This dataset contains data for the paper Janechek et al. Comprehensive Atmospheric Modeling of Reactive Cyclic Siloxanes and Their Oxidation Products, ACP, 2017.

Contacts:
Nathan Janechek: nathan-janechek@uiowa.edu
natejanechek@gmail.com (permanent)
Charles Stanier: charles-stanier@uiowa.edu

In the paper, cyclic volatile methyl siloxanes (cVMSs) were added to the CMAQ model to simulate the gas phase species. This dataset contains the edited CMAQ model code, run scripts, cVMS emission development, and hourly concentration and deposition fluxes of a subset of the modeled species.

Please contact the authors with questions or if you use the data. If you use the data, please cite both the ACP paper and this dataset.

At the time of data upload, the final ACP doi links have not been finalized. Below is the ACP Discussion citation to the article. The final ACP version should be available soon.

Janechek, N. J., Hansen, K. M., and Stanier, C. O.: Comprehensive Atmospheric Modeling of Reactive Cyclic Siloxanes and Their Oxidation Products, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2016-1159, in review, 2017.

List of Files

1. Modified gas-phase mechanism INCLUDE files created by CHEMMECH based on cb05cl_ae5_aq mechanism
    a. GC_ADV.EXT
    b. GC_CONC.EXT
    c. GC_DDEP.EXT
    d. GC_DEPV.EXT
    e. GC_DIFF.EXT
    f. GC_EMIS.EXT
    g. GC_G2AE.EXT
    h. GC_G2AQ.EXT
    i. GC_ICBC.EXT
    j. GC_SCAV.EXT
    k. GC_SPC.EXT
    l. GC_WDEP.EXT
    m. mech.def
    n. RXCM.EXT
    o. RXDT.EXT

2. Modified ebi_cb05cl_ae5 model code
   Files edited:
    a. hrg2.F

b. hrinit.F
c. hrprodloss.F
d. hrrates.F
e. hrdata_mod.F

3. Deposition model code changes
   a. acm2_inline
   Files edited:
      i. DEPVVARS.F
      ii. m3dry.F

   b. cloud_acm_ae5
   Files edited:
      i. hlconst.F

5. Emissions
   a. Data source is EPA 2011 Version 6.0 Air Emissions Modeling Platform downloaded from:
   ftp://ftp.epa.gov/EmisInventory/2011v6/v1platform/spatial_surrogates/

      i. US: CONUS36_2010_v4_20130827_surrogates.zip
      ii. MEX: CONUS36_2006CAN_2010v3MEX_surrogates.zip
      iii. CAN: 12US1_CAN2006_MEX2010v3_surrogates.zip

   b. cvms_emision_factors.xlsx
   Emission factors were calculated using ratios of Yucuis et al. (2013) Chicago measurements

   Yucuis, R. A., Stanier, C. O., and Hornbuckle, K. C.: Cyclic siloxanes in air, including identification of high levels in Chicago and distinct diurnal variation, Chemosphere, 92, 905-910, doi:10.1016/j.chemosphere.2013.02.051, 2013.

   c. cvms_emis.csv
   Combined population and cVMS emissions data. Format is (row, col, population, D4, D5, and D6 emissions). Emissions are in units of mole s^{-1}.

6. Boundary
   a. Month specific boundary conditions were developed by merging default "Profile" boundary conditions for default CMAQ species and cVMS boundary conditions derived from the DEHM modeled D5 as described in the paper.

      i. January: bcon_jan_mrg.nc
      ii. April: bcon_apr_mrg.nc
      iii. July: bcon_jul_mrg.nc
      iv. October: bcon_oct_mrg.nc

7. GRIDDESC domain definition
    a. GRIDDESC domain definition

        'CONUS36'
        'LAM_40N97W', -2736.D3, -2088.D3, 36.D3, 36.D3, 148, 112, 1

8. CMAQ run scripts
    a. JPROC
        i. bldit.jproc_seas
        ii. run.jproc_seas
    b. ICON
        i. bldit.icon_seas
        ii. run.icon_seas
    c. BCON (default "Profile")
        i. bldit.bcon_reg
        ii. run.bcon_reg
    d. BCON (DEHM cVMS values for 24 hours in m3conc mode)
        i. bldit.bcon_seas
        ii. run.bcon_seas
    e. CCTM
        i. bldit.cctm_seas
        ii. run.hppm.cctm_seas.csh
        iii. CONUS36_seas.csh

9. CMAQ Output
    a. ACONC – hourly average surface concentration in units of ppm for D4, D5, D6, o-D4, o-D5, o-D6, and SO2.
        i. January: jan_aconc_sub.ncf
        ii. April: apr_aconc_sub.ncf
        iii. July: jul_aconc_sub.ncf
        iv. October: oct_aconc_sub.ncf
    b. DRYDEP – cumulative hourly dry deposition (kg hectare^{-1}) for D4, D5, D6, o-D4, o-D5, o-D6, and SO2
        i. January: jan_drydep_sub.ncf
        ii. April: apr_drydep_sub.ncf
        iii. July: jul_drydep_sub.ncf
        iv. October: oct_drydep_sub.ncf
    c. WETDEP1 – cumulative hourly wet deposition (kg hectare^{-1}) for D4, D5, D6, o-D4, o-D5, o-D6, and SO2
        i. January: jan_wetdep_sub.ncf
        ii. April: apr_wetdep_sub.ncf
        iii. July: jul_wetdep_sub.ncf
        iv. October: oct_wetdep_sub.ncf