

RUN SPECIFICATION SHEET

HIGH-LEVEL AND LOW-LEVEL SOURCE APPORTIONMENT MODELING USING THE RepBase2 and 2028OTBa2 EMISSION SCENARIOS

WRAP Regional Haze Modeling Study
Revised September 29, 2020

Run Names:	RepBase2 High-Level Source Apportionment (H-L SA) 2028OTBa2 High-Level Source Apportionment (H-L SA) 2028OTBa2 Low-Level Source Apportionment for PM (L-L SA pm) (optional) 2028OTBa2 Low-Level Source Apportionment for ozone (L-L SA o3)
Model:	CAMx v7.0
Domains:	36US1 and 12WUS2 two-way nesting (see Figure 1)
Period:	2014 calendar year meteorology
Emissions:	RepBase2 and 2028OTBa2 updated emissions with RepBase Fires
Boundary Conditions:	WRAP Revised 2014 GEOS-Chem Base Case
Source Apportionment:	<u>H-L SA</u> : Natural sources, fires and anthropogenic emissions from U.S. and International sources <u>L-L SA</u> : 13 WRAP states for 5 anthropogenic source sectors
Purpose:	<p>The RepBase2 and 2028OTBa2 H-L Source Apportionment simulations have multiple uses:</p> <ul style="list-style-type: none"> • The RepBase2 H-L SA results with the fire contributions eliminated are used in the EPAwoF and ModMID 2028 visibility projection approaches (see draft WRAP visibility projection guidance document¹). • The RepBase2 and 2028OTBa2 H-L SA results are used in the TSS modeled express tools for source contributions.² • The RepBase2 and 2028OTBa2 H-L SA U.S. anthropogenic emission contributions are compared against the Dynamic Evaluation U.S. anthropogenic emissions impairment Glidepath developed using the 2002 H-L SA results. • The 2028OTBa2 H-L SA International anthropogenic emissions and Rx fire contributions are used to develop Adjusted URP Glidepaths (see draft WRAP URP Glidepath adjustment guidance document³). • The U.S. and international anthropogenic emissions, natural and fire contributions to ozone concentrations are also obtained. <p>The 2028OTBa2 L-L SA pm and (optional) L-L SA o3 results can be used as follows:</p> <ul style="list-style-type: none"> • State contributions to 2028 visibility impairment at Class I areas (CIAs) for total anthropogenic and 5 source sectors. • Total WRAP states EGU, non-EGU, O&G, Mobile and Other anthropogenic emissions contribution to visibility impairment at CIAs. • Similar contributions for ozone if and when this SA is completed.

¹ http://www.wrapair2.org/pdf/2028_Vis_Proj_WhitePaper_2020-07-24draft.pdf

² <https://views.cira.colostate.edu/tssv2/Express/ModelingTools.aspx>

³ http://www.wrapair2.org/pdf/URP_Glidepath_Adjust_WRAP_2020-07-24draft.pdf

DESCRIPTION

The RepBase2 and 2028OTBa2 High-Level Source Apportionment (H-L SA) CAMx simulations will conduct Particulate Source Apportionment Technology (PSAT) and Ozone Anthropogenic Precursor Source Apportionment (APCA) source apportionment. The RepBase2 and 2028OTBa2 emission scenarios both use the representative baseline fire emissions⁴ that were developed by the WRAP Fire and Smoke Work Group (FSWG⁵).

The CAMx RepBase2 and 2028OTBa2 PSAT and APCA H-L SA simulations will use the 36-km 36US1 and 12-km 12WUS2 domains shown in Figure 1 using two-way interactive grid nesting and will obtain contributions of anthropogenic, natural and fire emissions to PM and ozone concentrations and for PM, the resultant visibility at Class I Areas (CIAs) under RepBase2 and 2028OTBa2 conditions.

The CAMx 2028OTBa2 source sector Low-Level Source Apportionment (L-L SA) will conduct PSAT (and APCA, if conducted) source apportionment modeling to obtain separate contributions of 5 anthropogenic emission source sectors from each of the 13 WRAP states to SO₄ and NO₃ (and ozone, if conducted) concentrations.

