AIRSEA namelist

A.Pozzer, P. Jöckel, R. Sander,
J. Williams, L. Ganzeveld and J.Lelieveld

Air Chemistry Department
Max-Planck Institute of Chemistry
PO Box 3060, 55020 Mainz, Germany
pozzer@mpch-mainz.mpg.de

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```
! -*- f90 -*-
&CTRL
 l_tendency     = T  ! tendency of tracers
 l_whitecap     = F  ! Whitecap coverage calculations
 l_rain         = F  ! rain effect calculations
 l_turb         = F  ! Alternative calculation for turbulent velocity
 l_salt         = T  ! salinity climatology from other submodel
 param_kw       = 1  ! 1) Liss (1986)
                     ! 2) Wanninkhof (1992)
                     ! 3) Wanninkhof (1999)
                     ! 4) Nightingale (2000)
                     ! 5) Ho (2006)
/
&CPL
convect_rain    = 'convect','cv_precflx'
large_rain      = 'cloud','rainflux'
salinity        = 'offlem','salt_salt'
!!! NOTES:
!!! - MAX 100 TRACERS !!!
!***********************************
ASI_NAME(2)       = 'DMS'
HENRY_A(2)        = 4.8E-1
HENRY_B(2)        = 3100.
ALPHA(2)          = 1.
MOL_VOL(2)        = 77.4  !le bas
S_CONST(2)        = 0.
MOL_MASS(2)       = 62.13
USE_MOL_MASS(2)   = .TRUE.
EFFECT(2)         = .TRUE.
OUTPUT(2)         = .TRUE.
WATER_CON_CHN(2)  = 'offlem','airsea01_DMS_SEA',
SATURATION(2)     = .FALSE.
!***********************************
ASI_NAME(3)      = 'CH3OH'
HENRY_A(3)       = 2.2E2
HENRY_B(3)       = 5600.
ALPHA(3)         = 1.
MOL_VOL(3)       = 42.5
S_CONST(3)       = 0.
MOL_MASS(3)      = 32.04
USE_MOL_MASS(3)  = .TRUE.
OUTPUT(3)        = .TRUE.
EFFECT(3)        = .TRUE.
WATER_CON_CONST(3)  = 0.94
SATURATION(3)   = .TRUE.
!***********************************
```

Figure 1: Namelist example as implemented in AIRSEA submodel.

1 CTRL, main control part

All this variables are logical (i.e. can have only TRUE/FALSE value) with the exception of `param_kw`, which has an INTEGER value (between 1 and 5).

- `l_tendency`: Two emission/deposition methods can be selected with this variable.
  - If `l_tendency` is set to FALSE, the change of the mixing ratio during one model time-step is calculated from the calculated flux and applied to the corrisponding tracer.
  - If `l_tendency` is set to TRUE, a lower boundary condition for the vertical diffusive flux F_{vdiff} is calculated.

  See Kerkweg et al. (2006b, Emission method (1) and (2), sec.2.1) for more informations.
- `l_whitecap`: If TRUE, Eq.(8) in the manuscript is used to calculate K_w; if FALSE, one of the parametriation selected with `param_kw` will be used.
- `l_rain`: If TRUE, the rain effect is included, accordingly to Eqs.(10)-(11) in the manuscript; if FALSE, no rain enhancement will be added to the calculated transfer velocity
- `l_turb`: If TRUE, the aerodynamic resistance (R_a) and the quasi laminar boundary layer resistance (R_{bqr}) are calculated following Eqs.(13)-(14) in the manuscript; if FALSE the same approach of Kerkweg et al. (2006a, Eqs.(3) and (4)) is used.
- `l_salt`: If TRUE the submodel will search for input file which describes the salinity of the surface water (see `salinity`, later). If FALSE a constant salinity of 0.4 mol/L is used.
- `param_kw`: The submodel will use different parametrisation to calculate the transfer velocity K_w, accordingly to the INTEGER number given here, following Tab.(1) in the manuscript.

2 CPL, coupling part

