Information for mapping CESM2 (CAM-chem or WACCM) gas and aerosol species to WRF-Chem species for various mechanisms

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Example mozbc.inp for mapping CESM2/CAM-chem and WACCM6 output to WRF-Chem MOZART gas phase species:

```
&control
do_bc = .true.
do_ic = .true.
domain = 1
dir_wrf = '/glade/scratch/pfister/WRFreal_WACCM/'
dir_moz = './'
fn_moz = 'output_WACMM_0001.nc'
moz_var_suffix = ''
def_missing_var = .true.
spc_map = 'o3 -> O3', 'n2o -> N2O', 'no -> NO',
     'no2 -> NO2', 'nh3 -> NH3', 'hno3 -> HNO3', 'hno4 -> HO2NO2',
     'n2o5 -> N2O5', 'h2o2 -> H2O2',
     'ch4 -> CH4', 'co -> CO', 'ch3ooh -> CH3OOH',
     'hcho -> CH2O', 'ch3oh -> CH3OH', 'c2h4 -> C2H4',
     'ald -> CH3CHO', 'acet -> CH3COCH3', 'mgly -> CH3COCHO',
     'pan -> PAN', 'mpan -> MPAN', 'macr -> MACR',
     'mvk -> MVK', 'c2h6 -> C2H6', 'c3h6 -> C3H6', 'c3h8 -> C3H8',
     'c2h5oh -> C2H5OH', 'c10h16 -> MTERP',
     'isopr -> ISOP','acetol -> HYAC', 'mek -> MEK',
     'bigene -> BIGENE', 'bigalk -> BIGALK',
     'tol -> TOLUENE', 'benzene -> BENZENE', 'xylenes -> XYLENES',
     'cres -> CRESOL', 'dms -> DMS', 'so2 -> SO2'
```

For MOZCART gas species replace:

```
'tol -> TOLUENE', 'benzene -> BENZENE', 'xylenes ->XYLENES',
```

with

```
'tol -> TOLUENE+BENZENE+XYLENES',
```

VOC species mapping between MOZART and other mechanisms

MOZART-T1	SAPRC-99	RADM2	CBMZ
C2H6	ALK1	ETH	C2H6
C3H8	ALK2	HC3	PAR
BIGALK	ALK3+ALK4+ALK5	HC5	PAR
C2H4	ETHE	OL2	ETH
C3H6	OLE1		PAR
BIGENE	OLE2	OLET+OLEI	OLET, OLEI, PAR
TOLUENE	ARO1	TOL	TOL
XYLENES	ARO2	XYL	XYL
ISOP	ISOPRENE	ISO	ISOP
CH3OH	MEOH		CH3OH
CH2O	HCHO	HCHO	HCHO
CH3CHO	CCHO	ALD	ALD2
CH3COOH		ORA2	RCOOH
GLYOXAL		GLY	
GLYALD		ALD	ALD2
CH3OOH		OP1	CH3OOH
C2H5OOH		OP2	ETHOOH
CH3COOOH		PAA	
CH3COCH3	ACET	KET	AONE
HYAC		KET	AONE
CH3COCHO		MGLY	MGLY
ONIT+NOA+ALKNIT		ONIT	ONIT
MEK	MEK+PRD2	KET	AONE
MVK	MVK		ISOPRD
MACR	METHACRO		ISOPRD
MPAN			
HYDRALD			ISOPRD
BIGALD			OPEN
ONITR			ISOPN
CRESOL		CSL	CRES

MAM4 Aerosols [X. Liu, GMD, doi:10.5194/gmd-9-505-2016, 2016]

Aerosol Mode	CESM label	type	σ_g	Size range (μm)
Aitken	_a2	dst, ncl, so4, soa*, num	1.6	0.015 – 0.053
Accumulation	_a1	bc, pom, dst, ncl, so4, soa*, num	1.8	0.058 – 0.27
Coarse	_a3	dst, ncl, so4, num	1.8	0.8 – 3.65
Primary carbon	_a4	bc, pom, num	1.8	0.058 – 0.27

soa* = soa1, soa2, soa3, soa4, soa5 in mechanisms with VBS-SOA; =soa in MAM-SOA

num = total number (all aerosol types) for each mode

Matching the Modal Aerosol Model (MAM) in CESM (CAM-chem and WACCM) to WRF-Chem aerosol models

