SVOC (Version 1.0) User Manual

Semivolatile Organic Compounds

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SVOC is a new MESSy submodel to simulate tracers in the semivolatile organic group. All important cycling processes including emission, gas−particle partitioning, air−surface exchange, deposition, and degradation are calculated in the submodel through the calling sequence of process subroutines illustrated in Figure 1. A number of process parameterizations in the areas of gas−particle partitioning, soil volatilization, and the heterogeneous chemistry of benzo[a]pyrene (BaP) are available for use. Specifically, gas−particle partitioning is computed using one of four schemes: (1) Junge−Pankow (Junge, 1977; Pankow, 1987), (2) Finizio (Finizio et al., 1997), (3) Lohmann−Lammel (Lohmann and Lammel, 2004), and (4) Poly-parameter linear free energy relationships (ppLFER) (Goss and Schwarzenbach, 2001; Endo and Goss, 2014; Shahpoury et al., 2016). The soil volatilization is implemented using one of two parameterizations: the Jury scheme (Jury et al., 1983, 1990) and the Smit scheme (Smit et al., 1997). For BaP heterogeneous oxidation by O_3, four options are available for calculating the reaction rate: (1) Pöschl scheme (Pöschl et al., 2001), (2) Kwamena scheme (Kwamena et al., 2004), (3) Kahan scheme (Kahan et al., 2006), and (4) ROI-T scheme (Mu et al., 2018).

The following information lists major components in SVOC version 1.0, to be implemented within the ECHAM_v.5.3.0/MESSy_v2.50 model.

1 Namelist

The first step before running the submodel involves defining several input parameters in `svoc.nml` file. The template for this file can be seen in Figure 2.

1. Process switches:
   - `L_GP`: Switch to determine whether the calculations are for grid point (GP) tracers.
   - `L_LG`: Switch to determine whether the calculations are for Lagrangian (LG) tracers. The current SVOC version only works for grid-point representation (hence, `L_GP` should always be `.TRUE.`, and `L_LG` should be `.FALSE.`).
   - `l_svocpart`: Switch for gas−particle partitioning calculation. Default: `.TRUE.`
   - `l_svocvola`: Switch for volatilization from the surface. If this process is switched off, the AIRSEA submodel should also be turned off. Default: `.TRUE.`
   - `l_glacier`: Switch to include glacier compartment. Default: `.FALSE.`
   - `l_landsnow`: Switch to include snow compartment. Default: `.FALSE.`
   - `l_mode_partition`: If set to `.TRUE.`, the particulate-phase SVOC tracers will be discretized into the 7 aerosol modes applied in the GMXe and M7 submodels (*ns*: nucleation soluble, *ks*: Aitken soluble, *as*: accumulation soluble, *cs*: coarse soluble, *ki*: Aitken insoluble, *ai*: accumulation insoluble, and *ci*: coarse insoluble). Default: `.FALSE.` (the particle is treated as bulk species).

