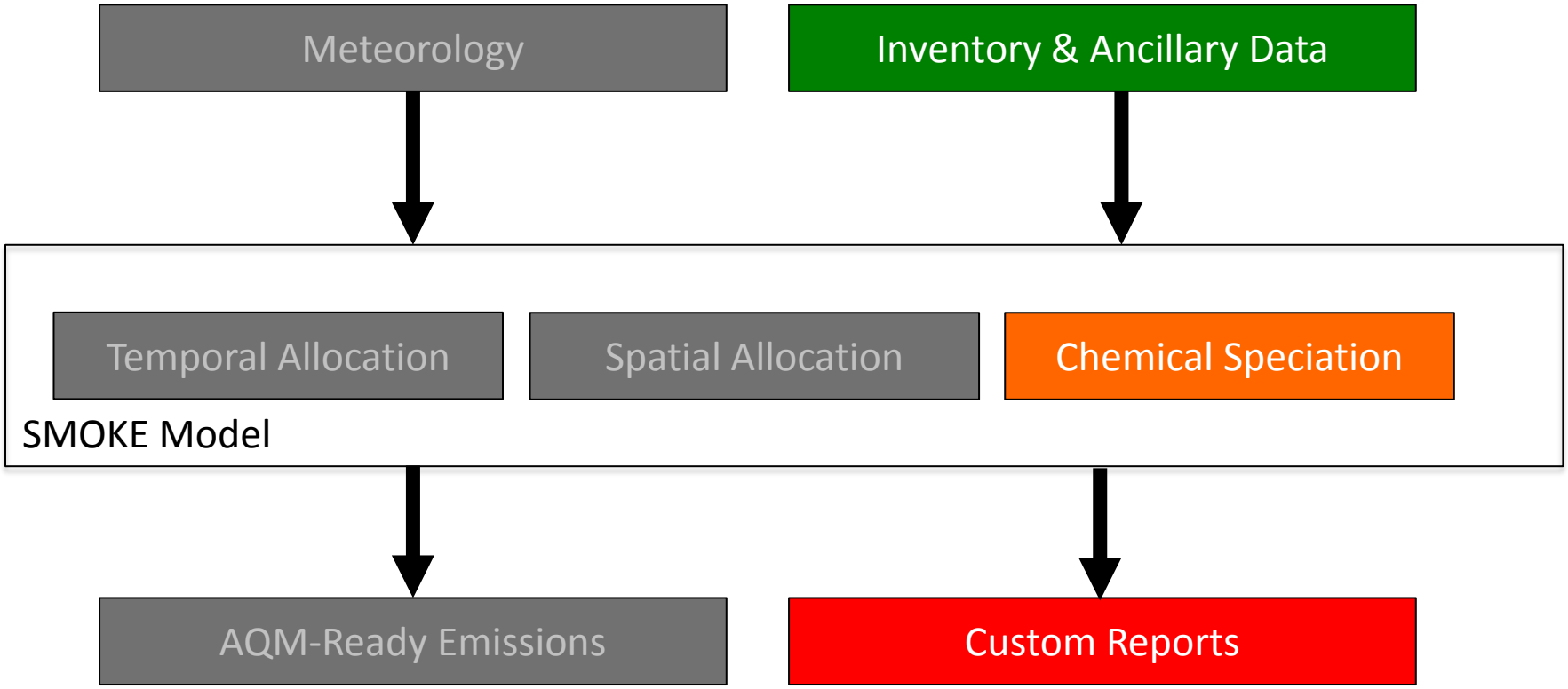
Project Background and Objectives

- Reactivity: Quantifies the relative contributions of individual volatile organic compounds (VOCs) to ozone formation (mass O3/mass VOC)
- 3-State Air Quality Study (3SAQS) project context:
  - Understand the contributions of individual emissions sources to rural and regional ozone
  - Analyze and improve emission inventories
- Objective: To develop an approach for analyzing emission inventories that considers VOC reactivity

Emissions Processing Schematic



Emissions Processing Schematic



Emissions Chemical Speciation

- Convert inventory pollutants to AQM species
  - PM2.5 → EC, OC, SO4, NO3, crustal PM species, other PM
  - VOC
    - Reactive organics (ROG) → Total organics (TOG)
    - TOG → Carbon Bond, SAPRC, RACM species

Emissions Chemical Speciation

- Speciation in SMOKE
  - Profile = characterization of the individual organics species from an emissions process
  - ROG2TOG = convert inventory VOC to TOG
  - Cross-reference = associate speciation profiles to inventory sources, e.g. by inventory pollutant, source code (SCC), location (country/state/county)

