Deutscher Wetterdienst
Wetter und Klima aus einer Hand

DWD

DKRZ
DEUTSCHES KLIMARECHENZENTRUM

KIT
Karlsruher Institut für Technologie

natESM

Federal Ministry of Research, Technology and Space

ICON-ART

Ali Hoshyaripour (KIT), Stefan Versick (KIT)

Empa
Materials Science and Technology

Training contents

1. **Overview of ICON-ART**
2. **Modeling primary aerosols**; lecture + exercise incl:
   Emission of dust, wildfire and sea salt aerosols
   Aerosol-radiation interaction

3. **Modeling air quality**; lecture + exercise incl:
   Full chemistry with MECCA
   Emission processing with emiproc
   Online emission module

4. **Modeling secondary aerosols & chemistry**; lecture + exercise incl:
   Point source emission for a volcanic eruption
   Aerosol dynamics (nucleation, condensation, coagulation)
   Simplified OH and LINOZ chemistry

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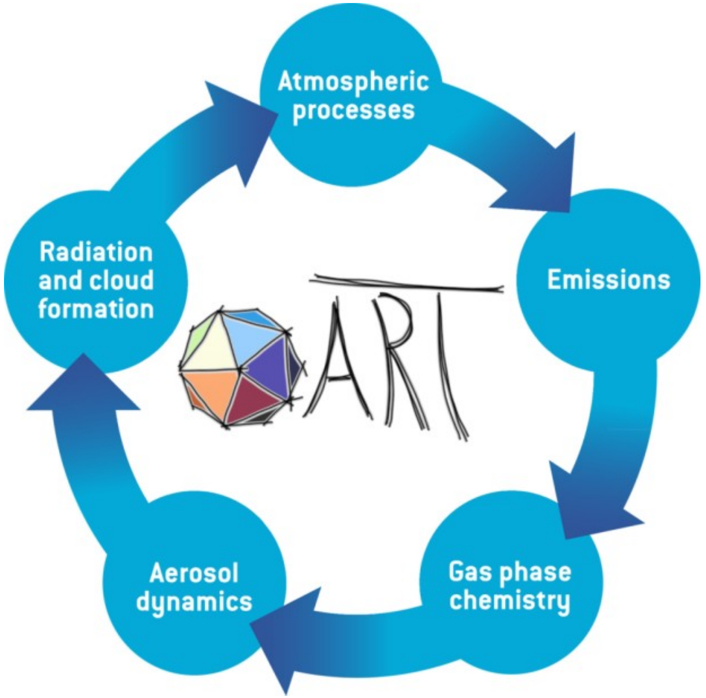
ICON-ART

Part 1: Overview

Ali Hoshyaripour (KIT), Stefan Versick (KIT)

ICON-ART



Aerosol and **R**eactive **T**race gases

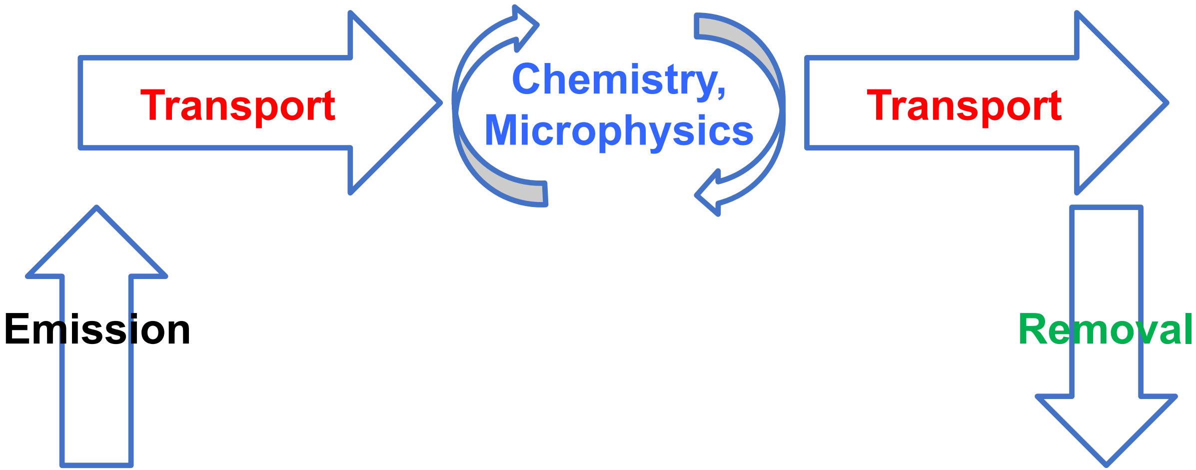
Rieger et al. (2015), Weimer et al. (2017)

A component of ICON modeling framework that enables prognostic treatment of atmospheric composition + interactions

Main features:

- Online fully-coupled for LEM, NWP and climate simulations
- Adaptable to global, nested and limited area configurations
- Fully modular and interoperable
- Scalable and flexible tracer structure, chemistry and aerosol dynamics

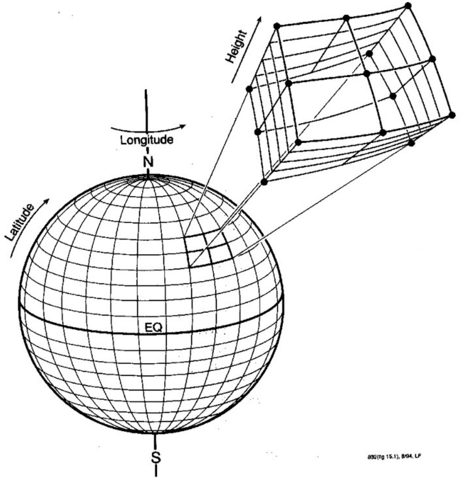
Atmospheric composition models



$$\frac{\partial \rho_i}{\partial t} = \left[\frac{\partial \rho_i}{\partial t}\right]_{adv} + \left[\frac{\partial \rho_i}{\partial t}\right]_{mix} + \left[\frac{\partial \rho_i}{\partial t}\right]_{conv} + \left[\frac{\partial \rho_i}{\partial t}\right]_{scav} + \left[\frac{\partial \rho_i}{\partial t}\right]_{chem} + \left[\frac{\partial \rho_i}{\partial t}\right]_{em} + \left[\frac{\partial \rho_i}{\partial t}\right]_{dep}$$

Modelling atmospheric composition

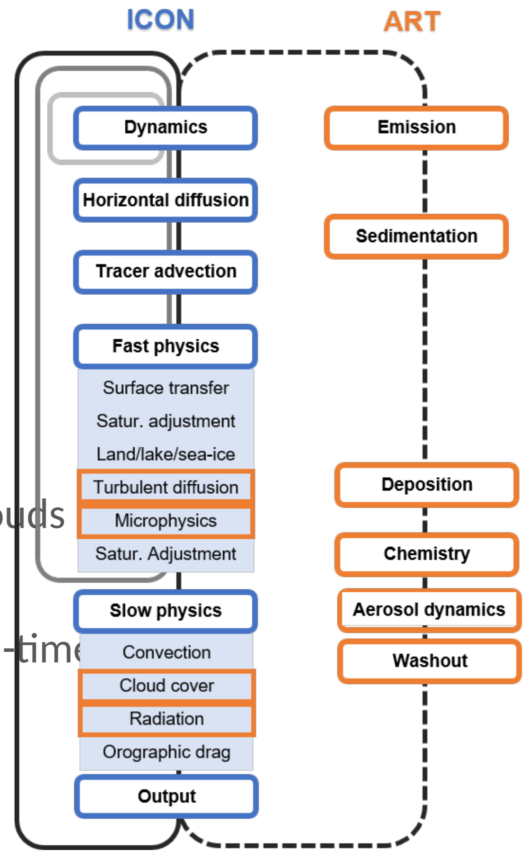
"Eulerian" atmospheric models solve mass balance (or continuity) equation in 3-D assemblage of gridboxes



Source: D. Jacob

ART - code parts and coupling

- **aerosol_dynamics** : condensation, nucleation, coagulation etc.
- **chem_init** : initialization of chemistry
- **chemistry** : chemical processes
- **emissions** : all emissions
- **externals** : external libraries
- **io** : read and write
- **phy_interact** : interaction with radiation and clouds
- **runctrl_examples** : a place to find examples 😊
- **shared** : modules for initialization and run-time
- **tools** : diagnostics and conversions



What do I need for an ICON-ART simulation

- Everything that you need for ICON simulation (grid, external parameters, initial conditions etc)
  - Config with --enable-art and compile
  - Prepare **input data** (initial conditions, boundary conditions, emission data)
  - Adapt the job script and submit it to HPC
  - Monitor the job and post-process the outputs

Enabling ART in a simulation

```
! run_nml: general switches ----------

&run_nml
 ltestcase        =        .FALSE.
 num_lev =        50
 ltransport       =        .TRUE.
………….
 lart             =        .TRUE.
```

ART Namelist

```
&art_nml
 lart_xxx          : LOGICAL → to switch processes on and off
 iart_yyy          : INTEGER → how to handle the details
 cart_zzz          : CHARACTER → where to find input data (e.g. XML)
```

e.g.

```
 lart_chem           =    .FALSE.
 lart_aerosol        =    .TRUE.
 iart_init_aero      =    0
 cart_aerosol_xml    =    '${INDIR}/tracers_aerosol.xml'
 cart_modes_xml      =    '${INDIR}/modes.xml'
```

General ART namelist parameters

Namelist parameter	Default	Description	If .TRUE. then needs
`lart_chem`	.FALSE.	Enables chemistry.	`lart_chemtracer = .TRUE.` OR `lart_mecca = .TRUE.`
`lart_chemtracer`	.FALSE.	Switch for simple OH chemistry	`cart_chemtracer_xml`
`lart_mecca`	.FALSE.	Switch for kpp chemistry	`cart_mecca_xml`
`lart_pntSrc`	.FALSE.	Enables addition of point sources	`cart_pntSrc_xml`

`lart_aerosol`	.FALSE.	Main switch for the treatment of atmospheric aerosol.	`cart_aerosol_xml`
			`cart_modes_xml`
			`cart_aero_emiss_xml`

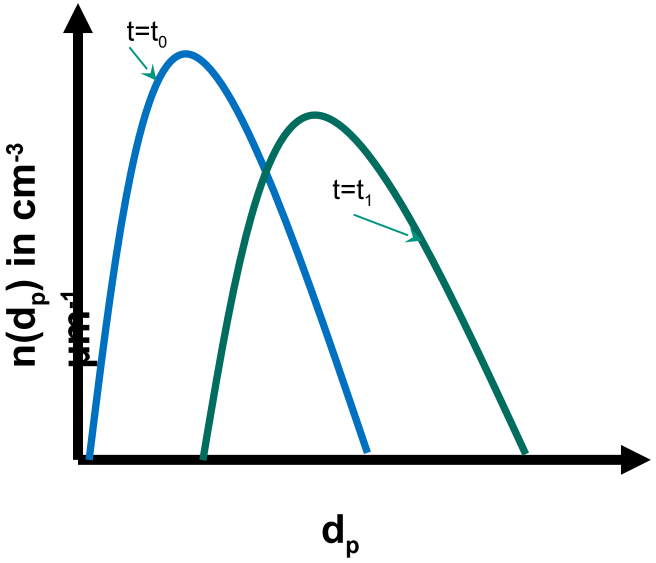
`lart_diag_out`	.FALSE.	Enables diagnostic output fields	`cart_diagnostics_xml`

The fundamental problem with aerosols

The size distribution of aerosol particles evolves continuously in the atmosphere as a result of *microphysical processes.*

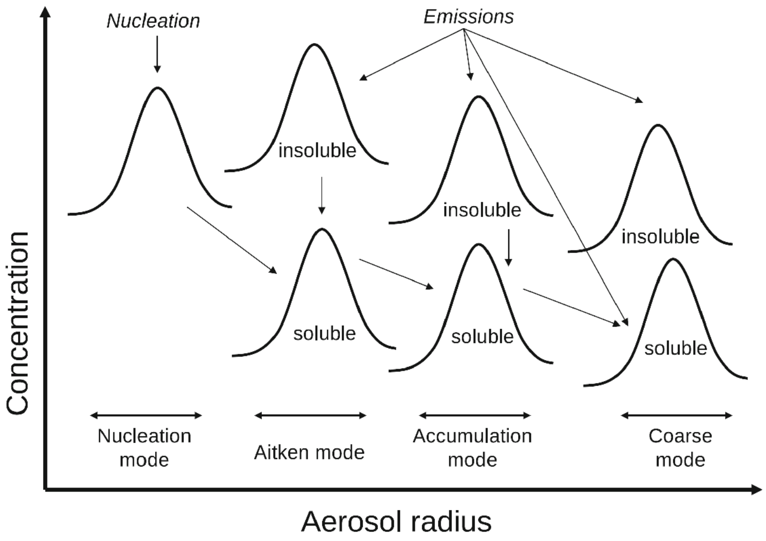
These processes are computationally challenging to represent in models

Processes of nucleation and aerosol-cloud interactions are highly non-linear.



Modal approach for modelling aerosols

- The modal approach results from a compromise that allows to represent the evolution of both the aerosol size distribution and the degree of mixing at an affordable computational cost but using a number of assumptions.



