Deutscher Wetterdienst
Wetter und Klima aus einer Hand

ICON-ART

Ali Hoshyaripour (KIT), Stefan Versick (KIT)

Federal Ministry of Research, Technology and Space

Empa Materials Science and Technology

Training contents

Part 1: Overview of ICON-ART

Part 2: Modeling primary aerosols; lecture + exercise incl:

Emission of dust, wildfire and sea salt aerosols

Aerosol-radiation interaction

Part 3: Modeling air quality; lecture + exercise incl:

Full chemistry with MECCA

Emission processing with emiproc

Online emission module

Part 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

Instructors

- Ali Hoshyaripour
  Group leader, IMKTRO, KIT

- Julia Bruckert
  Research Associate, IMKTRO, KIT

- Dominik Brunner
  Professor, EMPA

- Stefan Versick
  Research Associate, IMKASF, KIT

- Corina Keller
  Research Associate, EMPA

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

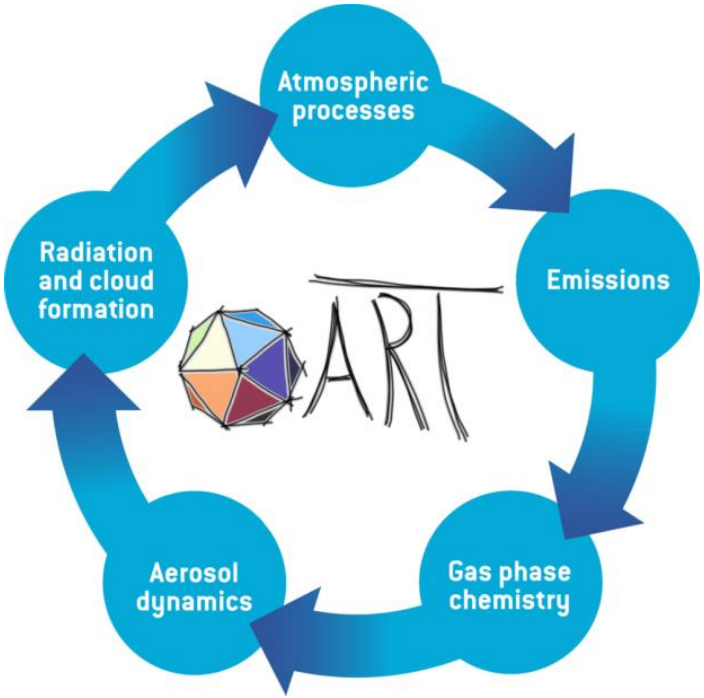
ICON-ART

Part 1: Overview

Ali Hoshyaripour (KIT), Stefan Versick (KIT)

Empa
Materials Science and Technology

ICON-ART



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

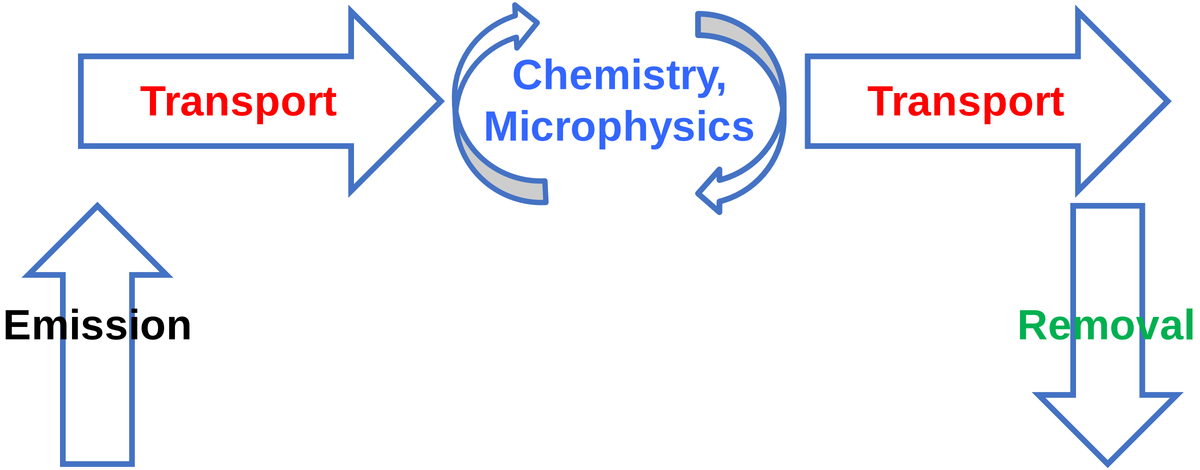
Rieger et al. (2015), Weimer et al. (2017)