Emissions Chemical Speciation

- Example calculation
  - Model Species = Inventory VOC * ROG2TOG * Profile Splits
  - 100 TPY VOC source
    - ROG2TOG = 1.639
    - 100 TPY VOC = 163.9 TPY TOG
  - Profile 1 = External Combustion Boiler – Residual Oil
    - 28% acetone = 45.9 TPY
    - 42% formaldehyde = 68.9 TPY
    - 11% methane = 18.0 TPY
    - 14% n-butane = 23.0 TPY
    - 5% n-hexane = 8.2 TPY
  - Additional layer of information parameterizes the actual organics to photochemical mechanism species

Speciation Resources

- Speciation Database
  - Database of VOC and $PM_{2.5}$ profiles for specific sources
  - Speciation Data Browser: http://cfpub.epa.gov/si/speciate/
- Speciation Tool
  - Database (Perl/PostgreSQL) system of TOG to chemical mechanism splits for > 1,500 profiles
- EPA CHIEF
  - Speciation x-ref assignments: Profile IDs to SCCs

Speciation Tool

- Open-source database of profile mass fractions and chemical mechanism lumping schemes
- Supported mechanisms
  - Carbon Bond IV, 05, 6
  - SAPRC 99, 07, 07T
  - SOA_CAMx45
  - CMAQ AE5 and AE6
- HAP/CAP integrate/no-integrate profiles
- Public release is imminent (http://www.cmascenter.org)

Reactivity Enhancements to Speciation Database

- Maximum Incremental Reactivity (MIR) estimates the max O3 change resulting from the addition of an incremental mass of VOC
  - ΔO3/VOC
  - Calculated for > 1,000 organic compounds
- Add MIRs to the Speciation Tool Database and calculate profile total MIR:

Reactivity Enhancements to Speciation Database

Speciation Profile 1 (External Combustion Boiler – Residual Oil) Example with 100 TPY source

Species	% weight	MIR	Fractional MIR
acetone	28	0.3559	0.0996
formaldehyde	42	9.4558	3.9714
methane	11	0.0144	0.0016
n-butane	14	1.1510	0.1611
n-hexane	5	1.2439	0.0622

Speciation Profile 1 Total MIR = 4.2960

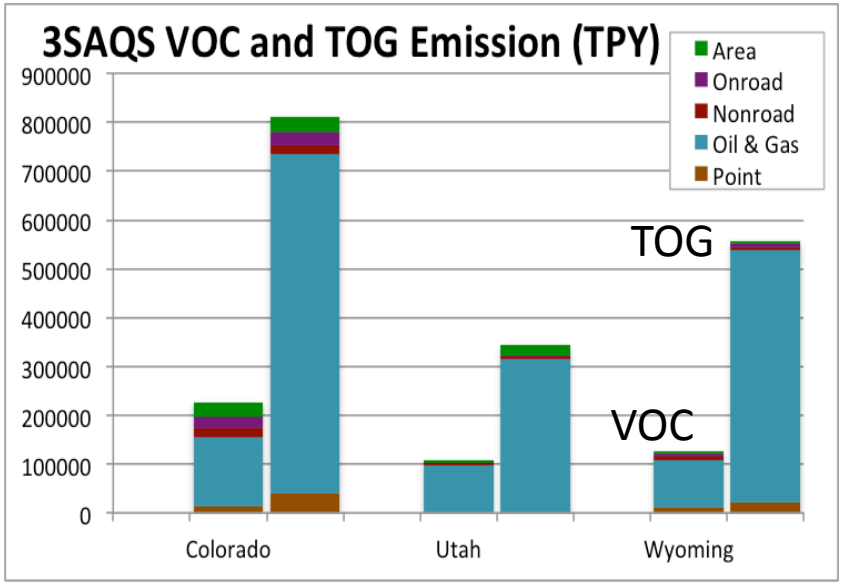
Reactive TOG = TOG * Total MIR = 163.9 * 4.2960 = 704.1 TPY O3

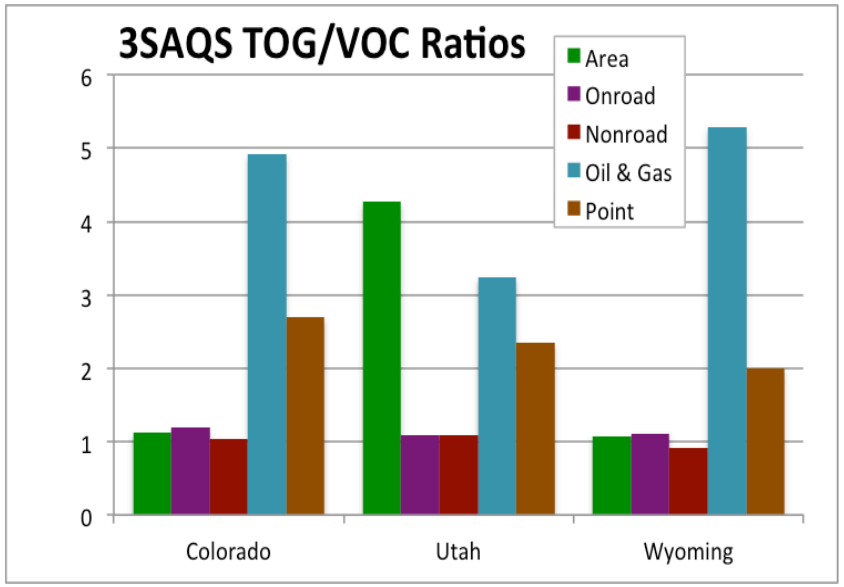
Reactivity Enhancements to Speciation Database

