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The box model **Hg_DomeC** simulates the diurnal and seasonal variations of mercury at Dome Concordia on the East Antarctic Plateau. The model is written in MATLAB® and details are described in the Song et al. paper which will be submitted soon (information will be updated then). This **readme.pdf** file provides a brief introduction to the model's parameterization.

The **main.m** is the main solving routine, which calls **fcn_vpbrox.m** (for estimating vertical profiles of BrO_x), and **fcn1.m** and **fcn2.m** (for calculating mercury concentrations and fluxes). As for the other routines, **fcn_reshape1.m** and **fcn_reshape2.m** are for array reshaping, **fcn_vplot.m** is for plotting vertical profiles of several variables, and **interp1gap.m** is for interpolation.

The input files for the box model are stored in the folder **./data/**. The CSV file **free_troposphere_hg_conc.csv** contains the modeled free tropospheric Hg^0 and Hg^{II} concentrations from two global chemical transport models (GEOS-Chem and GLEMOS). The MATLAB data file **mdatain_bro_monthly.mat** contains the modeled BrO concentrations from two global chemical transport model (GEOS-Chem and *p*-TOMCAT). The MATLAB data files **mdatain_MARorg.mat** and **mdatain_MARadj.mat** both contain the meteorological parameters (temperature, pressure, height, turbulent diffusion coefficients, surface layer turbulent kinetic energy) from the MAR model, and the turbulent diffusion coefficients and kinetic energy are different in the original and adjusted data files. The pressure at each vertical level is calculated based on the surface layer pressure, the depth of each layer, and the virtual temperature. The maximum/minimum values of turbulent diffusion coefficient and kinetic energy are set as 1E-5/20 $m^2 s^{-1}$ and 1E-2/0.5 $m^2 s^{-2}$ for the numerical stability of the solution. The MATLAB data files **mdatain_OXorg.mat** and **mdatain_OXadj.mat** respectively contain the temporal and vertical profiles of several oxidants (OH, HO_2, NO, NO_2, and O_3) calculated based on the original and adjusted meteorological data.

The input and output parameters and variables are respectively contained in MARLAB data files named **input.mat** and **output.mat**. under the folder **./data/**. The model is run for the year of 2013 with a spin up period of two months. **Table 1** shows the description of some parameters and variables in the mercury box model. **Table 2** shows the setup of parameters for different model scenarios.

Table 1. Description of parameters and variables in the mercury box model.

Parameter or Variable	Description	Values, Dimensions, or Notes
Logical or numerical parameters to set up in each scenario		
LBROX	Reaction rates for the Br oxidation mechanism	2: upper, 1: lower; 0: not included
LOHOX	Reaction rates for the OH oxidation mechanism	2: upper, 1: lower; 0: not included
LO3OX	Reaction rates for the O_3 oxidation mechanism	2: upper, 1: lower; 0: not included
LBRMR	Concentrations for Br	2: high; 1: low
LOHMR	Concentrations for OH	2: high; 1: default; 0: low
LO3MR	Concentrations for O_3	2: high; 1: default; 0: low
LMAR	Turbulent coefficients from MAR	0: original; 1: adjusted
TAU1	Lifetime of snow Hg^{II} photoreduction in summer	Number in days
TAU2	Lifetime of snow Hg^{II} dark reduction in the non-summer period	Number in days
Numerical parameters specified in the model		
BETA	Scaling factor of turbulent diffusion coefficients in surface snowpack	3×10^{-3} s
DT	Time step	1 minute
EDPTH	Surface snow layer depth	0.2 m
HG0DVD	Dry deposition rate for Hg^0	10^{-4} cm s^{-1}
HG2DVD	Dry deposition rate for Hg^{II}	1 cm s^{-1}
N0	Air number density at standard condition	2.68×10^{19} molecule cm^{-3}
R	Gas constant	287 J kg^{-1} K^{-1}
ROU	Snow density	300 kg m^{-3}
TS	All time step in a day	array [1:1:1440]
XX1	Linear array in time	array 1×240
XXh	Linear array in time	array 1×24
XXm	Linear array in time	array 1×1440
fac_br	Uncertainty of Br concentration	2.5
fac_oh	Uncertainty of OH concentration	0.5
fac_o3	Uncertainty of O_3 concentration	0.02
kbrdiff	Uncertainty of Br reaction rate constants	4
kohdiff	Uncertainty of OH reaction rate constants	8
Input or calculated parameters in the model		
DD	Depth of each air layer [m]	array nlay×1
DSWt DSWt2 DSWtm	Downward solar radiation [W m^{-2}]	DSWtm: array 1440×nday
FACSTP2LTP	Conversion factor from standard condition [ng m^{-3} STP] to local condition [molecule cm^{-3} LTP]	Estimated by local air density
Kzem Kze Kze2 Kzt	Turbulent diffusion coefficients [m^2 s^{-1}]	Kzem: array 1440×nday×nlay
Nair	Local air density [molecule cm^{-3} LTP]	Estimated by local pressure and temperature