Source: Boucher 2017

Continuity equation for aerosols number conc.

$$\frac{\partial n_i}{\partial t} + \nabla \bullet (\mathbf{v} n_i) = (\nabla \bullet \mathbf{K}_h \nabla) n_i$$

$$+ R_{emisn} + R_{depn} + R_{sedn} + R_{washn} + R_{nucn} + R_{coagn}$$

R_{emisn} = rate of surface or elevated emission
R_{depn} = rate of particle dry deposition to the surface
R_{sedn} = rate of sedimentation to the surface or between layers
R_{washn} = rate of washout to the surface or from one altitude down to another
R_{nucn} = rate of production of new particles due to homogeneous nucleation
R_{coagn} = rate of coagulation of number concentration

Source: Jacobson 2005

Continuity equation for aerosols volume conc.

$$\frac{\partial v_{q,i}}{\partial t} + \nabla \bullet (\mathbf{v} v_{q,i}) = (\nabla \bullet \mathbf{K}_h \nabla) v_{q,i}$$

$$+ R_{emisv} + R_{depv} + R_{sedv} + R_{washv} + R_{nucv} + R_{coagv}$$

$$+ R_{c/ev} + R_{dp/sv} + R_{ds/ev} + R_{eqv} + R_{aqv} + R_{hrv}$$

$R_{c/ev}$ = rate of change due to condensational growth (evaporation)
$R_{dp/sv}$ = rate of change due to depositional growth (sublimation)
$R_{ds/ev}$ = rate of change due to dissolutional growth (evaporation)
R_{eqv} = rate of change due to reversible chemical equilibrium reactions
R_{aqv} = rate of change due to irreversible aqueous chemical reactions
R_{hrv} = rate of change due to heterogeneous reactions on particle surfaces

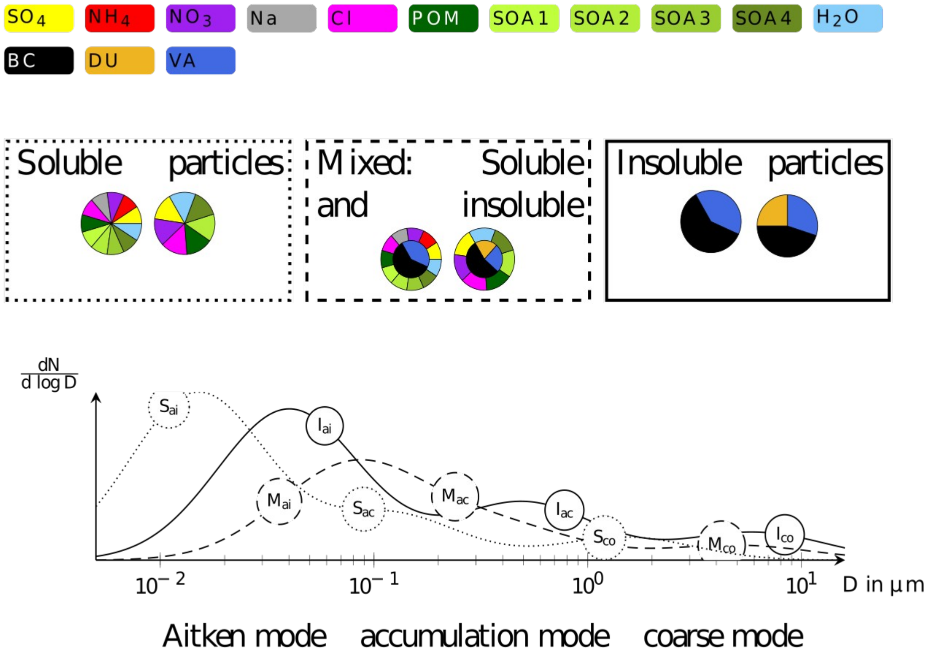
Source: Jacobson 2005

Aerosol Dynamics (AERODYN) in ICON-ART

- Flexible log-normal modes
- For each mode, prognostic equations for the number density and the mass concentration are solved:

$$\frac{\partial}{\partial t} M_{0,i} = -\mathrm{Ca}_{0,ii} - \mathrm{Ca}_{0,ij} + \mathrm{Nu}_0,$$
$$\frac{\partial}{\partial t} M_{3,i} = -\mathrm{Ca}_{3,ij} + \mathrm{Co}_{3,i} + \mathrm{Nu}_3,$$

- the ISORROPIA II for gas–aerosol partitioning



 Muser et al. (2020); Vogel et al. (2009); Fountoukis and Nenes (2007)

AERODYN in the ART Namelist

```
&art_nml
…
 iart_modeshift       = 1            ! 0 = off; 1 = on
 iart_isorropia       = 1            ! 0 = off; 1 = on
 cart_aerosol_xml     = '$path/tracers_aerosol.xml'
 cart_modes_xml       = '$path/modes.xml'
 cart_coag_xml        = '$path/coagulate.xml'
 cart_aero_emiss_xml = '$path/aero_emiss.xml'
```

Aerosol-cloud-radiation interactions

Interactions	Parameter	Value	ICON Namelist	.AND. in art_nml
Aerosol-cloud	inwp_gscp	6	nwp_phy_nml	iart_aci_warm = 0,1 iart_aci_cold = 0-7
Aerosol-radiation	irad_aero	9	radiation_nml	iart_ari = 1

NOTE: Use aerosol-cloud interactions with caution as they are not tested for all combinations. Please contact us if you are interested in such applications.

Continuity Equation for gases

$$\frac{\partial N_q}{\partial t} + \nabla \bullet (\mathbf{v} N_q) = (\nabla \bullet \mathbf{K}_h \nabla) N_q$$

$$+ R_{emisg} + R_{depg} + R_{washg} + R_{chemg}$$

$$+ R_{nucg} + R_{c/eg} + R_{dp/sg} + R_{ds/eg} + R_{hrg}$$

R_{emisg} = rate of surface or elevated emission
R_{depg} = rate of dry deposition to the ground
R_{washg} = rate of washout to the ground or from one altitude to another
R_{chemg} = rate of photochemical production or loss
R_{nucg} = rate of gas loss due to homogeneous or heterogeneous nucleation
$R_{\mathrm{c/eg}}$ = rate of gas loss (production) due to condensation (evaporation)
$R_{\mathrm{dp/sg}}$ = rate of gas loss (production) due to depositional growth (sublimation)
$R_{\mathrm{ds/eg}}$ = rate of gas loss (production) due to dissolutional growth (evaporation)
R_{hrg} = rate of gas loss (production) due to heterogeneous reactions

All rates are expressed in units of concentration per unit time (e.g., molec. cm^{-3} s^{-1}).

Jacobson 2005

Chemistry ODEs

$$\left[\frac{\partial \rho_i}{\partial t}\right]_{chem} = p_i - \ell_i \rho_i$$

- p_i [kg m-3 s-1] overall production rate constant
- ℓ_i [s-1] overall loss rate constant

- If p_i and ℓ_i are independent of the density ρ_i, the equation is linear and has a simple exponential solution.
- However, p_i and ℓ_i often depend on ρ_i due to coupling with other species in the chemical mechanism.
- One then needs to solve the equation as part of a system of coupled ODEs, one for each species in the mechanism.

Source: Brasseur and Jacob 2017

Chemistry in ICON-ART

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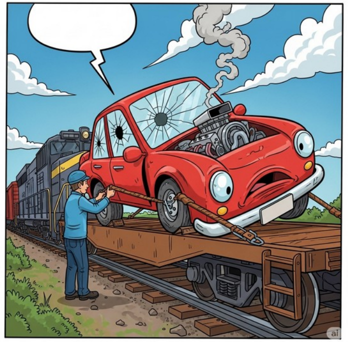
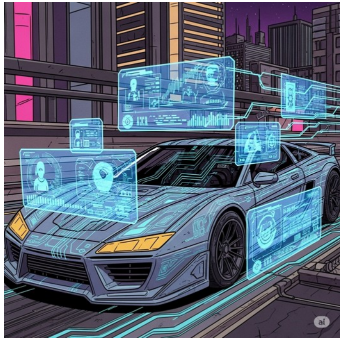




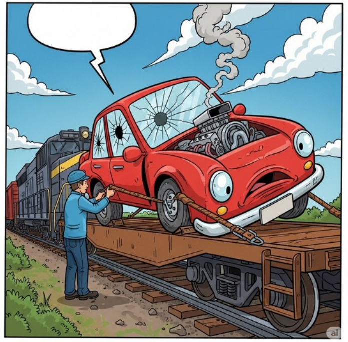



Passive -> Lifetime -> Simplified -> AI -> complex

Model complexity

Computing time

Passive Tracers



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- Only transported, no chemistry
- Emissions possible
- Useful for transport studies
    - E.g. in a current project we compare transport in different models and don’t want differences due to different chemistry

```xml
<chemtracer id="TRCO2aposGFED" full="FALSE" chemtr="TRUE">
  <tag001 type="char">chemtr</tag001>
  <mol_weight type="real">4.401E-2</mol_weight>
  <transport type="char"> hadv52aero </transport>
  <unit type="char">kg kg-1</unit>
  <c_solve type="char">passive</c_solve>
  <init_mode type="int">1</init_mode>
  <init_name type="char">TRCO2aposGFED_chemtr</init_name>
  <emiss_ANT type="char" inum_levs="1">CO2aposGFED_ANT_GFed2023CAMS</emiss_ANT>
</chemtracer>
```

Lifetime Tracers

- Exponential decay
- Globally uniform
- Useful for very fast simulations with mainly longlived tracers

```xml
<chemtracer id="TRCH4" full="FALSE" chemtr="TRUE">
  <tag001 type="char">chemtr</tag001>
  <mol_weight type="real">1.604E-2</mol_weight>
  <?source_lifetime Hayman et al., ACP, 2017 ?>
  <lifetime type="real">286977600</lifetime>
  <transport type="char"> hadv52aero </transport>
  <unit type="char">mol mol-1</unit>
  <c_solve type="char">lt</c_solve>
  <init_mode type="int">1</init_mode>
  <init_name type="char">TRCH4_chemtr</init_name>
  <emiss_ANT type="char" inum_levs="1">CH4_ANT_CAMSv5.3</emiss_ANT>
  <emiss_BIO type="char" inum_levs="1">CH4_BIO_CAMSv3.1</emiss_BIO>
</chemtracer>
```

Lifetime Tracers

- Parameterized lifetime for some tracers
    - Automatically applied when tracer name matches in `chemistry/mo_art_chemtracer.f90`

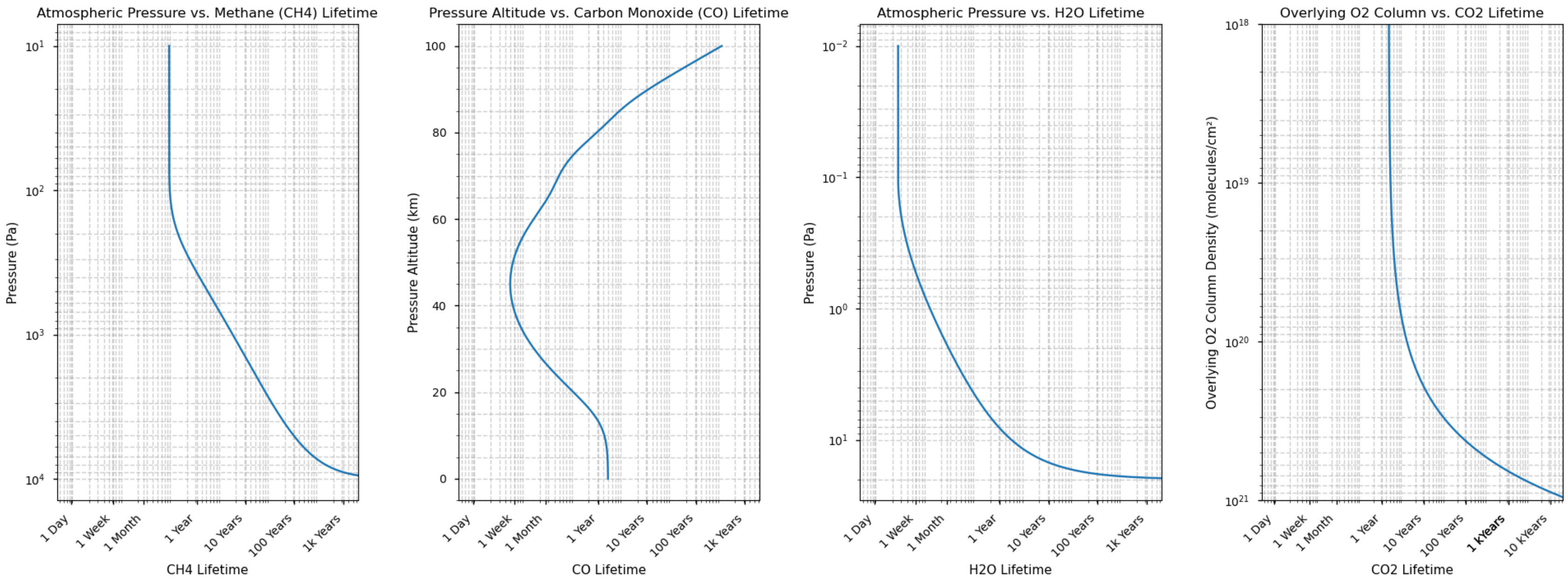
```
TYPE IS (t_chem_meta_lt)

  CALL tracer%set_tracer(p_tracer_now(:,:,:,jsp))

  IF (jsp == art_indices%iTRCH4) THEN
    CALL art_loop_cell_tracer(jg, tracer, art_get_CH4_des)
  ELSE IF (jsp == art_indices%iTRCO) THEN
    CALL art_loop_cell_tracer(jg, tracer, art_get_CO_des)
  ELSE IF (jsp == art_indices%iTRCO2) THEN
    CALL art_loop_cell_array(jg, art_param%o2_column, art_calc_o2_column)
    CALL art_loop_cell_tracer(jg, tracer, art_get_CO2_des)
  ELSE IF (jsp == art_indices%iTRCH3CN) THEN
    CALL art_loop_cell_tracer(jg, tracer, art_get_CH3CN_des)
  ELSE IF (jsp == art_indices%iTRH2O) THEN
    CALL art_loop_cell_tracer(jg, tracer, art_get_H2O_des)
  END IF
```