CESM with MAM4 -> MOSAIC 8-bin in WRF-Chem

```
      'oc_a01->0.0093*pom_a1+0.7510*soa1_a2+0.0093*soa1_a1+0.7510*soa2_a2+
0.0093*soa2_a1+0.7510*soa3_a2+0.0093*soa3_a1+0.7510*soa4_a2+0.0093*soa4_a1+
0.7510*soa5_a2+0.0093*soa5_a1;1.e9',
          'oc_a02->0.1123*pom_a1+0.2376*soa1_a2+0.1123*soa1_a1+0.2376*soa2_a2+
0.1123*soa2_a1+0.2376*soa3_a2+0.1123*soa3_a1+0.2376*soa4_a2+0.1123*soa4_a1+
0.2376*soa5_a2+ 0.1123*soa5_a1;1.e9',
          'oc_a03->0.3835*pom_a1+0.0113*soa1_a2+0.3835*soa1_a1+0.0133*soa2_a2+
0.3835*soa2_a1+0.0113*soa3_a2+0.3838*soa3_a1+0.0113*soa4_a2+0.3838*soa4_a1+
0.0113*soa5_a2+ 0.3838*soa5_a1;1.e9',
          'oc_a04->0.3783*pom_a1+0.0001*soa1_a2+0.3783*soa1_a1+0.0001*soa2_a2+
0.3783*soa2_a1+0.0001*soa3_a2+0.3783*soa3_a1+0.0001*soa4_a2+0.3783*soa4_a1+
0.0001*soa5_a2+ 0.3783*soa5_a1;1.e9',
          'oc_a05->0.1077*pom_a1+0.0000*soa1_a2+0.1077*soa1_a1+0.0000*soa2_a2+
0.1077*soa2_a1+0.0000*soa3_a2+0.1077*soa3_a1+0.0000*soa4_a2+0.1077*soa4_a1+
0.0000*soa5_a2+ 0.1077*soa5_a1;1.e9',
          'oc_a06->0.0087*pom_a1+0.0000*soa1_a2+0.0087*soa1_a1+0.0000*soa2_a2+
0.0087*soa2_a1+0.0000*soa3_a2+0.0087*soa3_a1+0.0000*soa4_a2+0.0087*soa4_a1+
0.0000*soa5_a2+ 0.0087*soa5_a1;1.e9',
          'oc_a07->0.0002*pom_a1+0.0000*soa1_a2+0.0002*soa1_a1+0.0000*soa2_a2+
0.0002*soa2_a1+0.0000*soa3_a2+0.0002*soa3_a1+0.0000*soa4_a2+0.0002*soa4_a1+
0.0000*soa5_a2+ 0.0002*soa5_a1;1.e9',
          'oc_a08->0.0000*pom_a1+0.0000*soa1_a2+0.0000*soa1_a1+0.0000*soa2_a2+
0.0000*soa2_a1+0.0000*soa3_a2+0.0000*soa3_a1+0.0000*soa4_a2+0.0000*soa4_a1+
0.0000*soa5_a2+ 0.0000*soa5_a1;1.e9',
          'bc_a01->0.0093*bc_a1+0.0093*bc_a4;1.e9',
          'bc_a02->0.1123*bc_a1+0.1123*bc_a4;1.e9',
          'bc_a03->0.3835*bc_a1+0.3835*bc_a4;1.e9',
          'bc_a04->0.3783*bc_a1+0.3783*bc_a4;1.e9',
          'bc_a05->0.1077*bc_a1+0.1077*bc_a4;1.e9',
          'bc_a06->0.0087*bc_a1+0.0087*bc_a4;1.e9',
          'bc_a07->0.0002*bc_a1+0.0002*bc_a4;1.e9',
          'bc_a08->0.0000*bc_a1+0.0000*bc_a4;1.e9',
          'so4_a01->0.7510*so4_a2+0.0093*so4_a1+0.0000*so4_a3;1.e9',
          'so4_a02->0.2376*so4_a2+0.1123*so4_a1+0.0000*so4_a3;1.e9',
          'so4_a03->0.0113*so4_a2+0.3835*so4_a1+0.0000*so4_a3;1.e9',
          'so4_a04->0.0001*so4_a2+0.3783*so4_a1+0.0002*so4_a3;1.e9',
          'so4_a05->0.0000*so4_a2+0.1077*so4_a1+0.0061*so4_a3;1.e9',
          'so4_a06->0.0000*so4_a2+0.0087*so4_a1+0.0934*so4_a3;1.e9',
          'so4_a07->0.0000*so4_a2+0.0002*so4_a1+0.4020*so4_a3;1.e9',
          'so4_a08->0.0000*so4_a2+0.0000*so4_a1+0.4983*so4_a3;1.e9',
          'nh4_a01->0.1410*so4_a2+0.0033*so4_a1+0.0000*so4_a3;1.e9',
          'nh4_a02->0.0446*so4_a2+0.0017*so4_a1+0.0000*so4_a3;1.e9',
          'nh4_a03->0.0021*so4_a2+0.0210*so4_a1+0.0000*so4_a3;1.e9',
          'nh4_a04->0.0000*so4_a2+0.0720*so4_a1+0.0000*so4_a3;1.e9',
          'nh4_a05->0.0000*so4_a2+0.0202*so4_a1+0.0011*so4_a3;1.e9',
          'nh4_a06->0.0000*so4_a2+0.0001*so4_a1+0.0175*so4_a3;1.e9',
          'nh4_a07->0.0000*so4_a2+0.0000*so4_a1+0.0755*so4_a3;1.e9',
          'nh4_a08->0.0000*so4_a2+0.0000*so4_a1+0.0935*so4_a3;1.e9',
          'no3_a01->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a02->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a03->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a04->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a05->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a06->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a07->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'no3_a08->0.0000*so4_a2+0.0000*so4_a1+0.0000*so4_a3;1.e9',
          'na_a01->0.2954*ncl_a2+0.0037*ncl_a1+0.0000*ncl_a3;1.e9',
          'na_a02->0.0935*ncl_a2+0.0442*ncl_a1+0.0000*ncl_a3;1.e9',
```

```
'na_a03->0.0045*ncl_a2+0.1509*ncl_a1+0.0000*ncl_a3;1.e9',
'na_a04->0.0000*ncl_a2+0.1488*ncl_a1+0.0000*ncl_a3;1.e9',
'na_a05->0.0000*ncl_a2+0.0424*ncl_a1+0.0024*ncl_a3;1.e9',
'na_a06->0.0000*ncl_a2+0.0034*ncl_a1+0.0367*ncl_a3;1.e9',
'na_a07->0.0000*ncl_a2+0.0000*ncl_a1+0.1582*ncl_a3;1.e9',
'na_a08->0.0000*ncl_a2+0.0000*ncl_a1+0.1960*ncl_a3;1.e9',
'cl_a01->0.4555*ncl_a2+0.0056*ncl_a1+0.0000*ncl_a3;1.e9',
'cl_a02->0.1441*ncl_a2+0.0681*ncl_a1+0.0000*ncl_a3;1.e9',
'cl_a03->0.0068*ncl_a2+0.2326*ncl_a1+0.0000*ncl_a3;1.e9',
'cl_a04->0.0000*ncl_a2+0.2295*ncl_a1+0.0000*ncl_a3;1.e9',
'cl_a05->0.0000*ncl_a2+0.0654*ncl_a1+0.0037*ncl_a3;1.e9',
'cl_a06->0.0000*ncl_a2+0.0055*ncl_a1+0.0567*ncl_a3;1.e9',
'cl_a07->0.0000*ncl_a2+0.0001*ncl_a1+0.2439*ncl_a3;1.e9',
'cl_a08->0.0000*ncl_a2+0.0000*ncl_a1+0.3023*ncl_a3;1.e9',
'oin_a01->0.7510*dst_a2+0.0093*dst_a1+0.0000*dst_a3;1.e9',
'oin_a02->0.2376*dst_a2+0.1123*dst_a1+0.0000*dst_a3;1.e9',
'oin_a03->0.0113*dst_a2+0.3835*dst_a1+0.0000*dst_a3;1.e9',
'oin_a04->0.0001*dst_a2+0.3783*dst_a1+0.0002*dst_a3;1.e9',
'oin_a05->0.0000*dst_a2+0.1077*dst_a1+0.0061*dst_a3;1.e9',
'oin_a06->0.0000*dst_a2+0.0087*dst_a1+0.0934*dst_a3;1.e9',
'oin_a07->0.0000*dst_a2+0.0002*dst_a1+0.4020*dst_a3;1.e9',
'oin_a08->0.0000*dst_a2+0.0000*dst_a1+0.4983*dst_a3;1.e9',
'num_a01->0.9502*num_a2+0.2509*num_a1+0.0000*num_a3;1.0',
'num_a02->0.0494*num_a2+0.4626*num_a1+0.0000*num_a3;1.0',
'num_a03->0.0004*num_a2+0.2470*num_a1+0.0007*num_a3;1.0',
'num_a04->0.0000*num_a2+0.0377*num_a1+0.0232*num_a3;1.0',
'num_a05->0.0000*num_a2+0.0016*num_a1+0.1886*num_a3;1.0',
'num_a06->0.0000*num_a2+0.0000*num_a1+0.4372*num_a3;1.0',
'num_a07->0.0000*num_a2+0.0000*num_a1+0.2935*num_a3;1.0',
'num_a08->0.0000*num_a2+0.0000*num_a1+0.0566*num_a3;1.0'
```