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

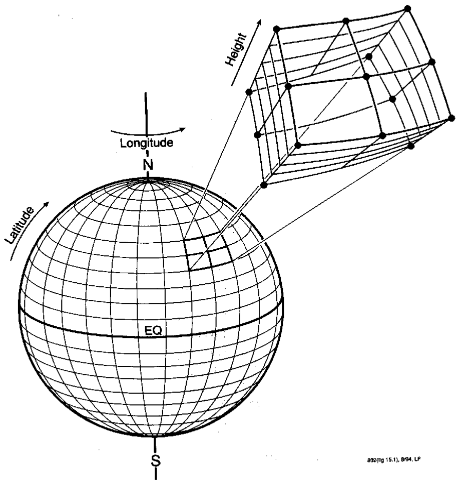
Atmospheric composition models



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

Modelling atmospheric composition

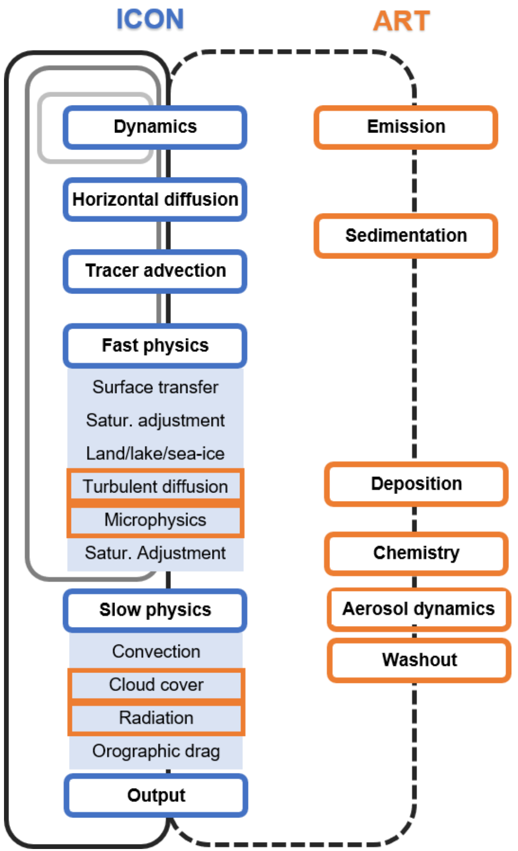
"Eulerian" atmospheric models solve mass balance (or continuity) equation in 3-D assemblage of gridboxes