Lifetime Tracers

- Example vertical profiles for some of the tracers



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Simplified chemistry

- Different schemes
  - Linoz: ozone
  - SimNOy: N2O
  - OH (included in the Aerosol experiment)
- Useful for fast simulations with good accuracy

```
<chemtracer id="TRO3" full="FALSE" chemtr="TRUE">
  <tag001 type="char">chemtr</tag001>
  <mol_weight type="real">4.800E-2</mol_weight>
  <?source_lifetime Ehhalt et al., IPCC, 2001, Chapte
  <lifetime type="real">1555200</lifetime>
  <transport type="char"> hadv52aero </transport>
  <init_mode type="int"> 1 </init_mode>
  <init_name type="char">O3</init_name>
  <feedback type="int"> 1 </feedback>
  <unit type="char">mol mol-1</unit>
  <c_solve type="char">linoz</c_solve>
</chemtracer>
```

```
<chemtracer id="TRCH4" full="FALSE" chemtr="TRUE">
  <tag001 type="char">chemtr</tag001>
  <mol_weight type="real">1.604E-2</mol_weight>
  <lifetime type="real">25920000</lifetime>
  <transport type="char"> hadv52aero </transport>
  <unit type="char">mol mol-1</unit>
  <c_solve type="char">OH</c_solve>
  <init_mode type="int">1</init_mode>
  <init_name type="char">CH4</init_name>
  <products type="char">TRCO;0.66*TRH2</products>
  <emiss_ANT type="char" inum_levs="1">CH4_ANT_CAMS
  <emiss_BBE type="char" inum_levs="1">CH4FIRE_BBE_
  <emiss_BIO type="char" inum_levs="1">CH4_BIO_CAMS
</chemtracer>
```

Simplified chemistry: Example Linoz

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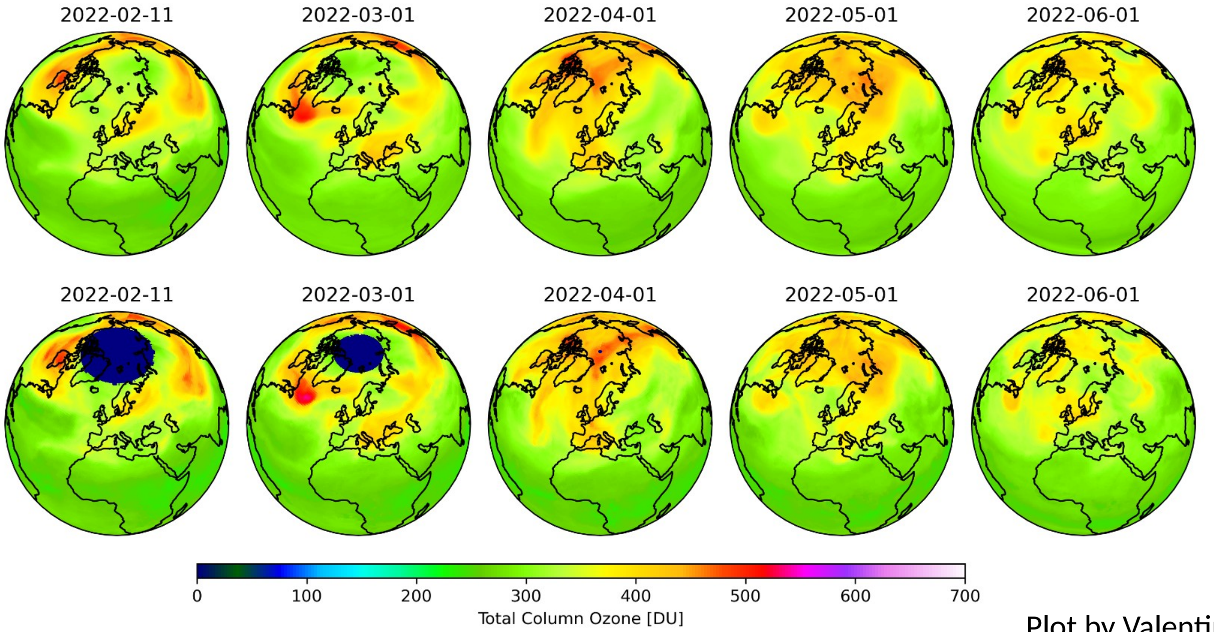
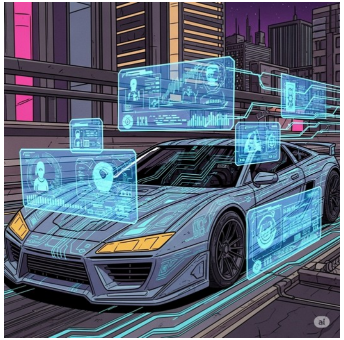


ICON-ART Linoz

NASA ozonewatch

Plot by Valentin Hanft

AI chemistry



- Not yet implemented in official branches
- Several developments ongoing
  - OH chemistry
  - Ozone
  - …
- Can be faster and/or more complex than simplified chemistry

Complex chemistry

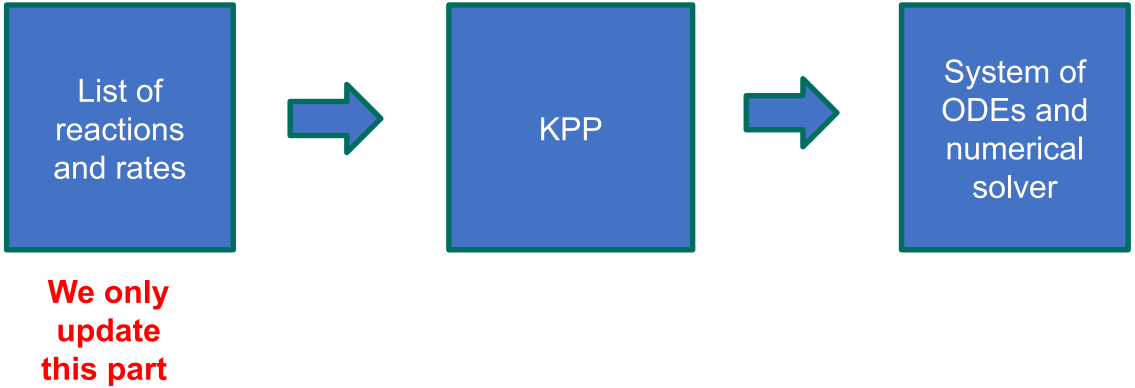
- MECCA based
- Needs pre-processing
- Can be very complex
- Most accurate
- You can easily achieve slowdowns of factor 100 or more of your simulations
- Best suited for short simulations or only local areas (Tutorial Experiment 2: Air Quality)

```
<meccatracer id="N2O" full="TRUE" chemtr="FALSE">
  <tag001 type="char">full</tag001>
  <mol_weight type="real">44.02E-3</mol_weight>
  <transport type="char">hadv52aero</transport>
  <number type="int"> 1 </number>
  <iconv type="int">1</iconv>
  <iturb type="int">1</iturb>
  <init_mode type="int">1</init_mode>
  <init_name type="char">N2O</init_name>
  <unit type="char">mol mol-1</unit>
  <c_solve type="char">mecca</c_solve>
</meccatracer>
```

KPP – Kinetic Pre-Processor

- Key challenge in chemistry modeling:
    - Any update (new species, reaction, rate parameter etc) ? complete revision of all ODEs ? error prone!

- KPP has solved this issue (Demian et al 2002)



Input data - Initial conditions

All input data should be "**cart_input_folder**" (in art_nml) remapped to ICON grid as NetCDF with the following name convention:

ART_XXX_icon-RnBkk-grid[-yyyy-mm-dd-hh]_cart_io_suffix.nc

XXX → type of data

RnBkk → ICON grid

[-yyyy-mm-dd-hh] → Optional

cart_io_suffix → grid specification defined by cart_io_suffix in art_nml

Species	Namelist switch	Options	XXX
Gas	iart_init_gas	0 (cold start), 1 (climatologies), 4 (external dataset), 5 (from ICON file)	ICE
Aerosol	iart_init_aero	0 (cold start), 5 (from file)	IAE

Emissions treated in ART

Volcanic


Biomass burning


Sea salt and DMS


Anthropogenic


Mineral dust


Biogenic


Pollen

Input data - Emissions

Type	Data	XXX
• **Point sources:**	XML-file	
• **Sea salt :**	no extra data necessary	
• **Mineral dust:**	Soil type data	ART_STY
• **Biogenic VOCs:**	Emissions/Vegetation	ART_BIO/ART_PFT
• **Anthropogenic emissions:**	Emission data sets	ART_ANT
• **Biomass burning:**	Satellite data	ART_BCF

Karlsruhe Institute of Technology

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PART 2:
Modeling primary aerosols

Ali Hoshyaripour

DKRZ DEUTSCHES KLIMARECHENZENTRUM MAX-PLANCK-INSTITUT FÜR METEOROLOGIE Deutscher Wetterdienst Wetter und Klima aus einer Hand DWD C2SM Center for Climate Systems Modeling

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ICON-ART

Part 2: Primary aerosols

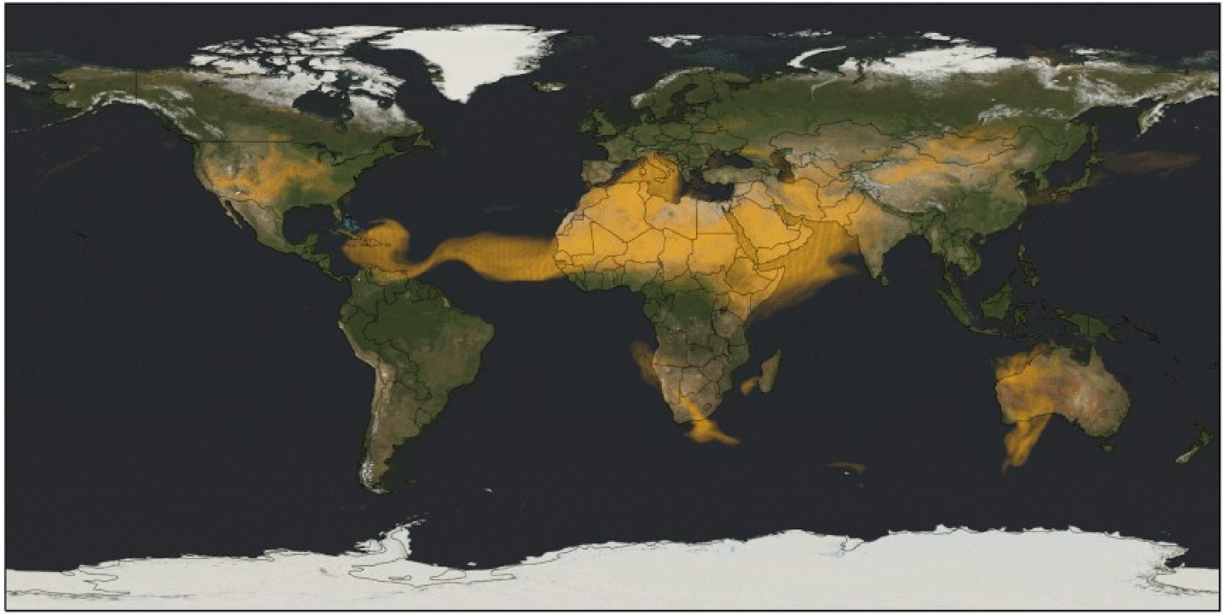
Ali Hoshyaripour (KIT), Julia Bruckert (KIT)

Empa Materials Science and Technology

Multi-aerosol simulations

R2B06

22-06-2019 00:00



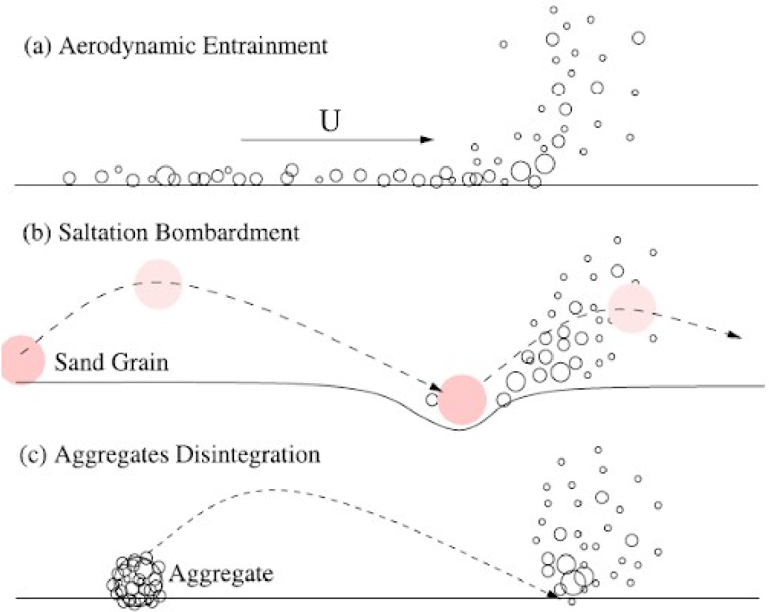
Mineral Dust

Sea Salt

Biomass Burning Aerosols

Mineral dust: emission mechanisms

- Most important dust emission mechanisms (Shao et al., 2011b)



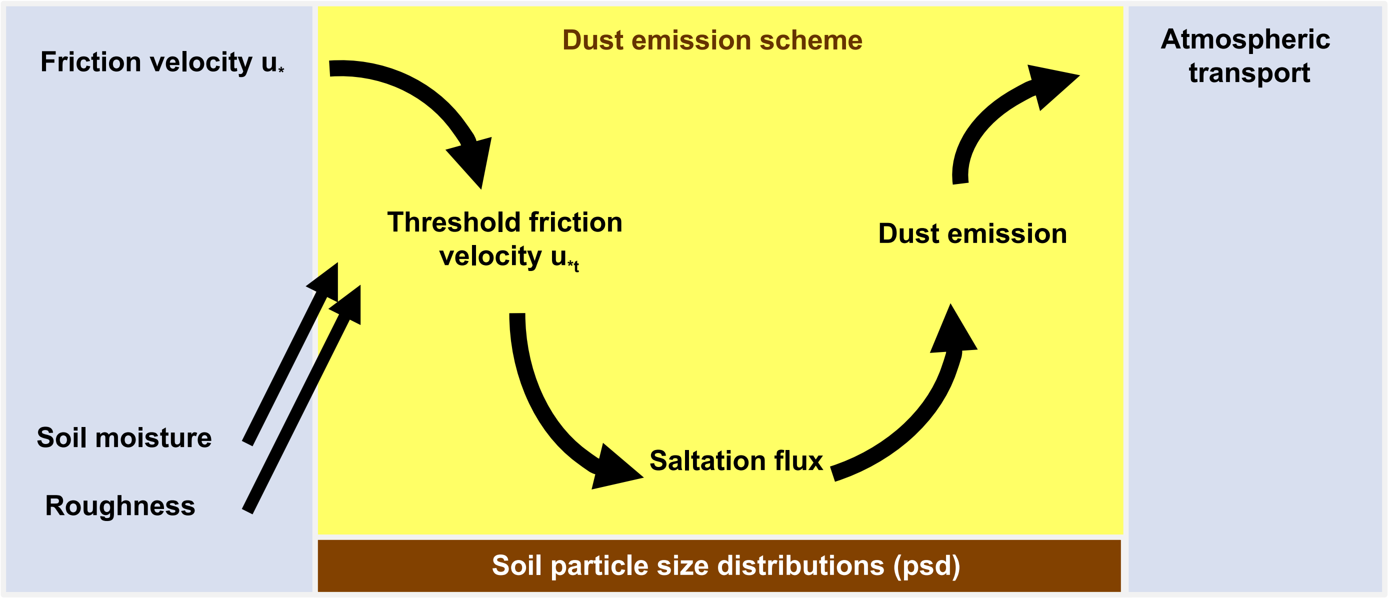
Mineral dust: implementation in ICON-ART