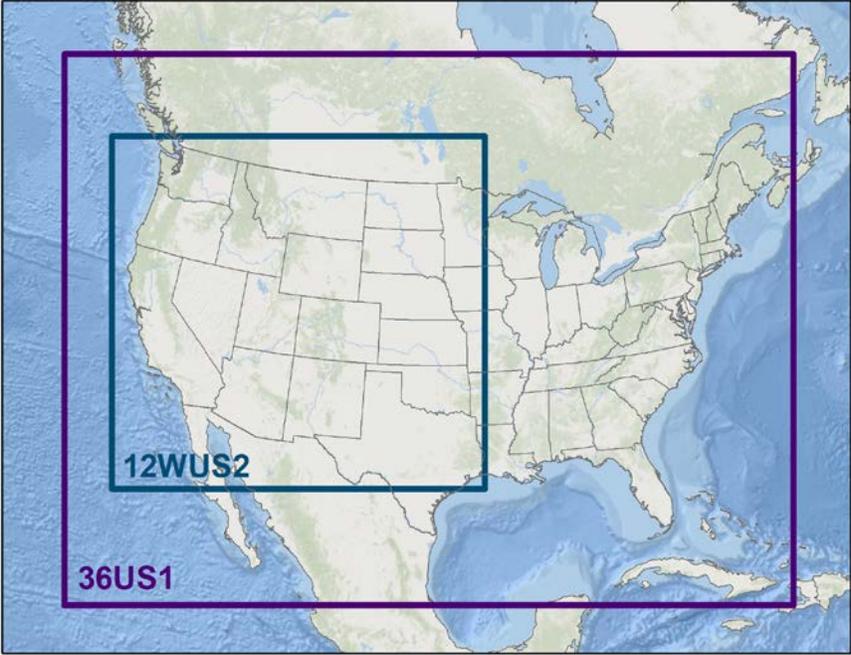


Figure 1. WRAP/WAQS 36-km 36US1 and 12-km 12WUS2 modeling domains used in the WRAP 2014v2, RepBase2 and 2028OTBa2 CAMx simulations.

HIGH-LEVEL SOURCE APPORTIONMENT SPECIFICATIONS

The RepBase2 and 2028OTBa2 H-L SA modeling will be performed in a consistent fashion. Besides the emissions (RepBase2 vs. 2028OTBa2), the only difference in the configuration of the two H-L SA runs is that RepBase2 H-L SA has one Source Group for all U.S. anthropogenic emissions, whereas 2028OTBa2 splits the U.S. anthropogenic emissions into two Source Groups: (1) WRAP states; and (2) non-WRAP states (note that both RepBase2 and 2028OTBa2 H-L SA have a separate Source Group for emission from Commercial

⁴ <http://wrapair2.org/RBFFSWG.aspx>

⁵ <http://wrapair2.org/FSWG.aspx>

Marine Vessels within 200 nautical miles [nmi] of the U.S. coast that are interpreted as U.S. anthropogenic emissions).

Source Apportionment Families of Tracers to be Used

The CAMx H-L SA modeling will apply the PSAT tool using the SO₄ (3), NO₃/NH₄ (8) and Primary PM (14) families of reactive tracers resulting in 25 total reactive tracers used to track PM source apportionment for each Source Group. The Secondary Organic Aerosol (SOA) family of PSAT tracers (which requires 14 tracers for each Source Group) will not be used because it would increase the run time by ~50% and the standard model output SOA species can be used to operationally⁶ estimate SOA due to anthropogenic (SOAA) versus biogenic (SOAB) precursors. This means we will not be able to distinguish whether the SOAA is due to U.S. or international anthropogenic emissions, but within the U.S. away from the border CIAs SOAA will be dominated by U.S. sources. We will also not be able to distinguish whether SOABB is from biogenic VOC or from fires, although since fire primary organic aerosol (POA) is much higher than fire VOC emissions so when fires are contributing to OA the fire POA dominates and it doesn't really matter whether the SOAB is biogenic or fire in origin.