 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
 iart_yyy
 cart_zzz
```

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

e.g.

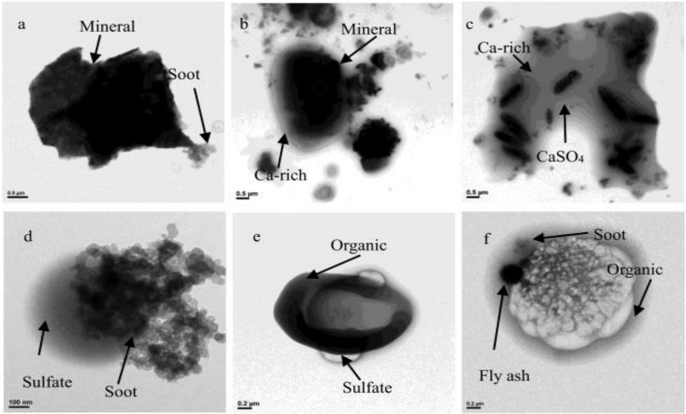
```
 lart_chem           =    .FALSE.
 lart_aerosol        =    .TRUE.
 iart_init_aero      =    0
 cart_aerosol_xml    =    '${INDIR}/tracers_aerosol.xml'
 cart_modes_xml      =    '${INDIR}/modes.xml'
```

General ART namelist parameters

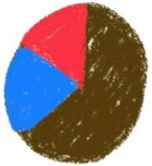
Namelist parameter	Default	Description	If .TRUE. then needs
`lart_chem`	.FALSE.	Enables chemistry.	`lart_chemtracer = .TRUE.` OR `lart_mecca = .TRUE.`
`lart_chemtracer`	.FALSE.	Switch for simple OH chemistry	`cart_chemtracer_xml`
`lart_mecca`	.FALSE.	Switch for kpp chemistry	`cart_mecca_xml`
`lart_pntSrc`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

Aerosol physicochemical properties

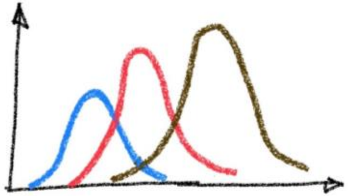
TEM image of (aged) aerosols



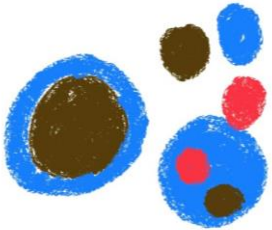
Chemical composition



Size distribution



Mixing state

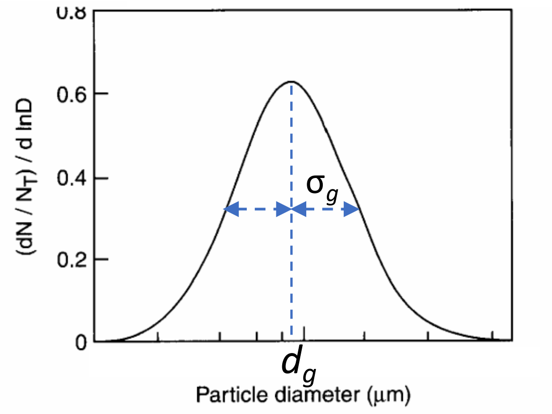


Morphology

Fan et al 2016

Modal approach for modelling aerosols

- The modal approach (based on lognormal distribution) 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.



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

To fully characterized the distribution we need to solve three equations:

$$\frac{\partial d_{pg}}{\partial t} = \cdots \qquad \frac{\partial \sigma_g}{\partial t} = \cdots \qquad \frac{\partial N}{\partial t} = \cdots$$

Instead we solve two equations for volume/mass and number concentration with fixed σ_g

 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.

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

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

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

$R_{c/ev}$ = 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

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
$R_{c/eg}$ = rate of gas loss (production) due to condensation (evaporation)
$R_{dp/sg}$ = rate of gas loss (production) due to depositional growth (sublimation)
$R_{ds/eg}$ = 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}).

 Source: Jacobson 2005

Chemistry ODEs

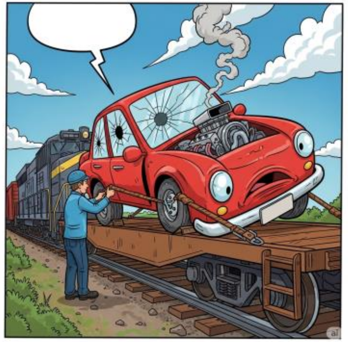
$$\left[\frac{\partial \rho_i}{\partial t}\right]_{chem} = p_i - \ell_i \rho_i$$

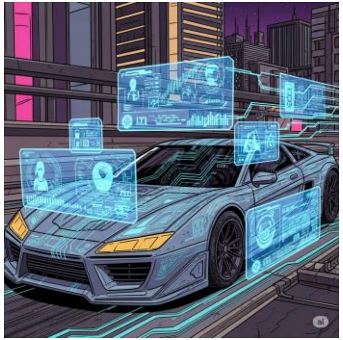
- p_i [kg m-3 s-1] overall production rate constant
- ℓ_i [s-1] overall loss rate constant

- 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



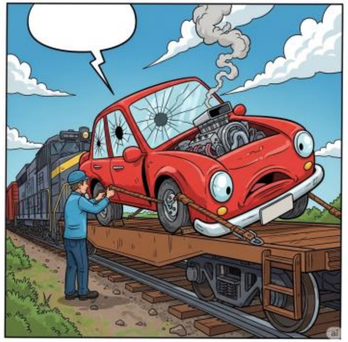


Passive -> Lifetime -> Simplified -> AI -> complex

Model complexity

Computing time

Passive Tracers



- 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