- Dust emission parameterizations (DEPs) in ICON-ART

DEP	Name	Based on
1	vogel2006	Vogel et al. (2006) and Shao (2004)
2	vogel2006s	Vogel et al. (2006) and Shao (2004)
3	shao2004	Shao (2004)
4	vogel2006_orig	Vogel et al. (2006)
5	vogel2006s_orig	Vogel et al. (2006)

- How to represent **source** and **force**.
- Only DEP1 is maintained and supported currently_

Mineral dust: implementation in ICON-ART



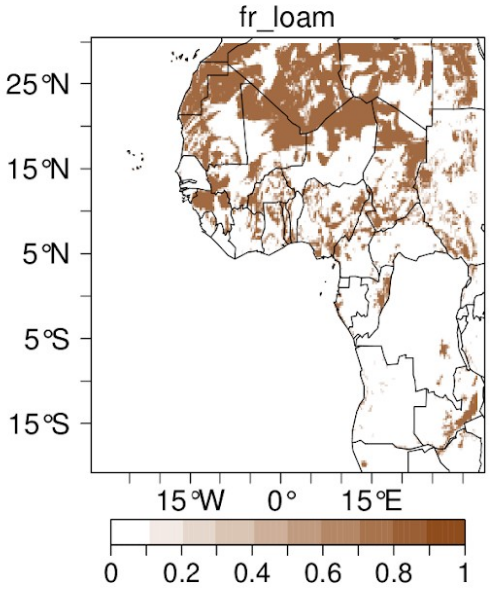
Mineral dust: implementation in ICON-ART

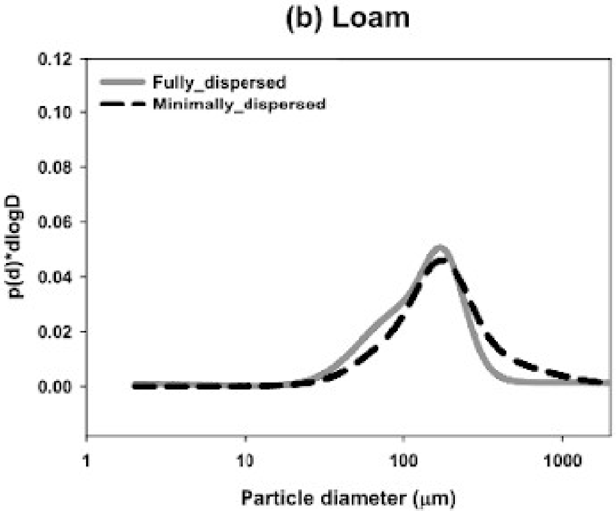
- **Input:**
  - friction velocity
  - soil moisture
  - vegetation cover
  - land use data
  - soil type (Harmonized World Soil Database, HWSD (2012))
  - soil particle size distributions (Shao et al., 2010)

- **Output:**
  - dust emission (µg m^{-2} s^{-1}) in **three lognormal modes**
  - additional information (e.g. threshold friction velocity)

Mineral dust: implementation in ICON-ART

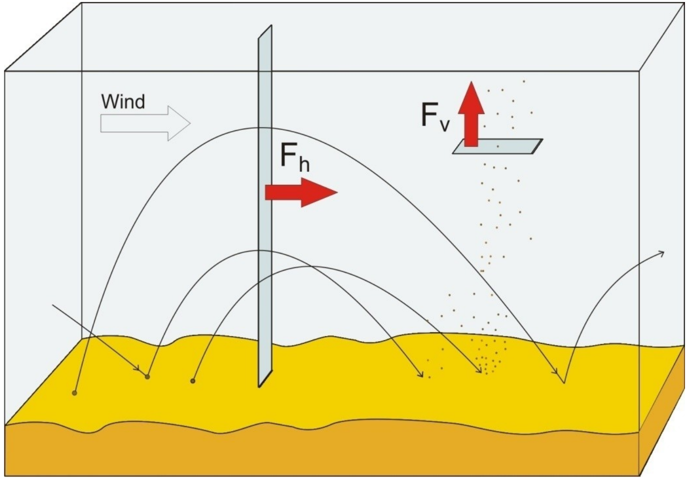
- Example **loam**: fraction of soil type (HWSD, 2012) and soil particle size distribution (Shao et al., 2010)





 Kang et al. 2011

Mineral dust emission in ICON-ART



$$u_{*ts}(d) = \sqrt{A_N\left(\frac{\rho_p}{\rho_{air}} g d + \frac{\gamma}{\rho_{air} d}\right)}$$

$$F_h(d) = C\frac{\rho_{air}}{g} u_*^3 \left(1 + \frac{u_{*t}}{u_*}\right)\left(1 - \frac{u_{*t}^2}{u_*^2}\right)$$

$$F_{vi}(d) = \frac{\pi}{6}\rho_p d^3_{dust,i} \frac{p_i(d) F_{kin}(d)}{e_i}$$

$$F_{vi} = \int_{d=0}^{d=\infty} F_{vi}(d) \frac{\frac{\pi}{4} d^2 n^*(\ln d)}{S_{tot}} dd$$

A_N, γ, C:	empirical parameters
$F_{kin}(d) = \beta . F_h(d)$	kinetic energy flux of saltation particles
e_i	binding energy of mode i

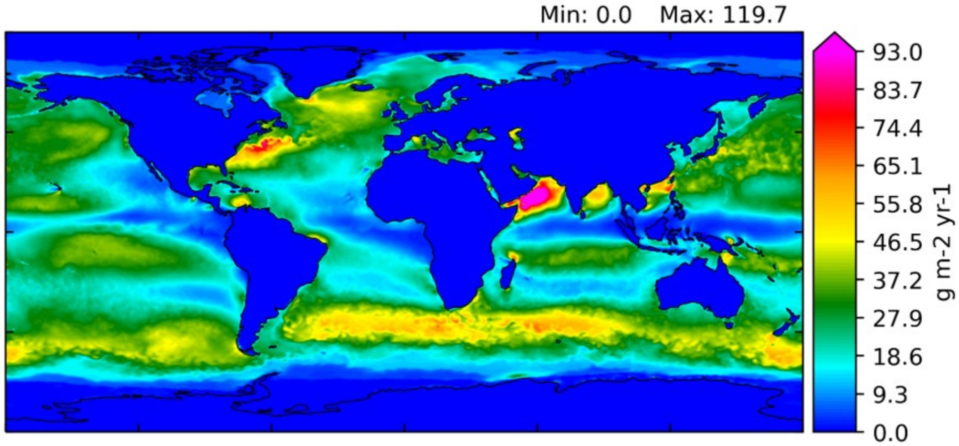
Three dust modes (d = 0.64, 3.45, 8.67 µm)

Vogel et al., 2006, Hoose, 2005

Sea salt

- Composition of sea spray aerosols:
  - Cl^- 55.0%
  - Na^+ 30.6%
  - SO_4^{2-} 7.7%
  - Mg^{2+} 3.7%
  - Ca^{2+} 1.2%
  - K^+ 1.1%
  - Br^- 0.19%
  - organics and iodine

Annual global sea salt emission simulated with ICON-ART

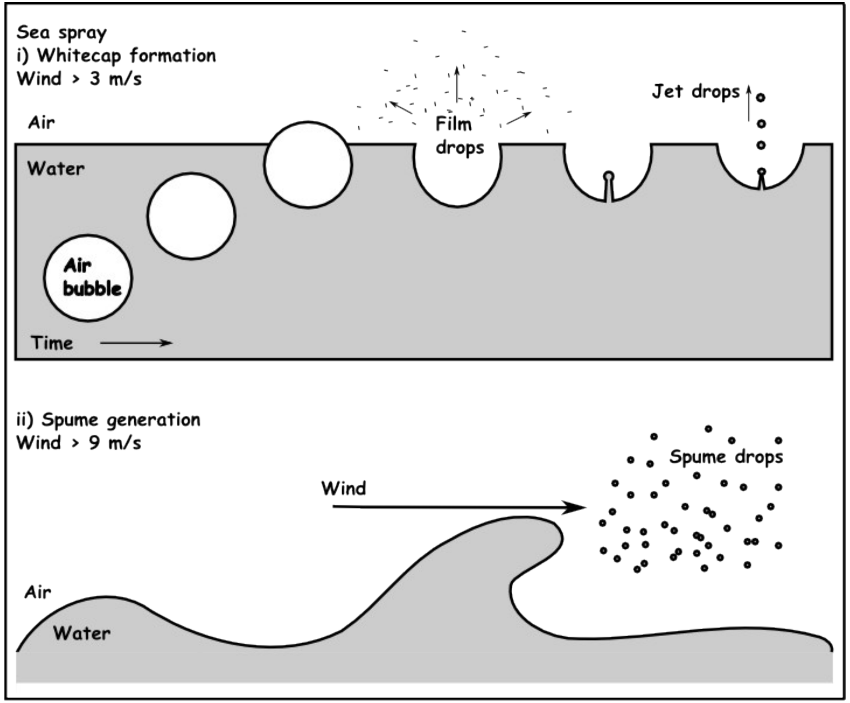


Emission of sea salt

Emission of sea salt particles is mostly driven by two mechanisms:

1- For wind > 3 m/s the air is entrained into seawater by wave-breaking. The resulting air bubbles rise and burst at the sea surface, injecting particles to the atmosphere (whitecap)

2- For wind > 9 m/s the spume generation occurs.



Lundgren et al., 2010

Sea salt

Representation in ICON-ART

- three modes with corresponding mean diameter and standard deviation

mode	diameter	σ	Process
A	0.1 µm	1.9	Film
B	3.0 µm	2.0	Jet
C	30.0 µm	1.7	Spume

- Three species are considered:
    - NaCl, Na_2SO_4, H_2SO_4

- calculation at each grid point (surface) over water and at each time step

Sea salt

Representation in ICON-ART

- Assumptions:
  - particles are emitted dry
  - freshly emitted particles are pure NaCl
  - no impact of salinity on emission
  - impact of sea surface temperature only as scaling/correction factor

- One parameterization for all modes

Sea salt emission in ICON-ART

$$\frac{\mathrm{d}F(D_\mathrm{p},U_{10},T)}{\mathrm{d}D_\mathrm{p}} = T_\mathrm{W}\cdot\Big[235\cdot U_{10}^{3.5}\exp(-0.55[\ln(\frac{D_\mathrm{p}}{0.1})]^2)$$

$$+\,0.2\cdot U_{10}^{3.5}\exp(-1.5[\ln(\frac{D_\mathrm{p}}{3})]^2)+6.8\cdot U_{10}^{3}\exp(-1[\ln(\frac{D_\mathrm{p}}{30})]^2)\Big]$$

D_p	particle diameters
U_{10}	10m wind speed
T_w	empirical parameter based on T

Grythe et al. 2014

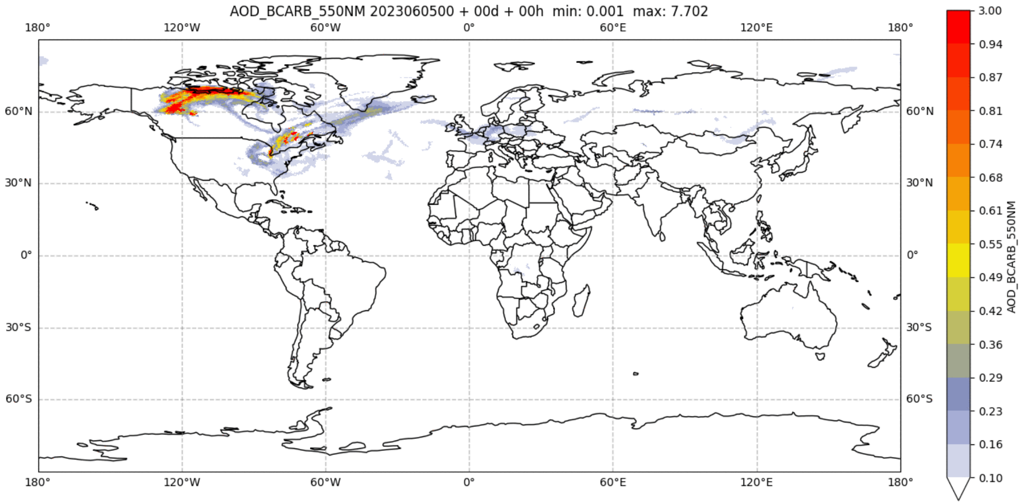
Biomass burning emissions

- The key parameters controlling biomass burning emissions:
  - Fuel availability and type
  - Weather conditions
  - Topography

- Satellite data provide some static information (daily) for fire activity.