Consequently to the selection made, some input from other submodels may be needed. Namely, informations about the submodel and the name of the element input may be necessary for salinity concentration (`salinity`), large scale precipitation (`large_rain`) and convective precipitation (`convect_rain`). This information must be given accordingly to the submodels used as input. In fig.1, the salinity field has been introduced from OFFLEM, while `large_rain` and `convect_rain` are from CLOUD and CONVECT submodel respectively. In the example in fig.1, only the salinity field is necessary (because `l_salt` has been set to TRUE) while the other two variabels are needed only in case `l_rain = T` .

Finally, for each tracer the following informations are necessary:

- `ASI_NAME` : is the name of the tracer on which the air-sea balance is calculated. The submodel will calculate the fluxes only if the tracer is present in the MESSy model.
- `HENRY_A`: is the Henry's law constant at 298.15 Kas described in Sander (1999) in M/atm
- `HENRY_B`: is the temperature dependency of the Henry's law constant as described in Sander (1999) in K
- `ALPHA` : is the reactivity coefficient use in Eq.(2) in the manuscript
- `MOL_VOL`: is the molar volume at normal boiling point, which can be obtained with the LeBas method (LeBas, 1915; Reid et al., 1984), in cm^3/mol
- `S_CONST` : is the Setschenow constant (L/mol). If 0 the theoretical value is calculated.
- `MOL_MASS` : is the molar mass of the considered tracer in g/mol.
- `USE_MOL_MASS` : is a logical switch. If TRUE the molar mass present in the AIRSEA namelist will be used; if FALSE the default molar mass of the tracer defined in MESSy is used.
- `EFFECT` : needed for testing reason, if this logical parameter is switch to FALSE no air-sea interaction is calculated.

- `OUTPUT` : if this logical parameter is TRUE, the transfer velocity is calculated also without any tracer initialized in the ECHAM5/MESSy model (see `ASI_NAME`)
- `WATER_CON_CHN`: This switch is needed to introduce the field of surface water concentration of the selected tracer. The file (in nmol/L) has to be read in by OFFLEM, and associate with the relative element in the MESSy interface. The values in the AIRSEA namelist have to be introduced accordingly to the OFFLEM setup.
- `WATER_CON_CONST`: In case of constant water concentration, a single value can be given here (in nmol/L).
- `SATURATION`: If a saturation value is used, this logical parameter has to be set to TRUE. In this case the `WATER_CON_CONST` (or the input file contained in `WATER_CON_CHN`) is used as saturation value for the water contents (i.e. 1 balance between gas and liquid phase, < 1 undersaturation of water phase with respect to the gas phase, > 1 oversaturation of water phase with respect to the gas phase). In Fig.1, as example, a saturation value of 0.94 has been selected for CH_3OH.

References

Kerkweg, A., Buchholz, J., Ganzeveld, L., Pozzer, A., Tost, H., and Jöckel, P.: Technical Note: An implementation of the dry removal processes DRY DEPosition and SEDImentation in the Modular Earth Submodel System (MESSy), Atmos. Chem. Phys., 6, 4617–4632, 2006a.

Kerkweg, A., Sander, R., Tost, H., and Jöckel, P.: Technical Note: Implementation of prescribed (OFFLEM), calculated (ONLEM), and pseudo-emissions (TNUDGE) of chemical species in the Modular Earth Submodel System (MESSy), Atmos. Chem. Phys., 6, 3603–3609, 2006b.

LeBas, G.: The Molecular Volumes of Liquid Chemical Compounds, in The Properties of Gases and Liquids, Monograph Longmans, Green, 1915.

Reid, R., Pransnitz, J., and Poling, B.: The Molecular Volumes of Liquid Chemical Compounds, in The Properties of Gases and Liquids, 3rd edition, McGraw Hill, New York, 1984.

Sander, R.: Compilation of Henry‘s law constant for inorganic and organic species of potential importance in environmental chemistry, `http://www.henrys-law.org`, 1999.