The CAMx APCA tool will also be used at the same time as PSAT in the H-L SA runs to obtain ozone contributions for the same Source Groups as PSAT. There are two versions of ozone source apportionment in CAMx, the Ozone Source Apportionment Technology (OSAT) and APCA. They differ in how ozone is attributed to natural sources (e.g., biogenic VOC and NO and lightning NO_x [LNO_x]). APCA will only assign ozone formed to the natural Source Group when it is due to natural NO_x emissions interacting with natural VOC emissions. In the case where ozone is formed due to chemical reactions involving natural VOC and anthropogenic NO_x emissions under VOC-limited ozone formation conditions where OSAT would assign the ozone formed to the natural emissions Source Group, APCA recognizes that natural emissions cannot be controlled so redirects the ozone formed to the anthropogenic emissions Source Group. APCA is used for the RepBase2 and 2028OTBa2 H-L SA as it provides more control strategy relevant information than OSAT.⁷

For each Source Group, APCA requires 10 reactive tracers to track ozone contributions. However, the PSAT NO₃ family has 5 reactive tracers in common with APCA so the addition of APCA only increases the number of reactive tracers need to track ozone formation from each Source Group by 5, from 25 (for PSAT alone) to 30 (PSAT + APCA) reactive tracers for each Source Group.

Boundary Conditions

The CAMx v7 source apportionment tool has a new capability to provide separate contributions due to stratified boundary conditions (BCs). Typically, these stratifications will be different source sectors from outside of the CAMx modeling domain. A BC source apportionment stratification pre-processor has been developed that can provide stratified BCs for the CAMx v7 source apportionment tool two ways: (1) processing of an existing larger scale source apportionment simulations into stratified BCs (i.e., one-way nesting among CAMx source apportionment runs); and (2) using global chemistry model base case and zero-out emission simulations processed for BCs to define BCs stratified as the zero-out component of the global model simulations. The CAMx v7 BC source apportionment pre-processor used this second approach with the 2014 GEOS-Chem base case (BASE), 2014 GEOS-Chem Natural (NAT, i.e., no anthropogenic emissions anywhere) and 2014 GEOS-Chem no international anthropogenic emissions (i.e., Zero-out Rest of World or ZROW) cases that were processed to generate lateral boundary conditions (BCs) for the CAMx 36-km 36US1 modeling domain. These three 2014 GEOS-Chem runs were processed to generate CAMx BC input files (i.e., GCBC_BASE, GCBC_NAT and GCBC_ZROW). They were then processed so that CAMx can separately track BC contributions due to natural sources (BC_{Natural}), International anthropogenic emissions

⁶ In the operational definition of SOAA and SOAB we are assuming that all SOA from isoprene, terpene and sesquiterpene species are biogenic and SOA from aromatic species are anthropogenic even though there are some anthropogenic isoprene emissions, but they are miniscule compared to the biogenic isoprene.

⁷ Note that APCA version of the CAMx ozone source apportionment is used in EPA's ozone transport assessments (e.g., CSAPR).

(BC_{Intl}) and U.S. anthropogenic emissions (BC_{US}). The CAMx BC tool has to be provided with the GEOS-Chem base case and the GEOS-Chem zero-out CAMx BCs for each of the source categories to be separately tracked. This results in the following BC zero-out emission inputs into the CAMx BC stratification source apportionment pre-processor so that separate tracking of International anthropogenic, U.S. anthropogenic and Natural sources could be obtained.:

- | | | |
|--------------------------------|---|------------------------------------|
| 1. BC_{Base} | = | GCBC_Base |
| 2. $BC_{Zero-OutNatural}$ | = | GCBC_Base - GCBC_NAT |
| 3. $BC_{Zero-OutIntl-Anthro}$ | = | GCBC_Base - GCBC_ZROW |
| 4. $BC_{Zero-Out_USA-Anthro}$ | = | GCBC_Base - (GCBC_ZROW - GCBC_NAT) |

This results in tracking three Source Groups for the lateral boundaries ($BC_{Natural}$, BC_{Intl} and BC_{US}). We also have to track the top concentration (TopCon) BC as well as Initial Concentrations (IC) so there are 5 total IC/BC tracers that need to be tracked in the RepBase2 and 2028OTBa H-L SA simulations. Note, it is expected, and the original RepBase H-L SA simulation verified, that the TopCon BC and IC contributions are negligible, but they still have to be separately tracked as the contributions due to all sources need to be accounted for in the CAMx source apportionment modeling.

Source Groups

When analyzing the contributions of geographic source regions and source emission sectors, the CAMx source apportionment tools (PSAT and APCA) allow the use of a source region map that defines the grid cell definitions of the source regions from which contributions will be tracked. Source Groups are defined as the intersection of the source regions and source categories. However, using the source region map can be inefficient as it may produce excessive computational time because you are tracking Source Groups that have no interest (e.g., state-specific biogenic emission contributions). Thus, for the RepBase2 and 2028OTBa2 H-L SA simulation we are providing separate emission inputs for each Source Group to be tracked.