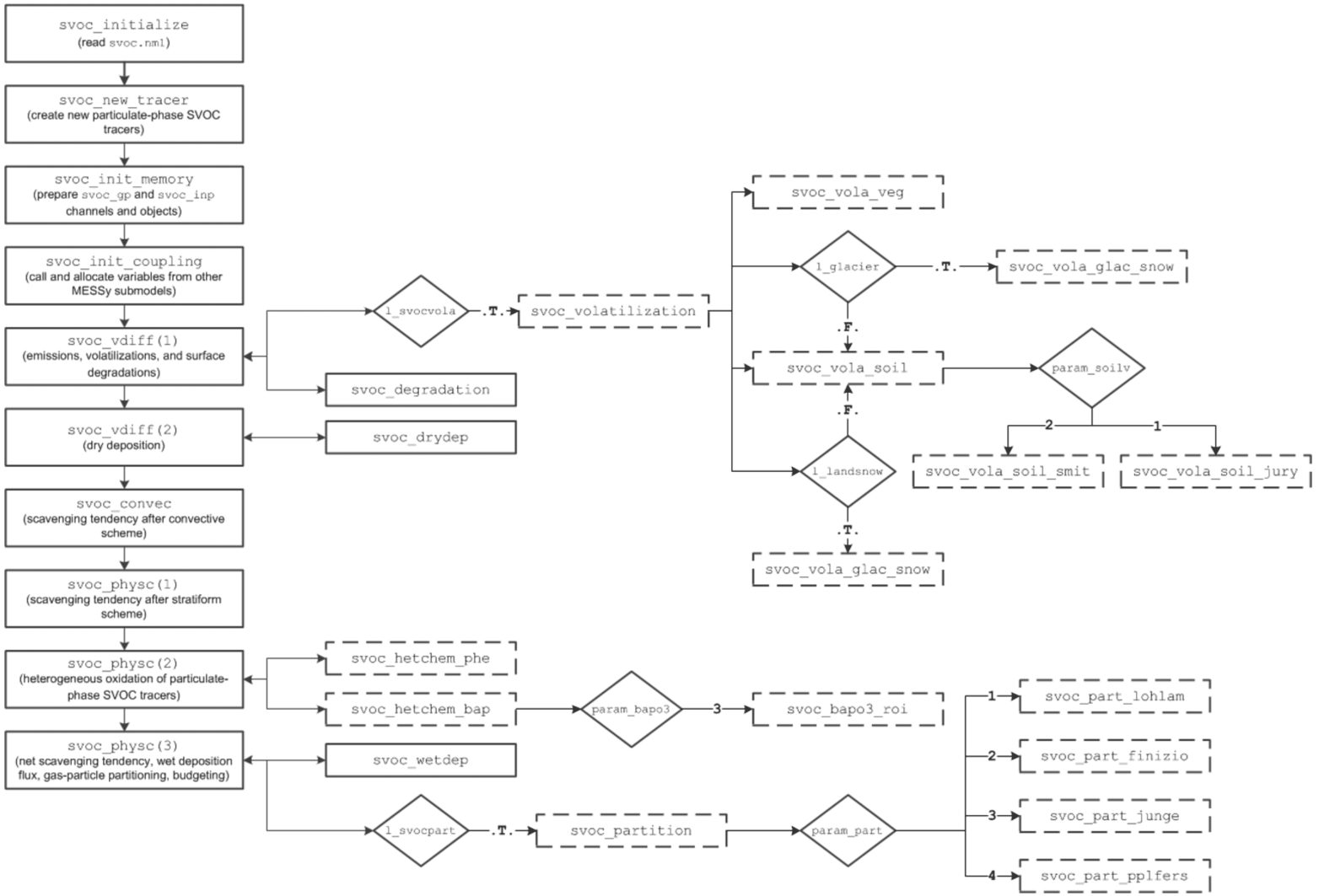

Figure 1: Calling sequence of process subroutines in SVOC submodel

```
! -*- f90 -*-

! ************************************************************************
! control namelist
! ************************************************************************

&CTRL

L_GP        = T ! SVOCs as grid-point tracers (default = T)
L_LG        = F ! SVOCs as lagrangian tracers (default = F)
l_svocpart  = T ! switch for gas-particle partitioning (default = T)
                ! if set to .false., l_mode_partition will be ignored
l_svocvola  = T ! switch for surface volatilization (default = T)
                ! caution: if set to .false., turn off airsea submodel
l_glacier   = T ! switch for (with or no) glacier compartment (default = F)
l_landsnow  = T ! switch for (with or no) snow compartment (default = F)

/

! ************************************************************************
! coupling namelist
! ************************************************************************

&CPL

l_mode_partition = T ! switch for modal partitioning (default = F)
                     ! if set to .false., use bulk partitioning and
                     ! ignore REMIS_MOD

param_part  = 4 ! scheme for gas-particle partitioning:
                ! 1 -> Lohmann-Lammel (2004)
                ! 2 -> Finizio (1997)
                ! 3 -> Junge-Pankow (1987)
                ! 4 -> ppLFER (Abraham, 1993; Goss 2005; Pourya et al., 2016)

param_soilv = 2 ! scheme for volatilization from soil (if l_svocvola = T):
                ! 1 -> Smit (1997)
                ! 2 -> Jury (1983)

param_bapo3 = 2 ! scheme for heterogeneous oxidation of bap by ozone:
                ! 1 -> Poeschl (2001)
                ! 2 -> Kwamena (2004)
                ! 3 -> ROI(T) (2018)
                ! 4 -> Kahan (2006)

aermod_str  = 'gmxe' ! 'm7' or 'gmxe'

! import sea spray  (AS mode) aerosol fluxes (channel, object)
! flux unit must be in kg m-2 s-1
imp_ss_as_flux = 'onemis','mss_as_lsce'

! import input data (channel, object)
imp_om_soil  = 'import_rgt','soil_foms'
imp_rho_soil = 'import_rgt','soil_rhos'
imp_mld_oce  = 'import_rgt','oce_ocn_mld'

! ************************************************************************
!
! NOTES:
! --> MAX 100 tracers
!
! SVOC_NAME(#) = tracer name, max 10 chars (should be the same with those
!                set in mecca)
! EMISS_IN(#) = import emission (channel name, channel object)
! MOLMASS(#)  = molar mass of tracer [g mol-1]
! MOLVOL(#)   = molar volume at boiling point [cm3 mol-1]
! RKSOIL(#)   = biotic and abiotic decay rate in soil [s-1]
! RKOCEAN(#)  = biotic and abiotic decay rate in ocean [s-1]
! RWSOL(#)    = water solubility [mg l-1] at 298 K
! RVAPP(#)    = saturated vapor pressure [Pa] at 298 K
! RHSOL(#)    = heat of solution [J mol-1] at 298 K
! RHVAP(#)    = heat of vaporisation [J mol-1] at 298 K
! RHSUB(#)    = heat of sublimation (condensation of sub-cooled liq)
!               at 298 K [J mol-1]
```