CESM -> MOSAIC 4 bin

Sum the 8-bin MOSAIC bins (above) for each aerosol type:

4bin_a01 = 8bin_a01 + 8bin_a02
4bin_a02 = 8bin_a03 + 8bin_a04
4bin_a03 = 8bin_a05 + 8bin_a06
4bin_a04 = 8bin_a07 + 8bin_a08

CESM/MAM4 -> GOCART in WRF-Chem

'BC1 -> 1.0*bc_a4;1.e9',
'BC2 -> 1.0*bc_a1;1.e9',
'OC1 -> 1.0*pom_a4;1.e9',
'OC2 -> 1.0*pom_a1;1.e9',
'SEAS_1 -> 1.0*ncl_a1+1.0*ncl_a2;1.e9',
'SEAS_2 -> 0.5*ncl_a3;1.e9',
'SEAS_3 -> 0.5*ncl_a3;1.e9',
'SEAS_4 -> 0.0*ncl_a3;1.e9'
'DUST_1 -> 0.02*dst_a3;1.e9',
'DUST_2 -> 0.93*dst_a3;1.e9',
'DUST_3 -> 0.05*dst_a3;1.e9',
'DUST_4 -> 0.0*dst_a3;1.e9',
'DUST_5 -> 0.0*dst_a3;1.e9',