- In ICON-ART we use one biomass-burning aerosol mode with d = 150 nm and sigma = 2

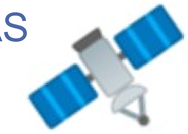
PermaStrom@DWD



Biomass burning emissions in ICON-ART

Emission rate:

GFAS

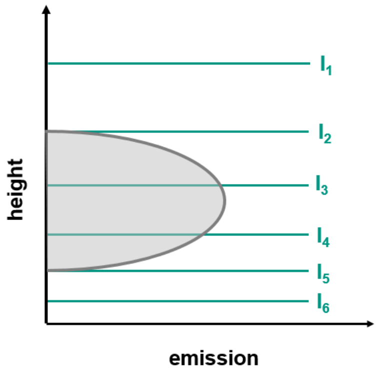


Kaiser et al., 2009

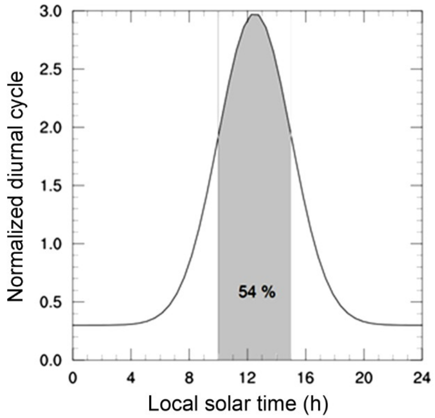
$$E(z) = M \cdot W_{emiss}(z) \cdot c_{emiss}$$

Diurnal cycle

Plume-rise Model



- **Input:**
  - atmospheric variables from ICON
    - T, p, u, v, q_v
  - heat flux
    - vegetation type



Walter et al. 2016

Freitas et al. 2006, 2007, 2010, Walter et al 2016

Experiment 1:
Primary aerosols

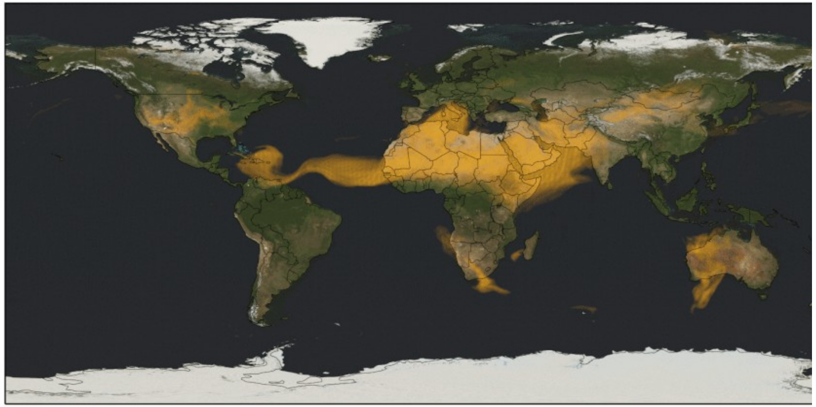
Julia Bruckert

Emission and transport of mineral dust, seasalt and soot aerosols

Objectives:

How to introduce aerosol tracers and modes

How to introduce online emissions for primary aerosols



Aerosol emission xml

```
<emiss>
    <routine id="dust">
        <nmodes type="int">3</nmodes>
        <d_g0_1 type="real">6.445E-7</d_g0_1>
        <d_g3_1 type="real">1.500E-6</d_g3_1>
        <sigma_g_1 type="real">1.700E+0</sigma_g_1>
        …
        <rho type="real">2.650E3</rho>
       <substances type="char">dust</substances>
    </routine>
    …
</emiss>
```

Aerosol emission xml

```
<emiss>
  <routine id="dust">
    <nmodes type="int">3</nmodes>
    <d_g0_1 type="real">6.445E-7</d_g0_1>
    <d_g3_1 type="real">1.500E-6</d_g3_1>
    <sigma_g_1 type="real">1.700E+0</sigma_g_1>
    …
    <rho type="real">2.650E3</rho>
   <substances type="char">dust</substances>
  </routine>
  …
</emiss>
```

Emission median diameter for zeroth and third moment and standard deviation for the lognormal distribution of the first mode

Modes xml

```xml
<modes>
  ...
  <aerosol id="insol_acc">
    <kind type="char">2mom</kind>
    <d_gn type="real">6.445E-7</d_gn>
    <sigma_g type="real">1.700E+0</sigma_g>
    <condensation type="int">0</condensation>
    <icoag type="int">0</icoag>
    <lut_optics type="char" >dust_a</lut_optics>
  </aerosol>
  ....
</modes>
```

Modes xml

```xml
<modes>
   …
   <aerosol id="insol_acc">
      <kind type="char">2mom</kind>
      <d_gn type="real">6.445E-7</d_gn>
      <sigma_g type="real">1.700E+0</sigma_g>
      <condensation type="int">0</condensation>
      <icoag type="int">0</icoag>
      <lut_optics type="char" >dust_a</lut_optics>
   </aerosol>
   ….
</modes>
```

Median diameter and standard deviation for the insoluble accumulation mode

Choose the optical properties of the mode from the file linked in cart_opt_props_nc (namelist)

Aerosol tracer xml

```
<tracers>
  …
  <aerosol id="dust">
    <moment type="int">3</moment>
    <mode type="char">insol_acc,insol_coa</mode>
    <sol type="real">0.0</sol>
    <mol_weight type="real">50.00E-3</mol_weight>
    <rho type="real">2.650E3</rho>
    <unit type="char">mug kg-1</unit>
    <transport type="char">hadv52aero</transport>
  </aerosol>
  …
</tracers>
```

Species ‘dust’ occurs in insoluble accumulation and insoluble coarse mode

Aerosol tracer xml

```
<tracers>
  …
  <aerosol id="dust">
    <moment type="int">3</moment>
    <mode type="char">insol_acc,insol_coa</mode>
    <sol type="real">0.0</sol>
    <mol_weight type="real">50.00E-3</mol_weight>
    <rho type="real">2.650E3</rho>
    <unit type="char">mug kg-1</unit>
    <transport type="char">hadv52aero</transport>
  </aerosol>
  …
</tracers>
```

Getting started

- Copy the Notebook and execute the cells to get the ICON-ART experiments:

  cp -r /work/bb1093/b380891/Copy_ICON-ART_Notebooks.ipynb ~/.

- Follow the instructions in *~/ICON-ART_experiments/Primary_Aerosols*

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

DWD

DKRZ
DEUTSCHES KLIMARECHENZENTRUM

KIT
Karlsruher Institut für Technologie

natESM

Federal Ministry of Research, Technology and Space

ICON-ART

Part 3: Air quality

Dominik Brunner (Empa), Corina Keller (Empa)

Empa
Materials Science and Technology

Importance of air pollution

Impacts on human health

- respiratory & cardiovascular diseases, lung cancer
- reduced life expectancy
- ~7 million pre-mature deaths yr^{-1} globally (WHO), 168000 – 346000 in Europe (EEA, 2020)

Impacts on ecosystems and agriculture

- acidification, eutrophication, oxidative damage
- reduced plant growth and crop production

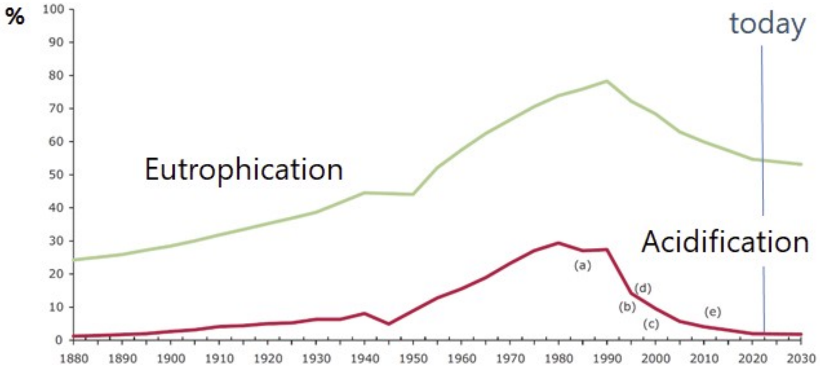
High external costs (health, agriculture, buildings)

-health costs ~600 billion EUR in Europe in 2017 (OECD 2016)

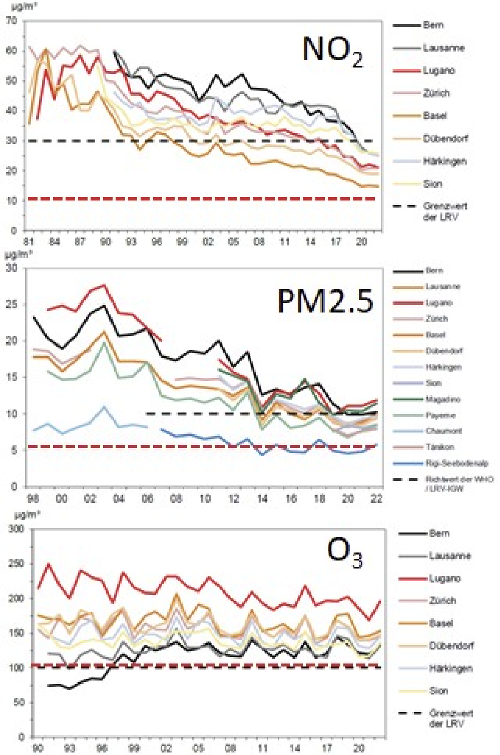
Air pollution trends

- Air quality improving in Europe; legal limits in CH met for NO_2 and PM_{10}, partially for $PM_{2.5}$, not met for O_3
- Target values proposed by WHO 2021 Air Quality Guidelines are not met
- Ecosystem impact through acidification was reduced, but eutrophication remains an issue due to NH_3

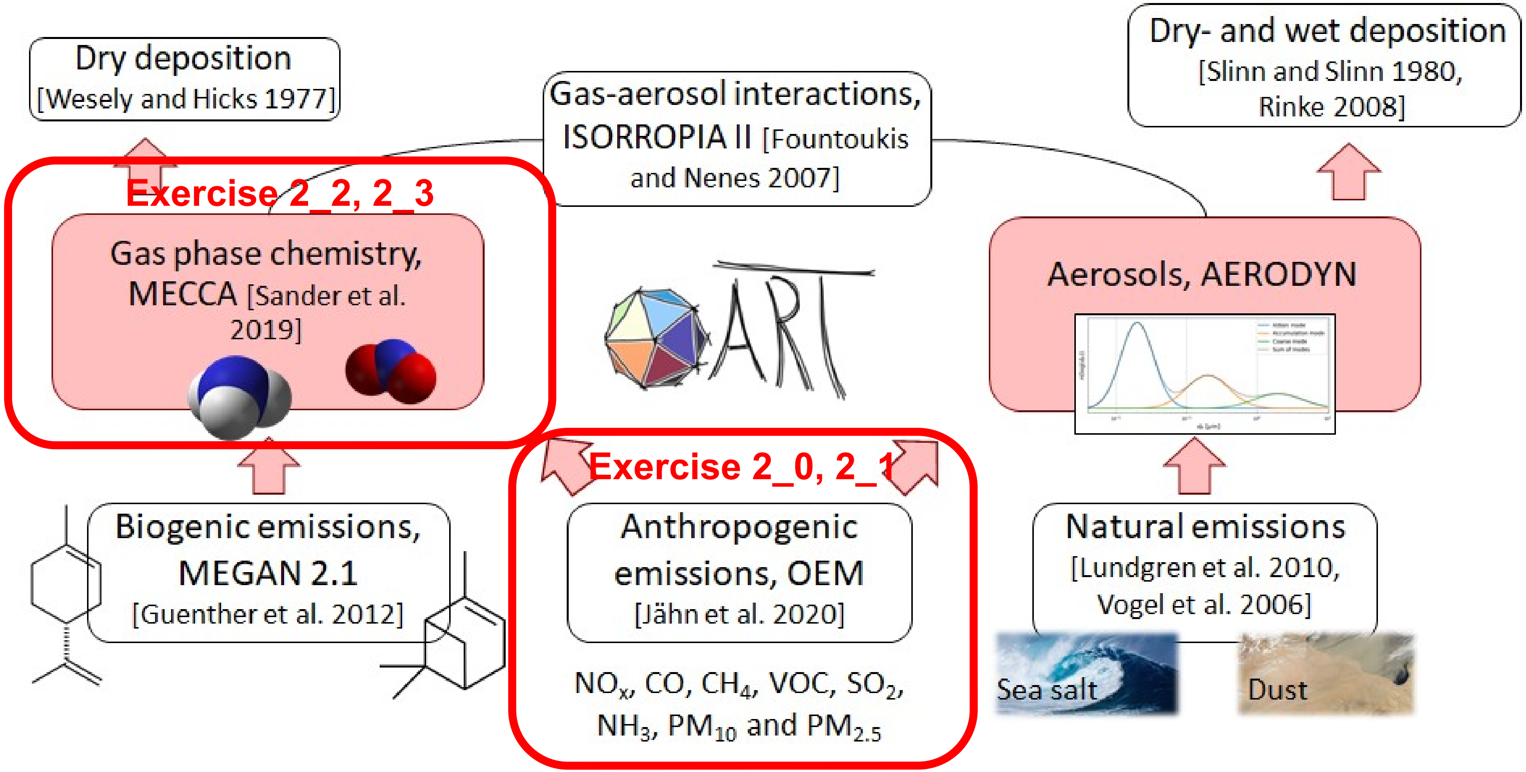
% ecosystem area in Europe with exceedance of critical loads



Trends in Switzerland



Full chemistry and aerosols in ICON-ART



Incorporating anthropogenic emissions using the Online Emissions Module (OEM)

- Originally developed for COSMO-ART/COSMO-GHG
  (Jähn et al., GMD 2020; https://gmd.copernicus.org/articles/13/2379/2020/)

- Applies temporal and vertical scaling of emissions online during simulation
  - Temporal: hour-of-day, day-of-week, month-of-year (or hour-of-year)
  - Vertical: sector-specific vertical emission profiles (e.g. for power plants)

- Integrated into ICON-ART and equipped with additional features
  - Online computation of CO_2 fluxes from vegetation
  - Online generation of ensemble of tracers driven by perturbed emissions and boundary conditions for inverse modeling

Online emissions module OEM

Set of fortran routines in *emissions* subdirectory of ART

- *mo_art_oem_types.f90*: Defines OEM data types
- *mo_art_oem_init.f90*: Initialize OEM, allocate memory, read input files
- *mo_art_oem_emission.f90*: vertical & temporal scaling, update of tracers
- (*mo_art_oem_vprm.f90*, *mo_art_oem_ensemble.f90*)