Table 1 lists the 15 and 16 Source Groups being tracked in the, respectively, RepBase2 and 2028OTBa2 H-L SA simulations. As noted above, they differ in that RepBase2 H-L SA tracks all U.S. anthropogenic emissions as a single Source Group while 2028OTBa2 H-L SA splits them between 13 WRAP states and non-WRAP state U.S. anthropogenic emissions in the continental U.S.

Table 1. Source Groups used in the RepBase2 (15) and 2028OTBa2 (16) H-L SA simulations.

No.	RepBase2	2028OTBa2	Description
1	BC _{Natural}	BC _{Natural}	Natural sources BC
2	BC _{Intl}	BC _{Intl}	International Anthropogenic Emissions BC
3	BC _{US}	BC _{US}	U.S. Anthropogenic Emissions BC
4	TopCon BC	TopCon BC	BCs from above top of the model (50 mb, ~19 km MSL)
5	IC	IC	Initial Concentrations
6	Natural	Natural	Biogenic, LNO _x , oceanic [SSA and DMS] and WBD
7	WF	WF	U.S. Wildfires (WF)
8	Rx Fires	Rx Fires	U.S. Prescribed Burns (Rx)
9	Ag Burning	Ag Burning	U.S. Agricultural Burning Fires (Ag)
10	Can/Mex Fires	Can/Mex Fires	Fires from Canada and Mexico (WF+Rx+Ag)
11	CMV ₂₀₀	CMV ₂₀₀	Commercial Marine Vessel (CMV) within 200 nautical miles (nmi) of the U.S. coast (i.e., the ECA zone of the coast of the U.S.)
12	CMV _{Intl}	CMV _{Intl}	CMV greater than 200 nautical miles off of the U.S. coast or off of the coast of Mexico or Canada
13	Mex Anthro	Mex Anthro	Mexico anthropogenic emissions
14	Can Anthro	Can Anthro	Canada anthropogenic emissions
15	U.S. Anthro	WRAP Anthro	<u>RepBase2</u> : All U.S. anthropogenic emissions <u>2028OTBa2</u> : 13 WRAP state anthropogenic emissions
16	NA	Non-WRAP Anthro	<u>RepBase2</u> : Not Applicable <u>2028OTBa2</u> : Non-WRAP state U.S. anthropogenic emissions

Computational Requirements

The previous RepBase H-L SA simulation with 14 Source Groups took 2.5 weeks to complete when not accounting for run stoppage. So the RepBase2 and 2028OTBa2 H-L SA runs will take approximately 19 and 20 days to complete, respectively, assuming no stoppage of the runs.

Use of Split WRAP vs. Non-WRAP State U.S. Anthropogenic in 2018OTBa2 H-L SA

The RepBase2 and 2028OTBa2 H-L SA are not using a source region map as they are providing separate emission input files for each of the 11 emission Source Groups in Table 1. However, Figure 2 is a source region map schematic that shows the geographic split of anthropogenic emissions in the 2028 H-L SA source apportionment simulation that tracks separate contributions of WRAP state, non-WRAP state, Mexico, Canada, CMV200 and remainder off-shore anthropogenic emissions. The source regions for the RepBase2 H-L SA is similar, only with the WRAP-state and non-WRAP state anthropogenic emissions are combined into one U.S. anthropogenic emissions Source Group.

