Supplement of

Modelling the water isotopes distribution in the Mediterranean Sea using a high-resolution oceanic model (NEMO-MED12-watiso-v1.0): Evaluation of model results against in-situ observations.

Study by

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Supplementary text

Text S1. Water isotope package, and NEMO-MED12-watiso-v1.0 used manual

Supplementary tables

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Text S1.

In this section we present a detailed description of the source code of the water isotopes package, a user manual to explain how to compile and launch a simulation using the NEMO-MED12-watiso-v1.0 model in the Mediterranean Sea. The code source and few examples of model boundary conditions and model output are available for downloading here: link zenodo (https://zenodo.org/records/10453745).

The Mediterranean regional high-resolution model NEMO-MED12

NEMO-MED12 is the Mediterranean regional version of the NEMO ocean modelling platform. Documentation of the model can be found at:

https://forge.ipsl.jussieu.fr/nemo/svn/NEMO/releases/release-3.4/NEMOGCM/

This document provides technical details on the "watiso" package which has been fully tested with versions 3.4 and 3.6 of NEMO. Upgrading to version 4.2 is readily made; useful information in that purpose may be found in the note Adding a tracer package in NEMO.

Code source of water isotope package

The water isotope package is implemented within the NEMO model using the TOP interface core functionalities by providing all the physical constraints/boundaries of $\delta^{18}O$ and δD and pseudo-salinity tracers. TOP interface are activated using key-top as presented below:

Available in the flowing directory

Ayache_et_al_20XX_GMD_sup/watiso_package

- **par_watiso.F90**

define additional arrays and public variables

- **trcini_watiso.F90**

initialized user defined namelists and the call to the external BGC model initialization

- **trcnam_watiso.F90**

called by trcini_my_trc and contain the initialization of additional namelists.

- **trcsms_watiso.F90**

Source-Minus-Sinks terms due to the biogeochemical processes of the external model

- **trcwri_watiso.F90**

This routine performs the output of the model tracers.

- **trcice_watiso.F90**

Prescribe the tracers concentrations in the sea-ice

- **namelist_watisoCTL**

additional trc diagnostics: short names, Isotopic ref ratio initialization (VSMOW) and reference salinity.

- **namelist_top-watiso**

```
!! NEMO/TOP1 :  1 - tracer definition                 (namtrc    )
!!              2 - tracer data initialisation        (namtrc_dta)
!!              3 - tracer advection                  (namtrc_adv)
!!              4 - tracer lateral diffusion          (namtrc_ldf)
!!              5 - tracer vertical physics           (namtrc_zdf)
!!              6 - tracer newtonian damping          (namtrc_dmp)
!!              7 - dynamical tracer trends           (namtrc_trd)
!!              8 - tracer output diagonstics         (namtrc_dia)
```

Compiling the model

The compilation of NEMO-MED12 is managed entirely through makenomo routine, so the generation of executable file is the same as described for NEMOv3.4, and NEMOv3.6 (cf. https://forge.ipsl.jussieu.fr/nemo/wiki/Users/ModelInstall). Before code compilation, the library netcdf and a Fortran compiler need to be installed. The compilation procedure is simply the following:

```
Cd NEMOGCM/CONFIG

./makenemo -m NAME_OF_YOUR_ARCHITECTURE_SYSTEM -n MED12_OFF_watiso -s NEMO
```

If the compilation is successful, then it creates the executable file, "opa" in the flowing directory.

```
/NEMOGCM /CONFIG/MED12_OFF_watiso/EXP00
```

In our study, NEMO-MED12 is compiled to run with 121 cores in parallel mode.

Running the model

Before running the model, the 3D surface boundary conditions for

- Freshwater flux INTO the ocean,
- Different isotopic signature of meteoric waters and freshwater inflow from ice sheets and continents,
- Boundary condition the buffer zone in the Atlantic close to the Gibraltar need to be generated.