Figure 2: SVOC namelist example

```
! RLOGKOW(#)  = octanol-water partition coefficient
! RKOAM(#)    = slope of temp-dependent gas-particle partition coeff [K]
! RKOAB(#)    = intercept of temp-dependent gas-particle partition coeff
! KAHENRY(#)  = henry parameter A [M atm-1]
! KBHENRY(#)  = henry parameter B [K]
! RLOSS(#)    = mass fraction loss directly to atmosphere
! RSPRAY(#)   = mass fraction applied (sprayed) to vegetation surface
! RDENS(#)    = aerosol density [kg m-3] at 293 K
! REMISP(#)   = fraction of (bulk) particles in emissions
! REMIS_MOD(#,NMODE) = fraction of mode-specific svoc in emissions
!                      (actual emission fraction: REMIS_MOD*REMISP)
!       where NMODE = 7 (follows m7 and gmxe), i.e.,
!                      'ns', 'ks', 'as', 'cs', 'ki', 'ai', 'ci'
!                      ns: nucleation soluble
!                      ks: aitken soluble
!                      as: accumulation soluble
!                      cs: coarse soluble
!                      ki: aitken insoluble
!                      ai: accumulation insoluble
!                      ci: coarse insoluble
! RPPLFER(#,6) = RBIGE, RBIGS, RBIGA, RBIGB, RBIGV, RBIGL (if param_part = 4)
!      RBIGE   = excess molar refraction
!      RBIGS   = polarizability
!      RBIGA   = solute H-bond acidity
!      RBIGB   = solute H-bond basicity
!      RBIGV   = McGowan molar volume
!      RBIGL   = log of hexadecane-air partition coeff.
!
! ********************************************************************

!!! phenanthrene
SVOC_NAME(1) = 'PHE'
EMISS_IN(1) = 'import_rgt', 'emiss_PHE'
MOLMASS(1)  = 178.2
MOLVOL(1)   = 199.2
RKSOIL(1)   = 5.17E-07
RKOCEAN(1)  = 5.4E-08
RWSOL(1)    = 1.1
RVAPP(1)    = 7.0E-02
RHSOL(1)    = 3.481E+04
RHVAP(1)    = 7.83E+04
RHSUB(1)    = 9.21E+04
RLOGKOW(1)  = 4.47
RKOAM(1)    = 3293.
RKOAB(1)    = -3.37
KAHENRY(1)  = 2.4E+01
KBHENRY(1)  = 6000.
RLOSS(1)    = 1.0
RSPRAY(1)   = 0.0
RDENS(1)    = 1174.
REMISP(1)   = 0.0
REMIS_MOD(1, :) = 0., 0., 0., 0., 0., 0., 0.
RPPLFER(1, :)   = 1.92, 1.28, 0., 0.29, 1.45, 7.71

/
```

Figure 2: continued

2. Physics and chemistry parameters:

   - `param_part`: Gas−particle partitioning scheme; 1=Lohmann−Lammel (default), 2=Finizio, 3=Junge-Pankow, or 4=ppLFER.
   - `param_soilv`: Soil volatilization scheme; 1=Smit (default), 2=Jury.
   - `param_bapo3`: Heterogeneous BaP oxidation with O_3; 1=Pöschl (default), 2=Kwamena, 3=ROI-T, or 4=Kahan.
   - `aermod_str`: MESSy submodel for aerosol microphysics (GMXe or M7).