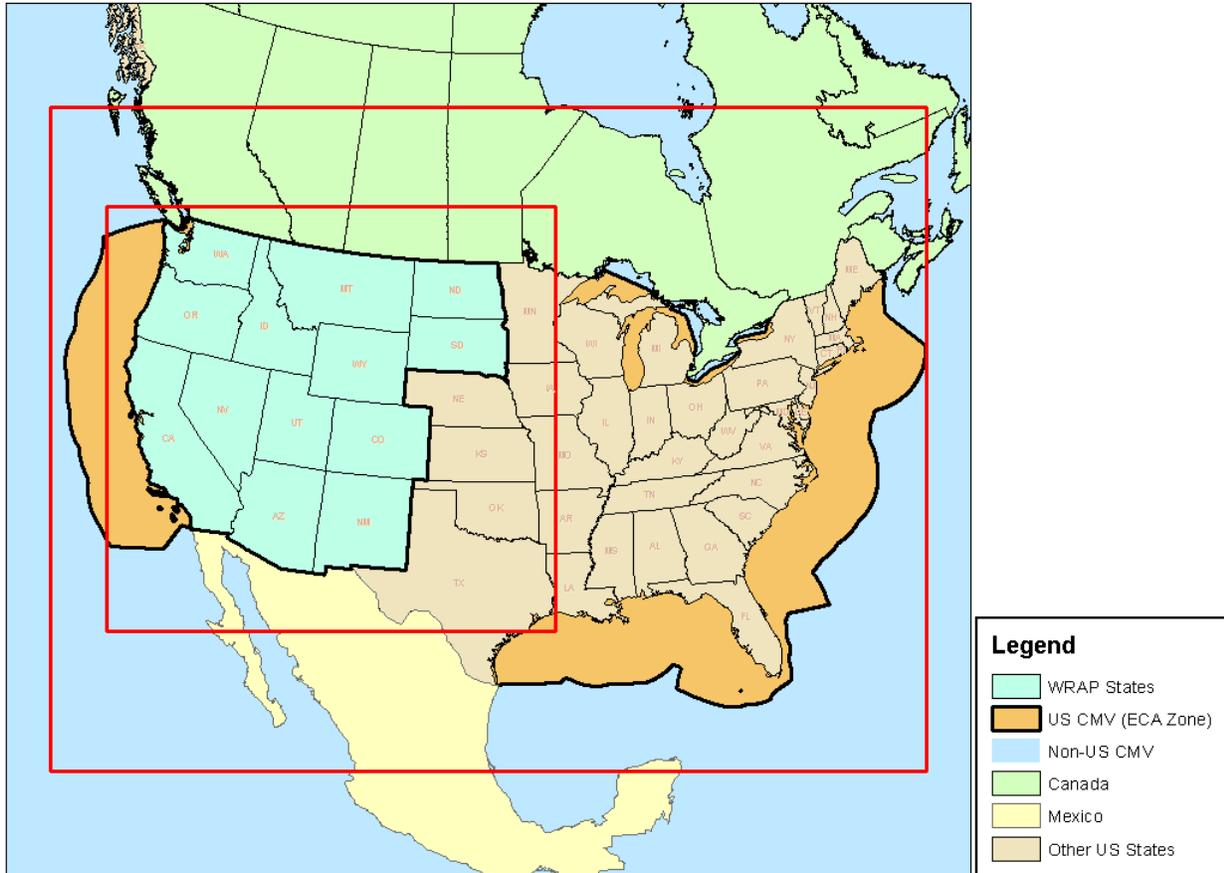


Figure 2. Schematic of the source regions used for anthropogenic emissions in the 2028OTBa2 H-L SA simulation.

LOW-LEVEL SOURCE SECTOR SOURCE APPORTIONMENT SPECIFICATIONS

WRAP is also conducting a CAMx 2028OTBa2 source sector Low-Level Source Apportionment (L-L SA) simulations to obtain the separate contributions of 5 source sectors from each of the 13 individual WRAP state anthropogenic emissions to PM (and ozone, if conducted) as follows:

- EGU Point
- Non-EGU Point
- Oil and Gas (Point and Non-Point)
- Mobile (On-Road and Non-Road)
- Remainder Anthropogenic (e.g., RWC, fugitive dust, agricultural, etc.)

The CAMx 2028OTBa2 L-L SA separate contributions for the 5 source sectors from 13 separate WRAP states will be combined with the CAMx 2028OTBa2 H-L SA results by replacing the H-L SA WRAP states anthropogenic Source Group (see Figure 2). When the 2028OTBa2 L-L and H-L SA results are combined this results in the effective anthropogenic emissions source regions shown in Figure 3, with the separate contributions of the 5 source sectors listed above obtained for each of the 13 WRAP states.