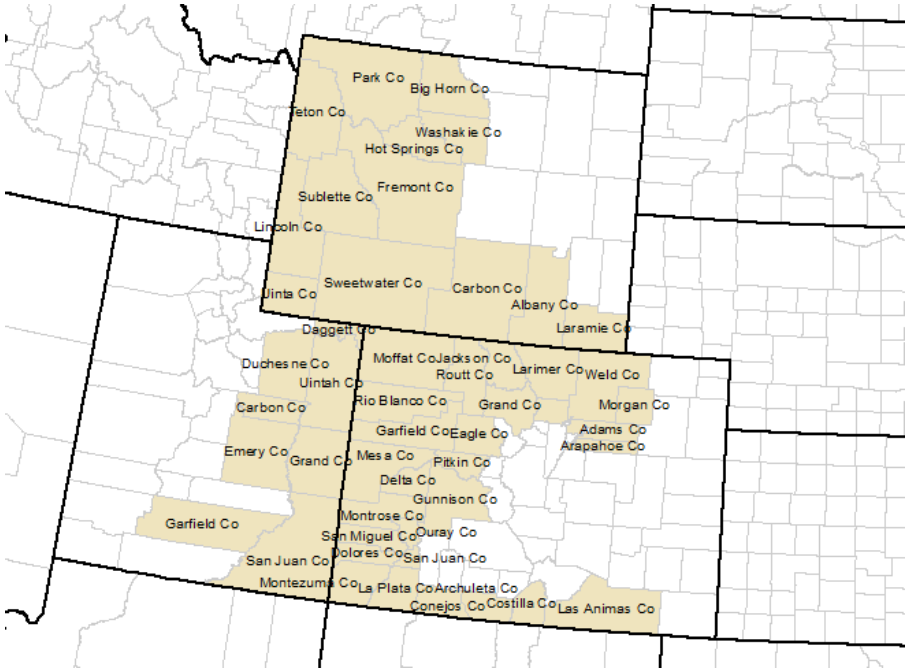
Profile #	Description	Total MIR
1	External Combustion Boiler - Residual Oil	4.2960
4	External Combustion Boiler - Refinery Gas	3.2322
5	External Combustion Boiler - Coke Oven Gas	1.1277
7	Natural Gas Turbine	2.8468
8	Reciprocating Diesel Fuel Engine	6.9601
11	By Product Coke Oven Stack Gas	2.9585

Inventory Reactivity Analyses

- Use SMOKE (Smkreport) to output tables of emissions by speciation profile.
  - Can also include: state, county, SCC, hour, and/or model grid cell
- Multiply TOG emissions associated with each speciation profile by total profile MIR to get reactive TOG (RTOG).
- Calculate total reactivity for inventory sectors in a county/state
- Example analyses:
  - Reactivity based inventory analysis
    - Compare RTOG to TOG within/across counties or spatial regions
    - Compare RTOG contributions of different inventory sectors/SCCs within a region (i.e. identify the most reactive sources contributing to O3 formation in a spatial region or inventory)
  - Emissions quality assessments
    - Does looking at the VOC emissions in the context of reactivity reveal any interesting trends?
    - Are we making the correct profile assignments to inventory sources (cross-referencing QA)
    - Are the profiles that we're assigning to sources representative of the source (profile QA)?







Total Anthro TOG/VOC Ratios

CO	=	3.60
UT	=	3.16
WY	=	4.40

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Next Steps

- Cooperate with Bill Carter to fill in the blanks for compounds/mixtures in the Speciate Database that don't have MIRs
  - 1,653 organic species in the database contribute to active speciation profiles
  - 47% of the species are missing MIRs (but small contributors to total emissions: median 8% of emissions across all profiles)
- Add a species MIR, MOIR, and EBIR tables to the Speciation Tool database and implement calculation of total profile MIR
- Apply profile MIRs to 3SAQS 2008 base emissions
- A similar approach could be used for toxicity by replacing species reactivity with species toxicity

Reactivity in Recent News

"Congratulations to Dr. William Carter, the first recipient of the Arthur C. Stern Award, for his pioneering work on ozone reactivity scales published in the July 1994 issue of ***JA&WMA***. This paper provided the foundation for requiring the use of reformulated gasoline to address the Nation's ozone pollution problem," says Dr. S. T. Rao, ***JA&WMA*** Technical Editor-in-Chief.