3. Channel and object names to access input data

   - `imp_ss_as_flux`: Sea salt in aitken-soluble mode
   - `imp_om_soil`: Fraction of organic matter in soil
   - `imp_rho_soil`: Soil density
   - `imp_mld_oce`: Ocean mixed layer depth

4. Tracer properties
   Table 1 lists all the required physicochemical properties for SVOC tracers, including tracer names, molecular weights, partition coefficients, Henry's law constants, and so forth. It also shows a subroutine name to denote which process utilizes the respective properties.

2 Coupling with other MESSy submodels

For its computations, SVOC requires some variables from other MESSy submodels:

- Dry deposition velocities of aerosol and gas-phase SVOC tracers from DDEP (Kerkweg et al., 2006).
- Aerosol wet radius from either GMXe (Pringle et al., 2010) or M7 (Vignati et al., 2004). If GMXe is used, SVOC will also import aerosol number concentration.
- Wet deposition fluxes of gas-phase and liquid-phase SVOC tracers and scavenging tendencies of black carbon (BC) from SCAV (Tost et al., 2006). To import the wet deposition fluxes, apply `out_string` = "[`SVOC_NAME`];[`SVOC_NAME`]`_l`" in `scav.nml`, whereas for the BC scavenging tendencies, apply `te_string` = "`BC_ks;BC_as;BC_cs;BC_ki`".
- Air−sea exchange fluxes of SVOC tracers from AIRSEA (Pozzer et al., 2006). To let AIRSEA calculate these fluxes, prepare all the necessary information in `airsea.nml`: tracer name, molar volume, Henry's law constants, and tracer concentration over the surface water. The last parameter is obtained from one of SVOC output variables (Table 3); hence user should set `WATER_CON_CHN`(#) = "`svoc_gp`","`CWAT_`[`SVOC_NAME`]" in `airsea.nml`.

Table 1: List of input parameters for tracer properties defined in `svoc.nml` file

Parameter	Description	Unit	Related subroutine(s)
`SVOC_NAME`	Tracer name		`svoc_new_tracer`
`EMISS_IN`	Import emission data (channel, object)		`svoc_init_coupling`
`MOLMASS`	Molecular mass	g mol^{-1}	`svoc_new_tracer`
`MOLVOL`	Molar volume	cm^3 mol^{-1}	not used in SVOC, but needed in AIRSEA
`RKSOIL`	1^{st} order degradation rate in soil	s^{-1}	`svoc_degradation`
`RKOCEAN`	1^{st} order degradation rate in ocean	s^{-1}	`svoc_degradation`
`RWSOL`	Water solubility	mg L^{-1}	`svoc_vola_glac_snow`
`RVAPP`	Saturated vapor pressure	Pa	`svoc_vola_veg`, `svoc_vola_glac_snow`, `svoc_part_lohlam`, `svoc_part_junge`
`RHSOL`	Heat of solution	J mol^{-1}	`svoc_vola_glac_snow`
`RHVAP`	Heat of vaporization	J mol^{-1}	see `RVAPP`, `svoc_part_pplfers`
`RHSUB`	Heat of condensation of sub-cooled liquid	J mol^{-1}	`svoc_vola_glac_snow`
`RLOGKOW`	Octanol−water partition coefficient	-	`svoc_vola_soil_smit`, `svoc_vola_soil_jury`
`RKOAM`	Slope of temperature-dependent octanol−air partition coefficient (K_{oa})	-	`svoc_part_lohlam`, `svoc_part_finizio`
`RKOAB`	Intercept of temperature-dependent K_{oa}	-	see `RKOAM`
`KAHENRY`	Henry coefficient at 25°C	M atm^{-1}	`svoc_drydep`, `svoc_vola_glac_snow`, `svoc_vola_soil_jury`, `svoc_vola_soil_smit`
`KBHENRY`	Constant for the temperature-correction of Henry coefficient		see `KAHENRY`
`RLOSS`	Fraction of emission release to the atmosphere	-	`svoc_vdiff(1)`
`RSPRAY`	Fraction of emission applied (sprayed) to surface	-	`svoc_vdiff(1)`
`RDENS`	SVOC particle density	kg m^{-3}	`svoc_new_tracer`
`REMISP`	Fraction of emission emitted as particles	-	`svoc_vdiff(1)`
`REMIS_MOD`	Fraction of `REMISP` assigned into each aerosol mode (7 comma-separated values)	-	`svoc_vdiff(1)`
`RPPLFER`	Solute descriptors for ppLFER (6 comma-separated values)		`svoc_part_pplfers`