Required input files

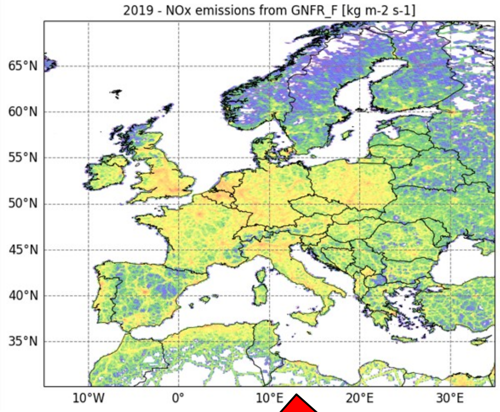
- **oem_gridded_emissions.nc**: emissions per species & sector; country masks
- Files with temporal scaling, one of the following options
    1) **dayofweek.nc, hourofday.nc, monthofyear.nc**: temporal profiles per species, sector and country
    2) **hourofyear.nc**: alternative temporal profiles
- **vertical_profiles.nc**: vertical profiles per species and sector

emiproc emission pre-processor

Open source python package (https://github.com/C2SM-RCM/emiproc)

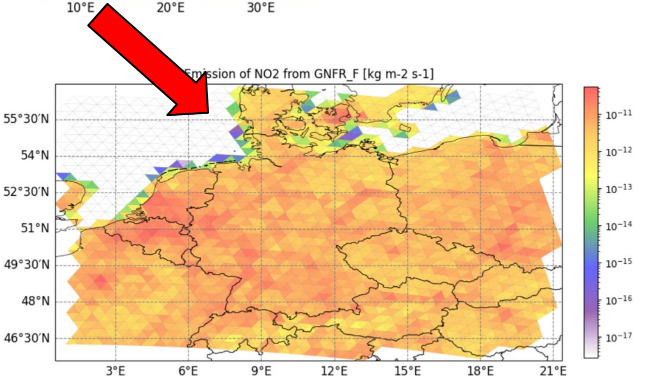
Features:

- Inventories: TNO, EDGAR, GFAS, ..
- Models: ICON, COSMO, WRF, ..
- Conservative remapping
- Merging of inventories
- Source-sector specific temporal and vertical emission profiles
- Speciation of NO_x and VOC
- Generate input files for OEM



TNO-CAMS regular grid

Traffic NO_x emissions

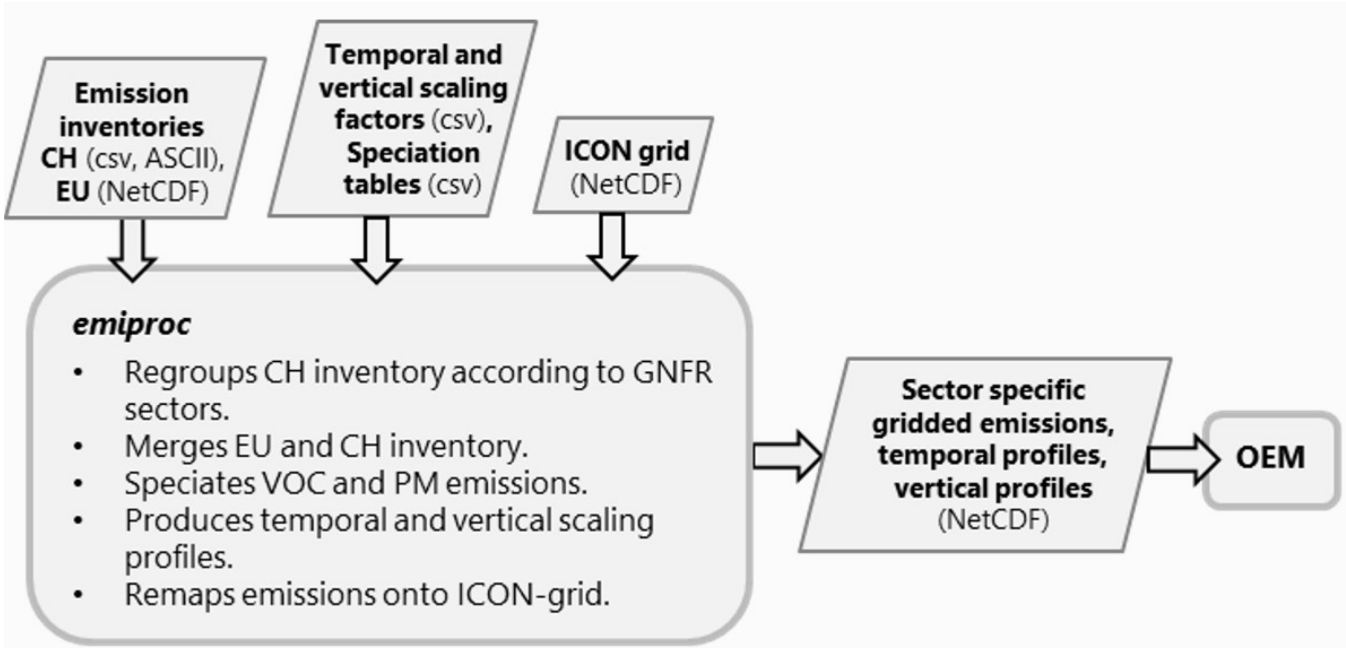


ICON triangular grid. Traffic NO_2 emissions

Constantin et al., JOSS 2025 (https://joss.theoj.org/papers/10.21105/joss.07509)

emiproc emission pre-processor

Example for preparing emissions for simulation over Switzerland



Using OEM tracers in ICON-ART

oem_type = emis: makes NH3 an OEM emis. tracer

Tracer xml-file

```
<meccatracer id="NH3" full="TRUE" chemtr="FALSE">
        <tag001 type="char">full</tag001>
        ...
        <oem_type type="char">emis</oem_type>
        <oem_tscale type="int">1</oem_tscale>
        <oem_cat type="char">GNFR_A-NH3, GNFR_B-NH3, GNFR_C-NH3, GNFR_D-NH3,
GNFR_E-NH3, GNFR_F-NH3, GNFR_H-NH3, GNFR_I-NH3, GNFR_J-NH3, GNFR_K-NH3,
GNFR_L-NH3</oem_cat>
        <oem_tp type="char">GNFR_A-NH3, GNFR_B-NH3, GNFR_C-NH3, GNFR_D-NH3, GNFR_E-
NH3, GNFR_F-NH3, GNFR_H-NH3, GNFR_I-NH3, GNFR_J-NH3, GNFR_K-NH3, GNFR_L-NH3</oem_tp>
        <oem_vp type="char">GNFR_A-NH3, GNFR_B-NH3, GNFR_C-NH3, GNFR_D-NH3, GNFR_E-
NH3, GNFR_F-NH3, GNFR_H-NH3, GNFR_I-NH3, GNFR_J-NH3, GNFR_K-NH3, GNFR_L-NH3</oem_vp>
</meccatracer>
```

oem_tscale = 1: hourofday+dayofweek+monthofyear
oem_tscale = 2: hourofyear

emission categories contributing to NH_3

Number of entries in oem_cat, oem_tp and oem_vp must be identical, so that for each category a corresponding temporal and vertical profile is defined

MOZART gas-phase chemistry with MECCA-KPP

Chemistry-transport model of NCAR

MOZART-4 chemistry scheme:

- 85 gas-phase species
- 157 gas-phase reactions
- 39 photolysis reactions

Detailed representation of VOC species and chemistry including oxidized VOCs and organic nitrates

Geosci. Model Dev., 3, 43–67, 2010
www.geosci-model-dev.net/3/43/2010/

Geoscientific Model Development

Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4)

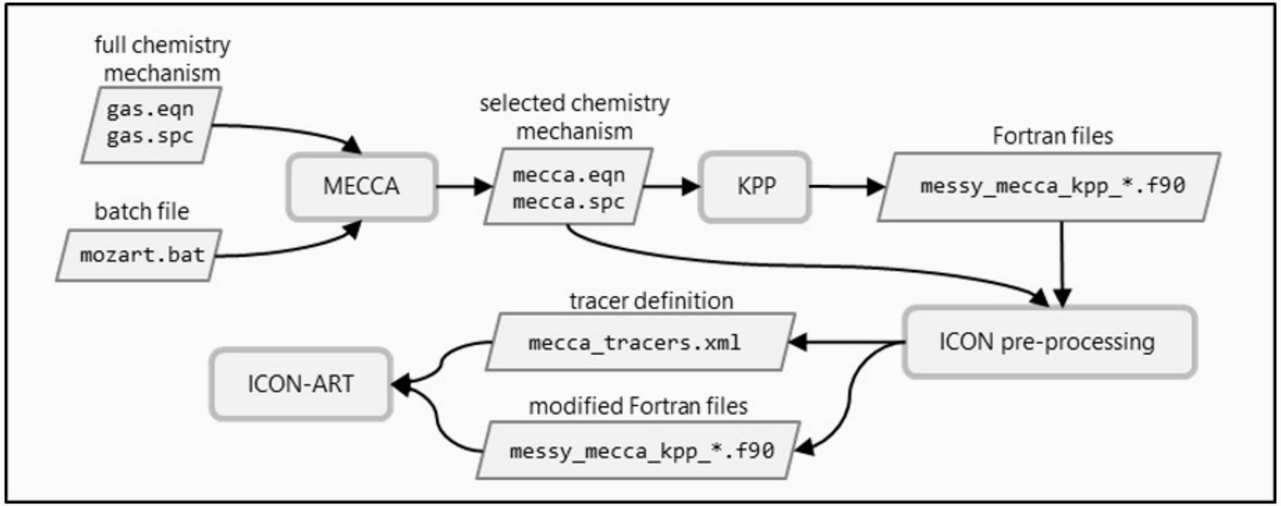
L. K. Emmons[1], S. Walters[1], P. G. Hess[1,*], J.-F. Lamarque[1], G. G. Pfister[1], D. Fillmore[1,], C. Granier[2,3], A. Guenther[1], D. Kinnison[1], T. Laepple[1,***], J. Orlando[1], X. Tie[1], G. Tyndall[1], C. Wiedinmyer[1], S. L. Baughcum[4], and S. Kloster[5,*]**

Example of C5 species In MOZART-4

C_5 species	BIGALK	C_5H_{12}	lumped alkanes C> 3
	ALKO2	$C_5H_{11}O_2$	
	ALKOOH	$C_5H_{11}OOH$	
	ISOP	C_5H_8	isoprene
	ISOPO2	e.g., $HOCH_2C(OO)CH_3CHCH_2$	peroxy radical derived from OH+ISOP
	ISOPOOH	e.g., $HOCH_2C(OOH)CH_3CHCH_2$	unsaturated hydroxyhydroperoxide
	HYDRALD	e.g., $HOCH_2CCH_3CHCHO$	lumped unsaturated hydroxycarbonyl
	XO2	e.g., $HOCH_2C(OO)CH_3CH(OH)CHO$	peroxy radical from OH+HYDRALD
	XOOH	e.g., $HOCH_2C(OOH)CH_3CH(OH)CHO$	
	BIGALD	$C_5H_6O_2$	unsaturated dicarbonyl, oxidation product of toluene
	ISOPNO3	$CH_2CHCCH_3OOCH_2ONO_2$	peroxy radical from NO3+ISOP
	ONITR	$CH_2CCH_3CHONO_2CH_2OH$	lumped isoprene nitrate

MOZART gas-phase chemistry with MECCA-KPP

Pre-processing steps for including MOZART chemistry in ICON-ART



Excerpt of file `gas.eqn`

```
<J3102> NO2 + hv = NO + O3P : {%UpStTrGJ} jx(ip_NO2);
<G1007> O3P + O2 {+M} = O3 {+M} : {%UpStTrG} kO_O2;
<G3109> NO + O3 = NO2 + O2 : {%UpStTrG} 3.00e-12*EXP(-1500./TEMP);
```

```
Up: upper atmosphere
St: stratosphere
Tr: troposphere
G: gas-phase
J: photolysis
```

Using MECCA tracers in ICON-ART

Tracer xml file *mecca_tracers_mozart4.xml*

```
<meccatracer id="NH3" full="TRUE" chemtr="FALSE">
          <tag001 type="char">full</tag001>
          <mol_weight type="real">17.0306E-3</mol_weight>
          <c_solve type="char">mecca</c_solve>
          <number type="int"> 4 </number>
          <transport type="char">hadv52aero</transport>
          <iconv type="int">1</iconv>
          <iturb type="int">1</iturb>
          <unit type="char">mol mol-1</unit>
          <init_name type="char">NH3_full</init_name>
          <init_mode type="int">1</init_mode>
          <latbc type="char">file</latbc>
          <oem_type type="char">emis</oem_type>
          ...
</meccatracer>
```

Molecular weight [kg mol^{-1}]

Tracer index used inside ART

Advection scheme
(“off” for short-lived species)

Activating biogenic emissions

Tracer xml file *mecca_tracers_mozart4.xml*

```
<meccatracer id="LTERP" full="TRUE" chemtr="FALSE">
          <tag001 type="char">full</tag001>
          <mol_weight type="real">136.238E-3</mol_weight>
          <c_solve type="char">mecca</c_solve>
          <number type="int"> 45 </number>
          <transport type="char">hadv52aero</transport>
          <iconv type="int">1</iconv>
          <iturb type="int">1</iturb>
          <unit type="char">mol mol-1</unit>
          <init_name type="char">LTERP_full</init_name>
          <init_mode type="int">1</init_mode>
          <latbc type="char">file</latbc>
          <emiss_onlBIO type="int" inum_levs="1">8</emiss_onlBIO>
</meccatracer>
```

Experiment 2:
Air quality

Corina Keller

Air Quality Simulations with MECCA Chemistry

Goal

Run ICON-ART simulation over Germany with full gas phase chemistry to **study the impact of emission mitigation on air quality**

- Simulation period: 2019-07-12 – 2019-07-14
- Chemistry mechanism: MOZART 4
- Emissions: Anthropogenic emissions (OEM) and biogenic emissions (MEGAN2.1)

Getting started

- Run the notebook **Exp_ART_AQ_getting_started.ipynb** to copy the Jupyter Notebooks and input data for this exercise

Air Quality Simulations with MECCA Chemistry

Overview

- **Task 0:** Setting up Python virtual environment
- **Task 1**: Emission processing with *emiproc*
  - **Group A**: Emission inventory for 2019
  - **Group B**: Modified emission inventory with half the NO_x emissions
- **Task 2**: Running ICON-ART simulation for 2 days over Germany ($\Delta x \approx 26$km)
- **Task 3**: Analysis of results
  - Mean 2D fields (surface level) for O_3 and NO_x
  - Comparison to ground-based observations
  - Influence of emissions inventories

Air Quality Simulations with MECCA Chemistry

Timetable

- **14:20 – 14:50 | Tasks 0, 1, and 2**
  Complete the initial tasks to prepare the simulation input data (emissions for OEM, tracer XML file) and start the simulation (*).
- **14:50 – 15:10 | Simulations in Progress**
  While simulations are running, we will review and discuss the ART namelist settings for air quality simulations.
- **15:10 – 15:30 | Task 3**
  Analyze the output data from the simulations and discuss the results.