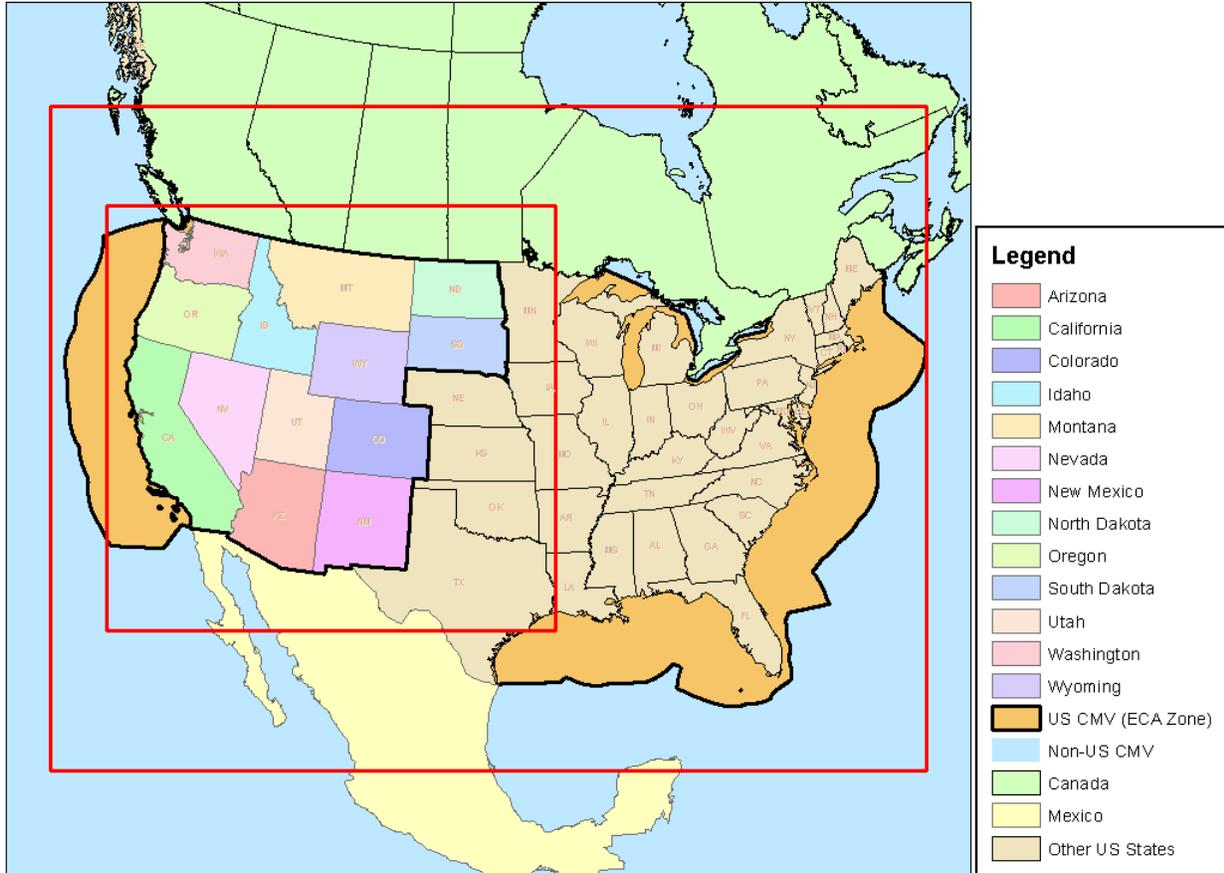


Figure 3. Anthropogenic source regions obtained by combining the CAMx 2028OTBa2 H-L and L-L SA modeling results.

Design of the CAMx 2028OTBa2 Low-Level Source Apportionment Runs

If we obtain the separate SO₄, NO₃, Primary PM (and ozone, if conducted) PSAT/APCA ozone contribution for 5 source sectors across 13 WRAP states using the 2014 36/12-km modeling database that would require 100 Source Groups and take four months to complete, which is too long. Thus we have divided the CAMx 2028OTBa2 L-L SA simulations into two runs as follows:

- CAMx 2028OTBa2 L-L SA PM run will run with just the PSAT SO₄ and NO₃ families of PSAT tracers and 13 WRAP states and 5 source sectors and require approximately 39 days to complete assuming no run stoppages.
- CAMx 2028OTBa2 L-L SA O₃ run will run (if conducted) with the ozone family of APCA tracers and 13 WRAP states and 6 source sectors and require approximately 42 days to complete assuming no run stoppage.

The CAMx 2028OTBa2 L-L SA PM will be highest priority in order to meet the schedule of the Regional Haze Rule planning deadlines.