3 Starting a simulation

To prepare an SVOC run, activate the submodel (set `USE_SVOC` = `.TRUE.` in `switch.nml`), fill in all input parameters in `svoc.nml` and other namelists, and setup the gaseous and liquid chemistry of SVOC tracers in MECCA and SCAV (more details in the manual of each submodel, Sander et al. (2011) and Tost et al. (2006), respectively).

4 Input and output

The following input data should be available in their desirable units: (a) Emission fluxes in kg m^{-2} s^{-1}, (b) soil density in kg m^{-3}, and (c) ocean mixed layer depth in m. Running EMAC-SVOC generates two output files in addition to other standard MESSy output: (a) [`EXP_NAME`]`_____yyyymmmddd_hhmm_svoc_inp` which stores the three input data after regridding, unit conversion, and other treatment (see Table 2), and (b) [`EXP_NAME`]`_____yyyymmmddd_hhmm_svoc_gp` which stores some diagnostic quantities, refer to the list in Table 3.

Table 2: List of variables in `svoc_inp` channel

Variable	Definition	Unit
`appl_[SVOC_NAME]`	Application/emissions	mol_{tr} mol_{air}^{-1} kg_{air} m^{-2} s^{-1}
`rhos`	Soil density	kg_{solid} m^{-3}
`foms`	Fraction of organic matter in soil	kg_{OM} kg_{solid}^{-1} m^{-3}
`ocn_mld`	Ocean mixed layer depth	m

Table 3: List of variables in `svoc_gp` channel

Variable	Definition	Unit	Dimension	Note
`Kp_[SVOC_NAME]`	Gas−particle partition coefficient (bulk)	$m^3\ \mu g^{-1}$	`LON,LAT,LEV`	
`Kp_[SVOC_NAME]_[cm]`	Gas−particle partition coefficient at mode `cm` (namely, `ns`, `cs`, `as`, `ks`, `ki`, `ai`, `ci`)	$m^3\ \mu g^{-1}$	`LON,LAT,LEV`	
`THETA_[SVOC_NAME]`	Particulate mass fraction (bulk)	-	`LON,LAT,LEV`	
`THETA_[SVOC_NAME]_[cm]`	Particulate mass fraction at mode `cm` (namely, `ns`, `cs`, `as`, `ks`, `ki`, `ai`, `ci`)	-	`LON,LAT,LEV`	
`BURD_[SVOC_NAME]`	Tracer burden in environmental compartments	$kg_{tr}\ m^{-2}$	`LON,LAT,LEV`	`LEV` (bottom to top): 1=soil, 2=vegetation, 3=ocean, 4=snow, 5=glacier, 6=atmosphere
`VOLA_[SVOC_NAME]`	Volatilization flux from surface compartments	$kg_{tr}\ m^{-2}\ s^{-1}$	`LON,LAT,LEV`	`LEV` (bottom to top): 1=soil, 2=vegetation, 3=ocean, 4=snow, 5=glacier
`DEPO_[SVOC_NAME]`	Deposition fluxes	$kg_{tr}\ m^{-2}\ s^{-1}$	`LON,LAT,LEV`	`LEV` (bottom to top): 1=dry, 2=wet, 3=total
`DEGR_[SVOC_NAME]`	Biotic degradation rate	$kg_{tr}\ m^{-2}\ s^{-1}$	`LON,LAT,LEV`	`LEV` (bottom to top): 1=soil, 2=vegetation, 3=ocean
`CWAT_[SVOC_NAME]`	Tracer concentration in the ocean	$kmol\ m^{-3}$	`LON,LAT`	

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