# README – POP2/Hg v1.0 Implementation Guide

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Ocean Mercury Biogeochemistry Module for CESM POP2

## 1. Introduction

### 1.1 Components

POP2/Hg is implemented within the CESM POP2 ocean model and coupled to MARBL for particle flux and ecosystem variables. Key model components include:

5 tracers:

- Dissolved elemental Hg0(aq)

- Divalent oxidized mercury HgII(aq)

- Particulate-bound mercury HgP

- Optional methylated species (MeHg, DMHg)

and 4 processes:

- Adsorption onto POC and release through remineralization

- Air–sea exchange

- Photochemical/dark/biochemical redox reactions

- Sinking and burial with biopump

All code provided in this repository is sufficient to **run, reproduce, and extend** the Hg module within CESM2.1.3.

### 1.2 CESM Configuration

POP2/Hg v1.0 supports CESM2.1.3 configurations, using:

- CESM version: CESM2.1.3 (cesm2_1_3)

- Varified compset: G compsets (active ocean + sea ice)

- OCN_TRACER_MODULES: must enable `"hg"` and `"ecosys"`

- Varified grid: T62_g37 / T62_g17 (module is grid-independent)

## 2. Setup Instructions

### Step 1: Modify buildcpp in source code

Copy buildcpp to $CESM/components/pop/cime-config/

### Step 2: Create a new CESM case

e.g.:

```
cd $CESM_ROOT/cime/scripts
./create_newcase --case $CASE --compset G --res T62_g37
```

### Step 3: Enable Hg module

In `$CASE/env_build.xml` :

```
<entry id="OCN_TRACER_MODULES" ...>...,hg,ecosys</entry>
```

### Step 4: add hg module files

Copy POP2/Hg source files to: $CASE/SourceMods/src.pop/

### Step 5: Build and submit CESM case

## 3. POP2/Hg Call Tree

This section describes how the Hg module is called within the POP2 time-stepping framework, including tracer initialization, reading forcing fields, and the full sequence of operations executed every model time step.

## 3.1 Initialization (Tracer Initialization & Forcing File Setup)

- `hg_init`
  This ensures that Hg tracers, surface fluxes, and diagnostics are fully prepared before entering the time-stepping loop.

## 3.2 Time-step Processing (POP Baroclinic Time Step)

Within each POP baroclinic time step, the Hg module is called in the following order:

## (1) Update surface forcing

- `hg_set_sflux`

- Reads or interpolates atmospheric Hg fluxes (monthly climatology or annual time series)

- Applies surface deposition or air–sea exchange to POP surface-tracer forcing arrays

## (2) Hg biogeochemical processes

- `hg_partition`
  Recomputes the dissolved–particulate partitioning of Hg(II) using updated POC concentrations.

- `hg_chemistry`
  Executes the full aqueous Hg chemistry mechanism using the KPP integrator (Hg$^o$ ↔ Hg(II), photochemical reactions, methylation/demethylation if active).

- `hg_biopump`
  Applies scavenging of Hg(II) to POC, downward transport via sinking POC flux, and release of Hg during POC remineralization at depth.

This structure ensures that transport, forcing, and internal biogeochemical transformations are all applied consistently at each model time step.

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# 4. Diagnostics Activation

## 4.1 POP tavg diagnostics

check the needed diagnostics for Hg tracers in:

$CASE/SourceMods/src.pop/gx3v7_tavg_contents (or dependent on grid)

## 4.2 MARBL diagnostics output

Make sure the needed MARBL diagnostics are listed in:
components/marbl/defaults/diagnostics_latest.yaml

# 5. File List

## 5.1 Hg Module Files (in src.pop)

```
hg_mod.F90
hg_init.F90
hg_partition.F90
hg_chem.F90
hg_chem_kpp.F90
hg_chem_rates.F90
hg_biopump.F90
hg_forcing.F90
hg_tavg.F90
```

## 5.2 KPP-generated chemistry mechanism (in src.pop)

```
ocean_hg_Initialize.F90
ocean_hg_Integrator.F90
ocean_hg_Rates.F90
ocean_hg_Parameters.F90
ocean_hg_Function.F90
ocean_hg_Global.F90
ocean_hg_Jacobian.F90
ocean_hg_JacobianSP.F90
```

## 5.3 POP modifications (in src.pop)

```
passive_tracers.F90
tavg.F90
gx3v7_tavg_contents or gx1v7_tavg_contents
```

## 5.4 MARBL-related modifications (in src.pop)

```
ecosys_driver.F90
ecosys_tracers_and_saved_state_mod.F90
marbl_interface_private_types.F90
marbl_interior_tendency_mod.F90
settings_latest.yaml / json
```

## 5.5 CESM build configuration

```
buildcpp   (copied to component/pop/cime-config)
env_build.xml   (modify OCN_TRACER_MODULES)
```