(*) Note

If you don't finish Tasks 0-2 within the first 30 minutes, please use the notebook Exp_chem_AQ_sim.ipynb to initiate the simulation.

Air Quality Simulations with MECCA Chemistry

ART namelist settings

```
! art_nml: Aerosols and Reactive Trace gases extension
&art_nml
 lart_chem                 =                         .TRUE.
 lart_mecca                =                         .TRUE.
 iart_init_gas             =                         4
 cart_cheminit_type        = 'ERA'
 cart_cheminit_file        = 'IC_2019021200.nc'
 cart_cheminit_coord       = 'IC_2019021200.nc'
 cart_mecca_xml            = 'mecca_tracers_mozart4.xml'
 cart_input_folder         = '${EXPDIR}'
/
```

Initialize tracers according to values in xml-file

File combines meteorological and chemical initial fields

Folder PFT is inside this input folder and contains file describing plant functional types

Air Quality Simulations with MECCA Chemistry

OEM namelist settings

```
! oem_nml: online emission module
&oemctrl_nml
     gridded_emissions_nc        =   'oem_gridded_emissions.nc'
     vertical_profile_nc         =   'vertical_profiles.nc'
     hour_of_day_nc              =   'hourofday.nc'
     day_of_week_nc              =   'dayofweek.nc'
     month_of_year_nc            =   'monthofyear.nc'
/
```

PART 4:
Aerosol processes and interactions

Ali Hoshyaripour

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

DKRZ
DEUTSCHES KLIMARECHENZENTRUM

KIT
Karlsruher Institut für Technologie

natESM

Federal Ministry of Research, Technology and Space

ICON-ART

Part 4: Secondary aerosols

Ali Hoshyaripour (KIT), Julia Bruckert (KIT)

Empa
Materials Science and Technology

Continuity Equation for aerosols

Continuity equation for particle number concentration

$$\frac{\partial n_i}{\partial t} + \nabla \bullet (\mathbf{v} n_i) = (\nabla \bullet \mathbf{K}_h \nabla) n_i$$
$$+ R_{emisn} + R_{depn} + R_{sedn} + R_{washn} + \boxed{R_{nucn} + R_{coagn}}$$

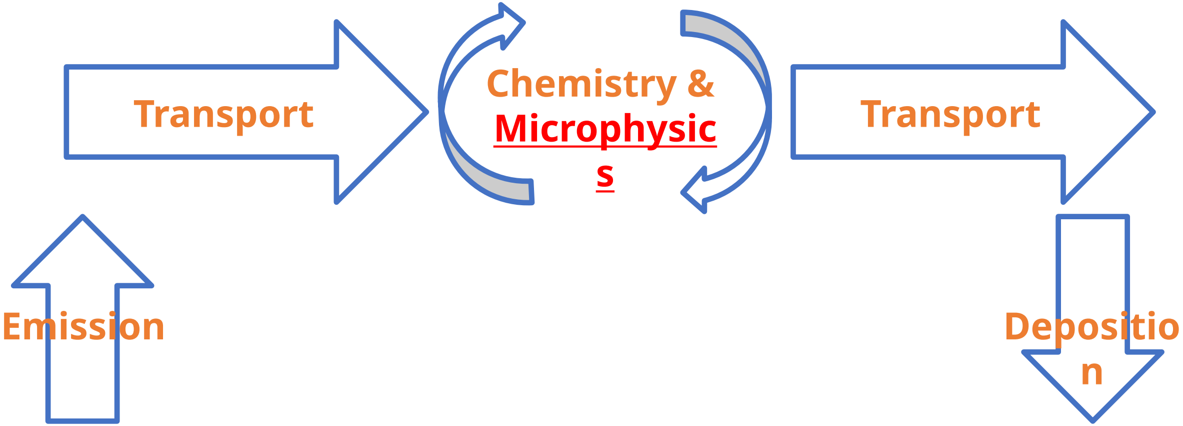
Continuity equation for particle volume concentration

$$\frac{\partial v_{q,i}}{\partial t} + \nabla \bullet (\mathbf{v} v_{q,i}) = (\nabla \bullet \mathbf{K}_h \nabla) v_{q,i}$$
$$+ R_{emisv} + R_{depv} + R_{sedv} + R_{washv} + \boxed{R_{nucv} + R_{coagv}}$$
$$+ \boxed{R_{c/ev} + R_{dp/sv} + R_{ds/ev}} + R_{eqv} + R_{aqv} + R_{hrv}$$

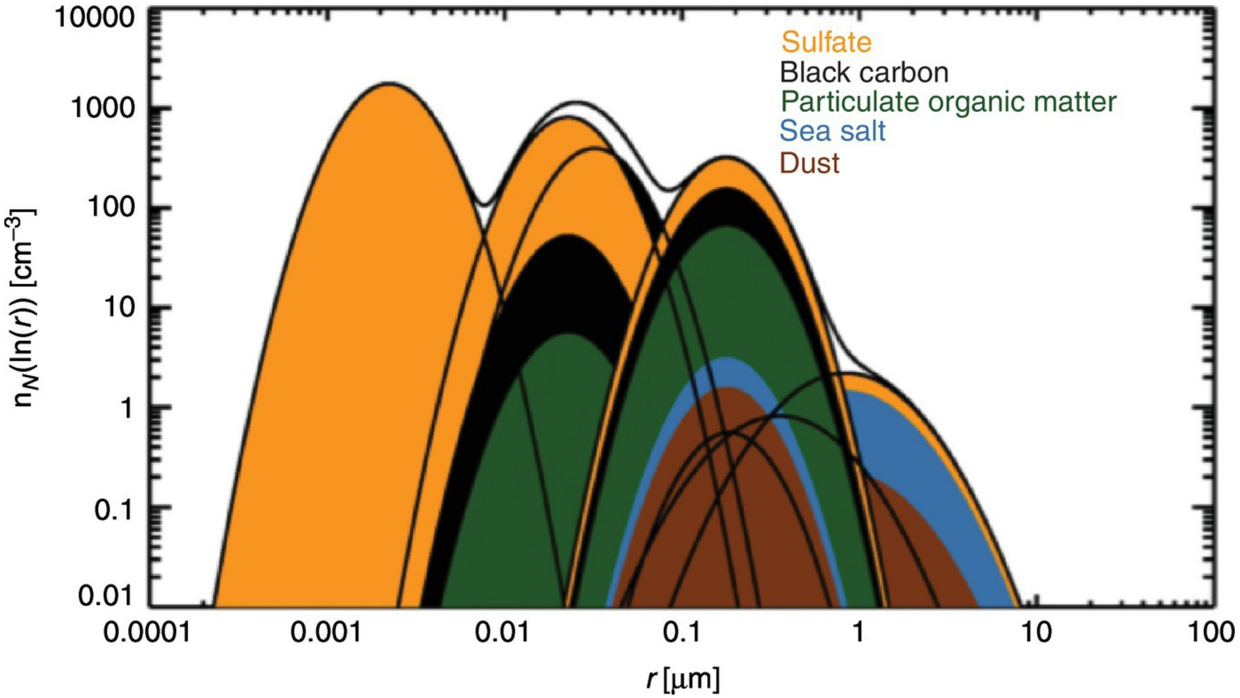
Source: Jacobson 2005

Aerosol Microphysics

- (micro-)physical processes that change the properties of aerosol particles like:
  - Concentration (number and mass)
  - Composition
  - Size
  - Morphology



Typical distributions of aerosols - modes



Source: Brasseur and Jacob 2017

Log-normal distribution

$$n_l(d_P) = \frac{N_{Pl}}{\sqrt{2\pi} d_P \ln\sigma_{g,l}} \exp\left(- \frac{\left(\ln d_P - \ln d_{g,l}\right)^2}{2\ln^2\sigma_{g,l}} \right)$$

$$n_l^*(\ln d_P) = \frac{N_{Pl}}{\sqrt{2\pi} \ln\sigma_{g,l}} \exp\left(- \frac{\left(\ln d_P - \ln d_{g,l}\right)^2}{2\ln^2\sigma_{g,l}} \right)$$

$$\ln\sigma_{g,l} = \left(\frac{1}{N_{Pl}} \int_0^\infty n_l(d_P)\left(\ln d_P - \ln d_{g,l}\right)^2 dd_P \right)^{\frac{1}{2}}$$

with:

d_p: particle diamater

$d_{g,l}$: geometric median diamater

$\sigma_{g,l}$: geometric standard deviation

Definition of moments of distributions

$$N_P = M_0$$

$$M_k = \int_0^{\infty} d_P^k n(d_P) dd_P$$

$$S = \pi M_2$$

$$V = \frac{\pi}{6} M_3$$

$$\ln d_{g,l,k} = \ln d_{g,l} + k \ln^2 \sigma_{g,l}$$

$$M_k = \int_{-\infty}^{\infty} d_p^k n_l^*(\ln d_P) d(\ln d_P) = N_{Pl} d_{g,l}^k \exp\left(\frac{k^2}{2} \ln^2 \sigma_{g,l}\right)$$

$$d_{g,l} = \left(\frac{M_3}{M_0 \exp(\frac{9}{2} ln^2 \sigma_g)}\right)^{1/3}$$

with:

d_p: particle diamater

$d_{g,l}$: geometric median diamater

$\sigma_{g,l}$: geometric standard deviation

We need to solve three equations

$$\frac{\partial N}{\partial t} = \cdots$$

$$\frac{\partial \sigma_g}{\partial t} = \cdots$$

$$\frac{\partial d_{pg}}{\partial t} = \cdots$$

Assumption:

Geometric standard deviation is kept constant!

Generalized aerosol microphysics equations

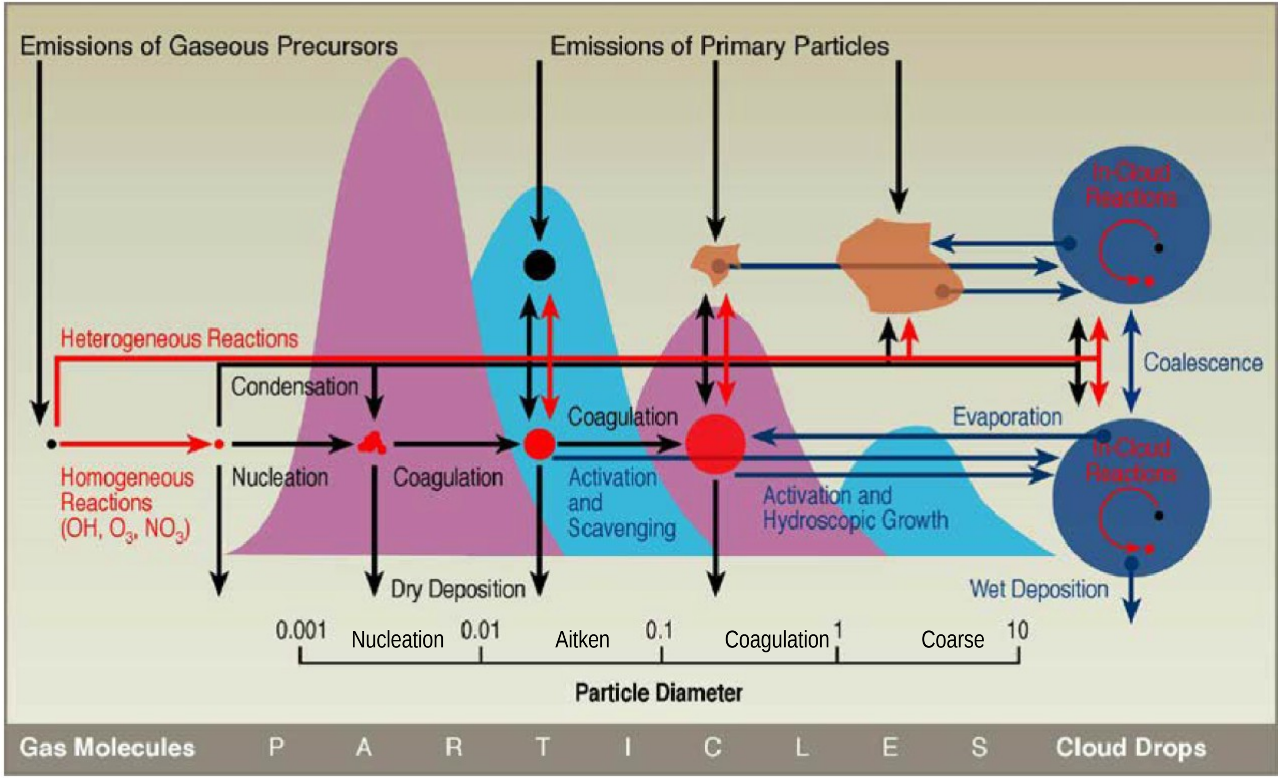
$$\frac{\partial}{\partial t} M_{0,i} = -Ca_{0,ii} - Ca_{0,ij} + Nu_0$$