PPt PPt3	Pressure in each air layer [mb]	PPt3: 12×24×nlay
TKEtm TKEt TKEt2	Turbulent kinetic energy in surface air layer [m^2 s^{-2}]	TKEtm: array 1440×nday
TTt TTt3	Temperature in the air layers [K]	TTt3: array 12×24×nlay
ZZ ZZt	Depth of air layers [m]	ZZ: array nlay×1
avg_bro	Monthly averaged BrO concentration [pptv]	array 12×1
boxin	Temporary data structure	structure; similar for boxout
cnt	Temporary parameter for counting	similar for cnt1 and cnt2
dmc_mavg	Input observational data of O_3 and NO_x	array 12×12×24; similar for dmc_mavg2
jo1d	Normalized O_3 photolysis rate	array 1440×nday
k1max k1min k3 k4_br k4_bro k4_ho2 k4_no2 k4_oh k5max k5min k6max k6min keq12	Rate constants or equilibrium constants for corresponding reactions or reaction pairs; details given in the main.m routine	
kbrox	Oxidation rates for the Br mechanism	array 12×24×nlay; similar for ktox, ko3ox, and kohox
ktoxm	Total oxidation rates of Hg^0 [s^{-1}]	array 1440×nday×nlay
ksn1m	Rate of photoreduction [s^{-1}]	Estimated by TAU1 and DSW
ksn2m	Rate of dark reduction [s^{-1}]	Estimated by TAU2 and NO_x levels
moBr	Concentrations of Br	array 12×24×nlay; similar for moO3, moNO, moNO2, moOH, moHO2, moBrO, moBrOc, moHO2c, moNO2c, moNOc, moO3c, moOHc
nday	Number of days for calculation	426 (365 days in 2013 and 61 days for spinup)
nlay	Number of layers in the atmosphere	33
snHg0int snHg2cint snHgmint hg0int hg2int	Initial concentrations or masses for Hg^0 and Hg^{II}	
tmp tmp1 tmp2 tmpfac tmpPP tmpTT junk c	Temporary arrays	
upHg0m	Free tropospheric Hg^0 concentration	array 1440×nday; similar for upHg2m
upHg0	Free tropospheric Hg^0 concentration	array 12×1; similar for upHg2
	Parameters in model output	
svairHg0	Atmospheric Hg^0 concentrations	array 1440×nday×nlay

svairHg2	Atmospheric Hg^{II} concentrations	array 1440×nday×nlay
svHg0dep	Hg^0 dry deposition flux	array 1440×nday; unit
svHg2dep	Hg^{II} dry deposition flux	array 1440×nday
svHg0exg	Hg^0 exchange flux from free troposphere	array 1440×nday
svHg2exg	Hg^{II} exchange flux from free troposphere	array 1440×nday
svHg0sne	Hg^0 reemission flux from surface snowpack	array 1440×nday
svHg2sn1	Surface snow Hg^{II} photoreduction flux	array 1440×nday
svHg2sn2	Surface snow Hg^{II} dark reduction flux	array 1440×nday
svsnHg0	Surface snow Hg^0 concentrations	array 1440×nday
svsnHg2m	Surface snow Hg^{II} mass	array 1440×nday

Table 2. Set up of parameters for different model scenarios.

Scenario	LBROX	LOHOX	LO3OX	LBRMR	LOHMR	LO3MR	LMAR	TAU1	TAU2
O3_HH_3d	0	0	2	1	1	2	1	3	1.00E+10
O3_HH_7d	0	0	2	1	1	2	1	7	1.00E+10
O3_HH_14d	0	0	2	1	1	2	1	14	1.00E+10
O3_HH_21d	0	0	2	1	1	2	1	21	1.00E+10
OH_HH_3d	0	2	0	1	2	1	1	3	1.00E+10
OH_HH_7d	0	2	0	1	2	1	1	7	1.00E+10
OH_HH_14d	0	2	0	1	2	1	1	14	1.00E+10
OH_HH_21d	0	2	0	1	2	1	1	21	1.00E+10
BR_HH_3d	2	0	0	2	1	1	1	3	1.00E+10
BR_HH_7d	2	0	0	2	1	1	1	7	1.00E+10
BR_HH_14d	2	0	0	2	1	1	1	14	1.00E+10
BR_HH_21d	2	0	0	2	1	1	1	21	1.00E+10
BR_HL_3d	1	0	0	2	1	1	1	3	1.00E+10
BR_HL_7d	1	0	0	2	1	1	1	7	1.00E+10
BR_HL_14d	1	0	0	2	1	1	1	14	1.00E+10
BR_HL_21d	1	0	0	2	1	1	1	21	1.00E+10
BR_LH_3d	2	0	0	1	1	1	1	3	1.00E+10
BR_LH_7d	2	0	0	1	1	1	1	7	1.00E+10
BR_LH_14d	2	0	0	1	1	1	1	14	1.00E+10
BR_LH_21d	2	0	0	1	1	1	1	21	1.00E+10
BR_LL_3d	1	0	0	1	1	1	1	3	1.00E+10
BR_LL_7d	1	0	0	1	1	1	1	7	1.00E+10
BR_LL_14d	1	0	0	1	1	1	1	14	1.00E+10
BR_LL_21d	1	0	0	1	1	1	1	21	1.00E+10
BR_S1	2	0	0	2	1	1	0	14	1.00E+10
BR_S2	2	0	0	2	1	1	1	14	365
BR_S3*	2	0	0	2	1	1	1	14	1.00E+10

* For the scenario BR_S3, the concentrations of BrO for March and April are reduced by a factor of 3.