Examples of this boundary condition are available in the following directory:

```
Ayache_et_al_20XX_GMD_sup/FORCING

    1-  LMDZ-ISOT-144_143_ORCA_2009.nc
!  Atmospheric forcing from LMDZ
!  -1  preH2O       Precipitation H2O. [kg/(s*m2)]
!  -2  preO18       Precipitation., isotope O18 [kg/(s*m2)]
!  -3  preHDO       Precipitation, isotope HDO [kg/(s*m2)]
!  -4  evaH2O       evaporation H2O [kg/(m2*s)]
!  -5  evaO18       evaporation O18 [kg/(m2*s)]
!  -6  evaHDO       evaporation HDO [kg/(m2*s)]

    2-  river_runoff_clim__bassin.nc
! sorunoff        Runoffs monthly  [kg/(m2*s)]
```

If you run the NEMO-MED12-watiso-v1.0 model in offline coupling mode. In this method the fields of physics variables are read from files and interpolated at each model time step, i.e., the circulation fields (U, V, W) previously computed by the dynamical model are read daily and interpolated to give values for each 20 min time step, and must be provided in the forcing directory.

Technical aspects relative to the tracers in NEMO/TOP interface are not addressed here; they may be found in the companion report “TOP_manual-vxx”.

To run a simulation, you can use a bash script adapted from your CPU architecture system. It must contain some center-specific instructions for the management of environmental variables, including the necessary pathways for the model’s preferences and allocation of computing resources. The script is executed with a time step of one day, month or year (depending on the aims of your study).

Examples of model output are available in the following directory:

Ayache_et_al_20XX_GMD_sup/OUTPUT

1- MED12__watiso.200912.diad_T.nc
   H2Oflx: ‘Evap - Precip – Runoff’
   O18flx: ‘Net surface flux O18’
   HDOflx : ‘Net surface flux HDO’
   d18O : ‘Seawater delta O18’
   dD : ‘Seawater delta D’
2- MED12__watiso.200912.ptrc_T.nc
   WSEL: ‘"Pseudo salt tracer’

Table S.1 Standard output fields for the watiso package

Field	Type	Dim	Units	Description
R18O	ptrc	3-D	-	$^{18}\mathcal{R}$ ratio
RHDO	ptrc	3-D	-	D/H ratio
WSEL	ptrc	3-D	-	pseudo-salinity
d18O	diad	3-D	‰	δ^{18}O
dD	diad	3-D	‰	δD
d-excess	diad	3-D	‰	deuterium excess
H2Oflx	diad	2-D	$kg/m^2/s$	$\mathcal{E} - \mathcal{P} - \mathcal{R}$
O18flx	diad	2-D	$kg/m^2/s$	Net surface flux of ^{18}O
HDOflx	diad	2-D	$kg/m^2/s$	Net surface flux of D

Table S.2: Water fluxes in the different configurations of NEMO. Individual E and P are not available in NEMO when off-line mode; contains E (evaporation) −P (precipitation) −R (runoff)−I (net freshwater flux associated to sea-ice), expl (explicit, i.e. dilution/concentration by mean oc actual flux through the sea-surface), impl (implicit, i.e. dilution/concentration resulting from changes in the volume of the ocean), vvl: for the non-linear free-surface (variable volume)

NEMO-v3.4					
	Stand-alone			Coupled	
Offline	T	F		-	-
VVL	F	F	T	F	T
$\mathcal{E}$	-	expl	impl	expl	impl
$\mathcal{P}$	-	expl	impl	expl	impl
$\mathcal{E}-\mathcal{P}$	expl	expl	impl	expl	impl
$\mathcal{R}$	expl	impl	impl	impl	impl
$\mathcal{I}$	expl	expl	expl	expl	expl
Water fluxes in Eq.5 MUST be provided by					
$\mathcal{R}$	any	OGCM	OGCM	Land Mod	Land Mod
$\mathcal{E}$	any	any	OGCM	AGCM	AGCM
$\mathcal{P}$	any	any	OGCM	AGCM	AGCM
$\mathcal{I}$					

Reference:

Ayache, M., Dutay, J.-C., Mouchet, A., Tachikawa, K., Risi, C., & Ramstein, G. (2024). Model and output for Ayache et al "Modelling the water isotopes distribution in the Mediterranean Sea using a high-resolution oceanic model (NEMO-MED12-watiso-v1.0): Evaluation of model results against in-situ observations ". https://doi.org/10.5281/zenodo.10453745