Intra-modal coagulation, Inter-modal coagulation, Nucleation

$$\frac{\partial}{\partial t} M_{3,i} = -Ca_{3,ij} + Co_{3,i} + Nu_3$$

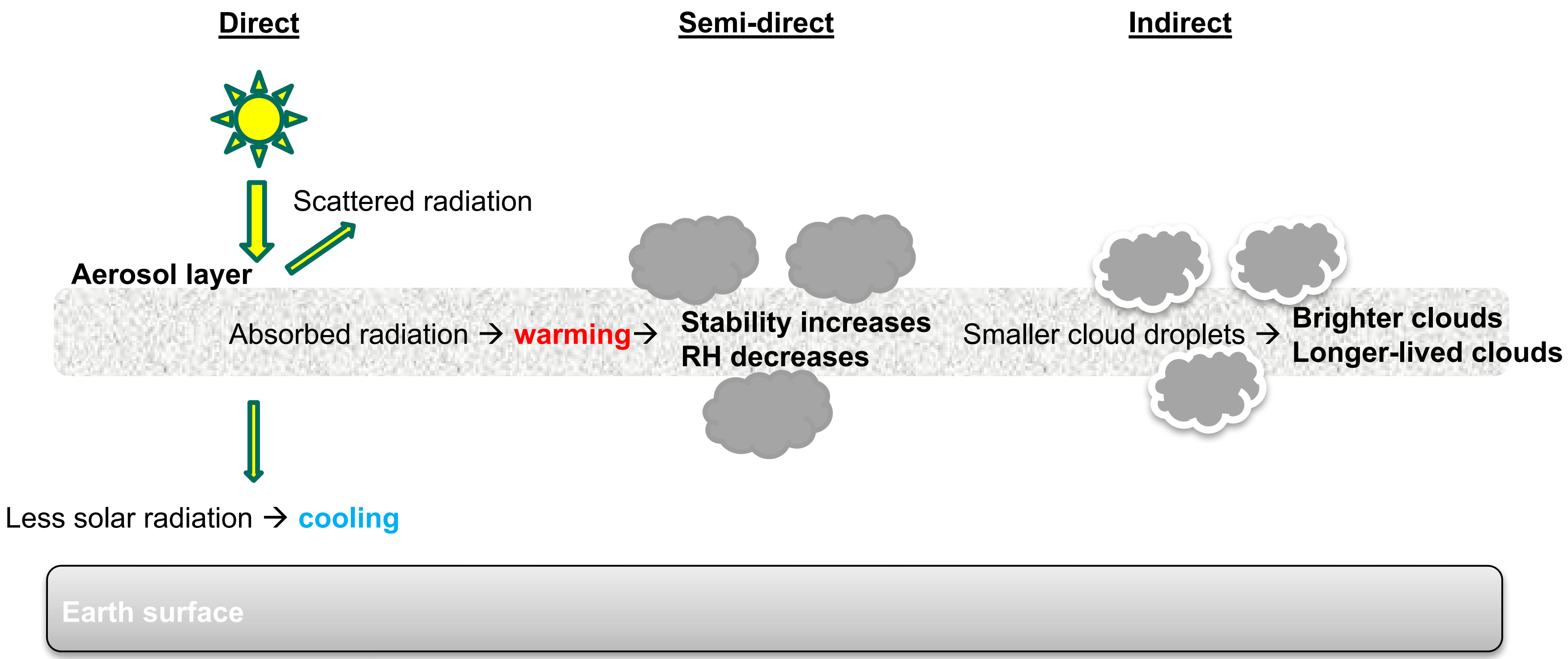
inter-modal coagulation, condensation, Nucleation

Aerosol microphysical processes



Heintzenberg et al 2003

Aerosol effects on the atmosphere



Aerosol optical properties in ICON-ART

- Natural aerosols as externally mixed:

  Saharan Dust, 3 modes, Shape

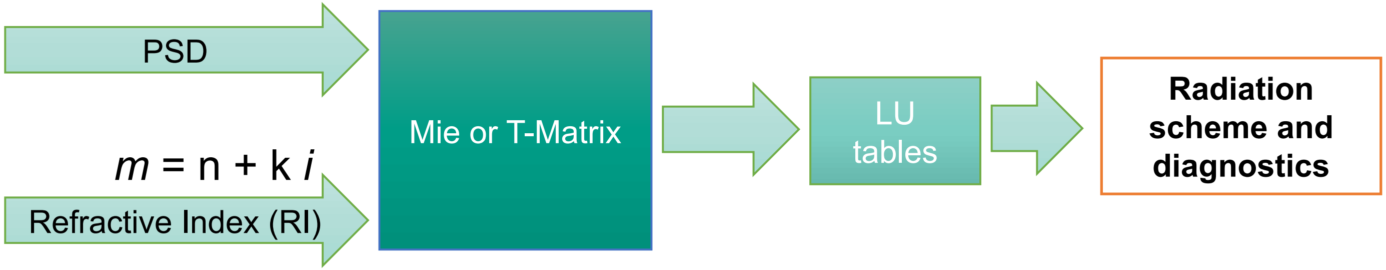
  Volcanic Ash 3 modes, Shape, composition

  Sea Salt 3 modes, RH = 70%

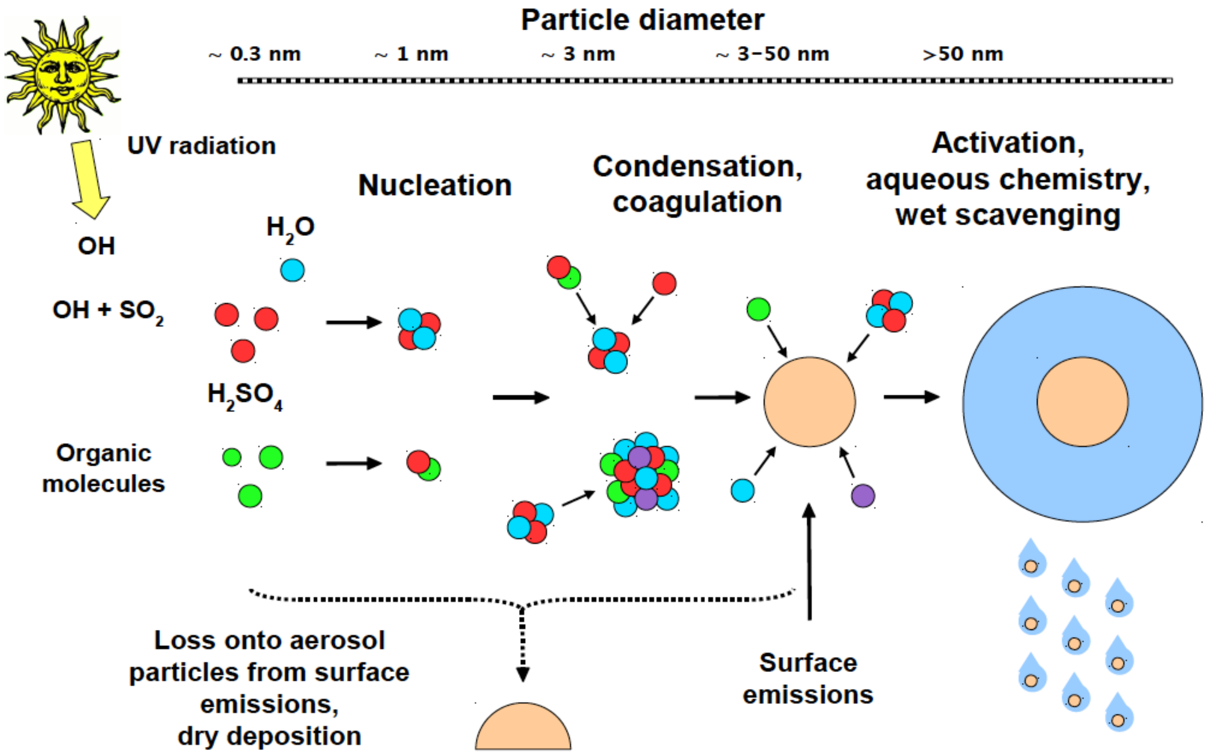
  Biomass Burning 1 mode Composition (OC/BC = 30), shape: sphere

- Natural aerosols as internally mixed:

  Volcanic Aerosols Aerodyn, Core-Shell



From aerosol microphysics to CCN activation



Source: J. Kazil slides

Experiment 3: Secondary Aerosol

Julia Bruckert

Emission and aerosol aging after the Raikoke 2019 eruption

Objectives:

How to use the point source for emissions

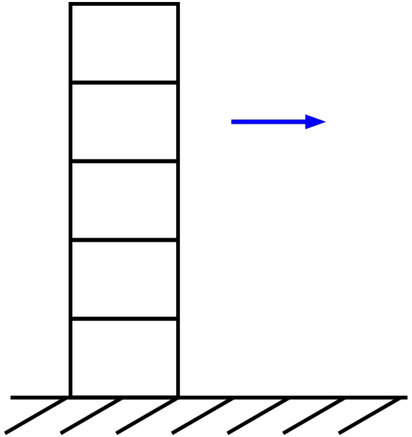
How to activate aerosol dynamical processes (nucleation, condensation, coagulation)

https://earthobservatory.nasa.gov/images/145226/raikoke-erupts

Point Source

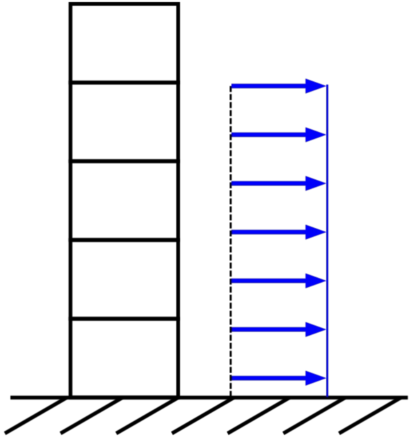
(A)

- **Emission in single point**



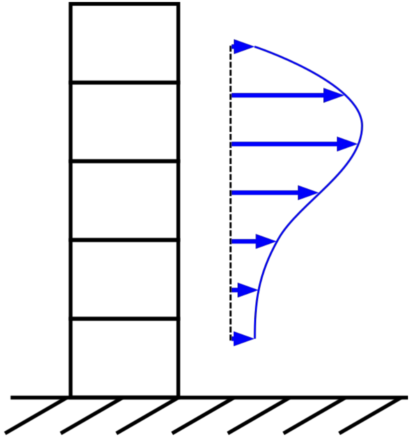
(B)

- **Emission with uniform profile**



(C)

- **Emission with user defined profile**



pntSrc.xml case (A)

```xml
<sources>
    <pntSrc id="testtracer">
        <lon type="real">10.1</lon>
        <lat  type="real">49.9</lat>
        <substance type="char">testtr</substance>
        <height type="real">2000.0</height>
        <source_strength type="real">150.0</source_strength>
        <unit type="char">kg s-1</unit>
    </pntSrc>
</sources>
```

pntSrc.xml case (B)

```
<sources>
    <pntSrc id="testtracer">
        <lon type="real">10.1</lon>
        <lat  type="real">49.9</lat>
        <substance type="char">testtr</substance>
        <height type="real">-2000.0</height>
        <source_strength type="real">150.0</source_strength>
        <unit type="char">kg s-1</unit>
    </pntSrc>
</sources>
```

negative height: allows emission with uniform profile from surface to |<height>|

pntSrc.xml case (C)

```
<sources>
  <pntSrc id="testtracer">
    <lon type="real">10.1</lon>
    <lat  type="real">49.9</lat>
    <substance type="char">testtr</substance>
    <height type="real">2000.0</height>
    <height_bot type="real">500.0</height_bot>
    <source_strength type="real">150.0</source_strength>
    <unit type="char">kg s-1</unit>
  </pntSrc>
</sources>
```

pntSrc.xml case (C)

```xml
<sources>
    <pntSrc id="testtracer">
        <lon type="real">10.1</lon>
        <lat  type="real">49.9</lat>
        <substance type="char">TRSO2</substance>
        <height type="real">2000.0</height>
        <height_bot type="real">500.0</height_bot>
        <source_strength type="real">150.0</source_strength>
        <emiss_profile type="char">0.1*[z_star] – sqrt(pi)*erf([z_star])</emiss_profile>
        <unit type="char">kg s-1</unit>
    </pntSrc>
</sources>
```

modes.xml

```
<modes>
  <aerosol id="insol_acc">
      <kind type="char">2mom</kind>
      <d_gn type="real">0.2E-6</d_gn>
      <sigma_g type="real">2.0</sigma_g>
      <condensation type="int">0</condensation>
      <icoag type="int">0</icoag>
  </aerosol>
  <aerosol id="insol_coa">
…
  </aerosol>
  <aerosol id="giant">
…
  </aerosol>
</modes>
```

Activation of aerosol dynamical processes

tracer_aerosol.xml

```
<tracers>
  <aerosol id="nmb">
…
  </aerosol>
  <aerosol id="so4">
                <moment type="int">3</moment>
                <mode type="char">sol_ait</mode>
                <sol type="real">1.</sol>
…
      <inucleation type="int">0</inucleation>
  </aerosol>
…
</tracers>
```

Activation of H_2SO_4 nucleation to sulfate aerosols

Externally mixed aerosols

- Simulation of the Raikoke eruption in June 2019 with internally mixed aerosols and simplified OH chemistry

	Aitken	Accumulation	Coarse	Giant
Ash	/	insoluble, mixed	insoluble, mixed	insoluble
so4	soluble	mixed, soluble	mixed	/

- Follow the instructions in *~/ICON-ART_experiments/Secondary_Aerosols/*

https://earthobservatory.nasa.gov/images/145226/raikoke-erupts

Wrap up

Ali Hoshyaripour

Best-practice recommendations

1. Always follow '**Trust, but verify**' principal. Before re-cycling some old runscript or XMLs from a colleague, check the latest namelists and XMLs to make sure nothing is outdated. Keep in mind that there is no globaly-valid namelist for ICON, ART or any other model. Settings must be adopted according to the model version, resolution and configurations. A good place to start is here.
2. Use git and keep using it! The last thing you need is an outdated local branch that no one can test, debug and understand including yourself. Update your local branch(es) at least after each release which means twice a year.
3. Use the GNU/GCC compiler especially in debugging mode. Intel is fast but compiles every possible garbage.
4. Use the checksuit and SAMOA very frequently to make sure that your branch is physically sound and is not producing garbage.

Resources

ICON-ART website (key info about the model and research)

https://www.icon-art.kit.edu/

ICON-ART user guide (how to use the model)

https://www.icon-art.kit.edu/userguide/

ICON Website (latest release and news)

https://icon-model.org/

Python tools for pre- and post-processing

https://github.com/alihoshy/art_pytools.git

Workflow management

auto-icon / auto-icon · GitLab (dkrz.de)