For both the CAMx 2028OTBa2 L-L SA runs we will use a source region map that has 14 source regions and feed them the source sectors that we want contributions for. For the 2028OTB L-L SA PM PSAT run there will be 6 source sectors: EGU Point, non-EGU Point, O&G, Mobile, Remainder Anthropogenic and everything else (e.g., natural and fires). With 14 source regions and 6 source sectors plus two Source Groups for IC

and BC that makes 86 Source Groups. As noted above, we are just running the L-L SA pm run with the SO4 and NO3 PSAT families as adding the primary PM family would increase the run time from 39 to 90 days.

Because APCA needs natural sources to be their own source sector, the CAMx 2028OTBa2 L-L SA O3 run (if conducted) will use 7 source sectors and 14 sources regions resulting in 100 Source Groups and require 45 days to complete.

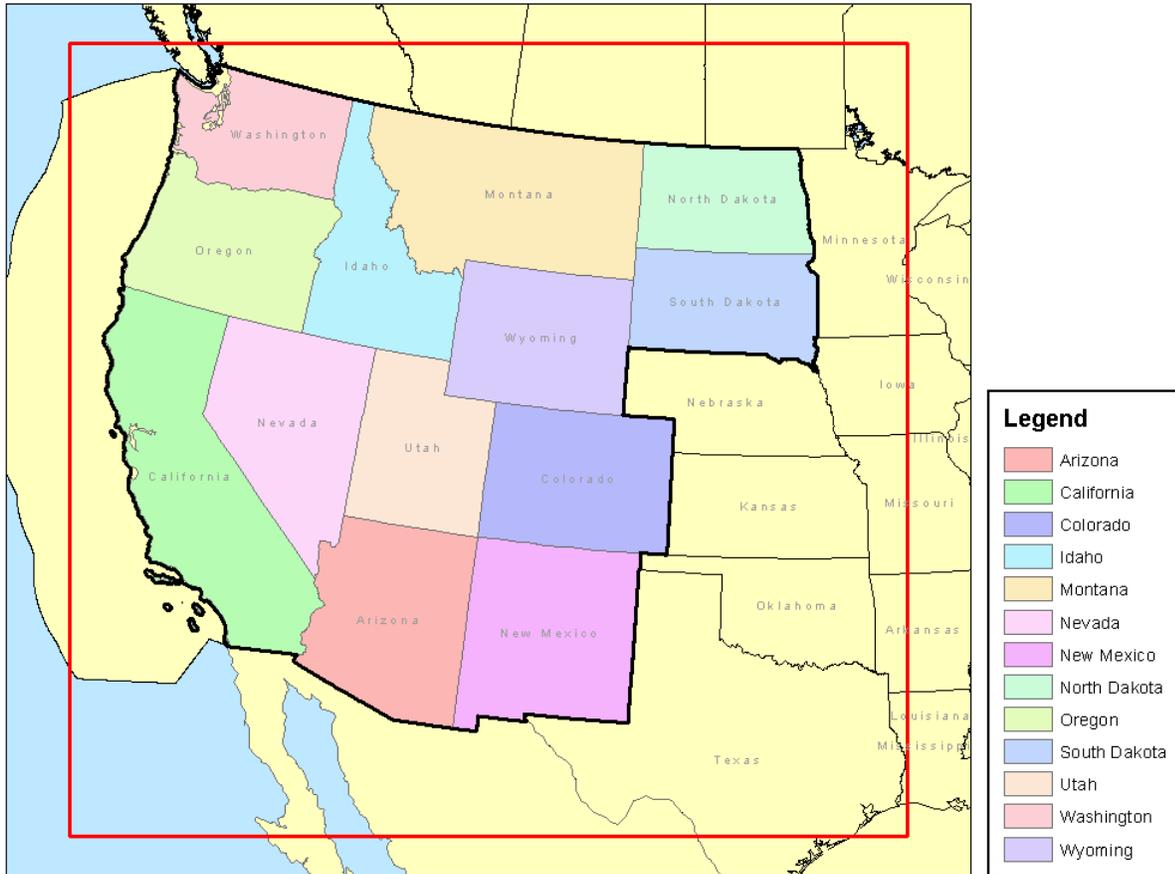


Figure 4. Source region map used in the CAMx 2028OTBa2 L-L SA runs that obtain separate contributions from 13 WRAP states and everywhere else.