```
<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

```
<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

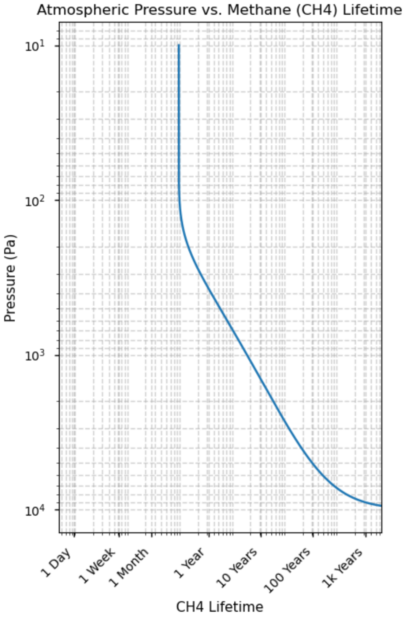
    `chemistry/mo_art_chemtracer.f90`

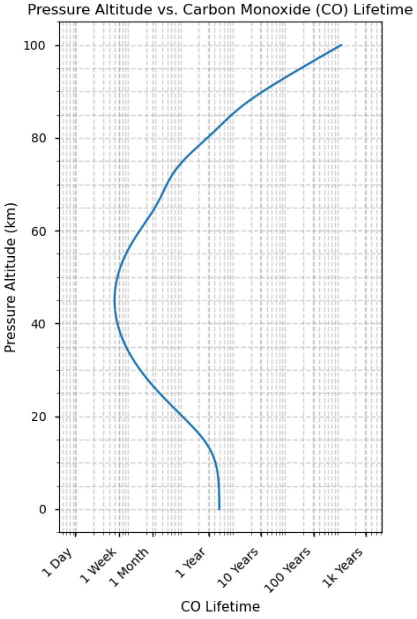
```
TYPE IS (t_chem_meta_lt)

  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
```

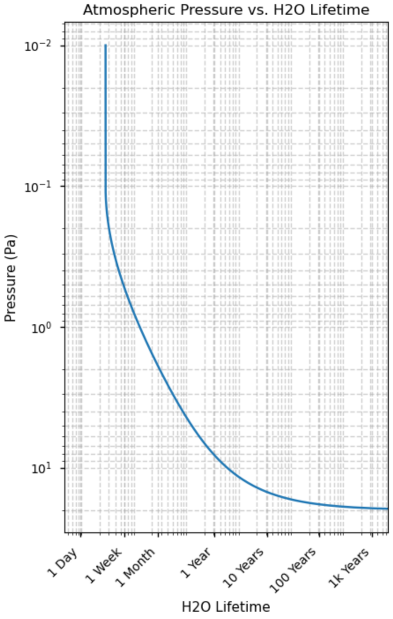
Lifetime Tracers

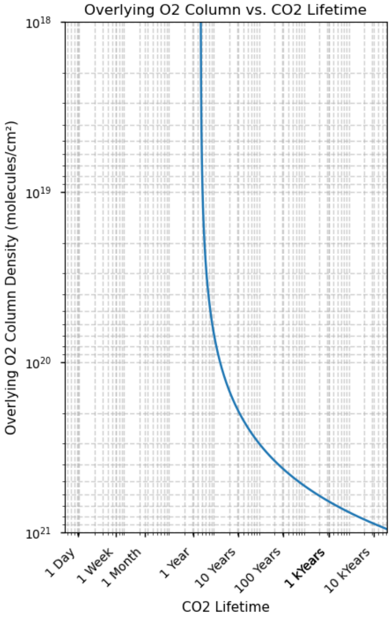
DWD
Deutscher Wetterdienst
Wetter und Klima aus einer Hand
DKRZ
KIT
natESM

- Example vertical profiles for some of the tracers









Simplified chemistry

Deutscher Wetterdienst
Wetter und Klima aus einer Hand
DWD
DKRZ
KIT
natESM

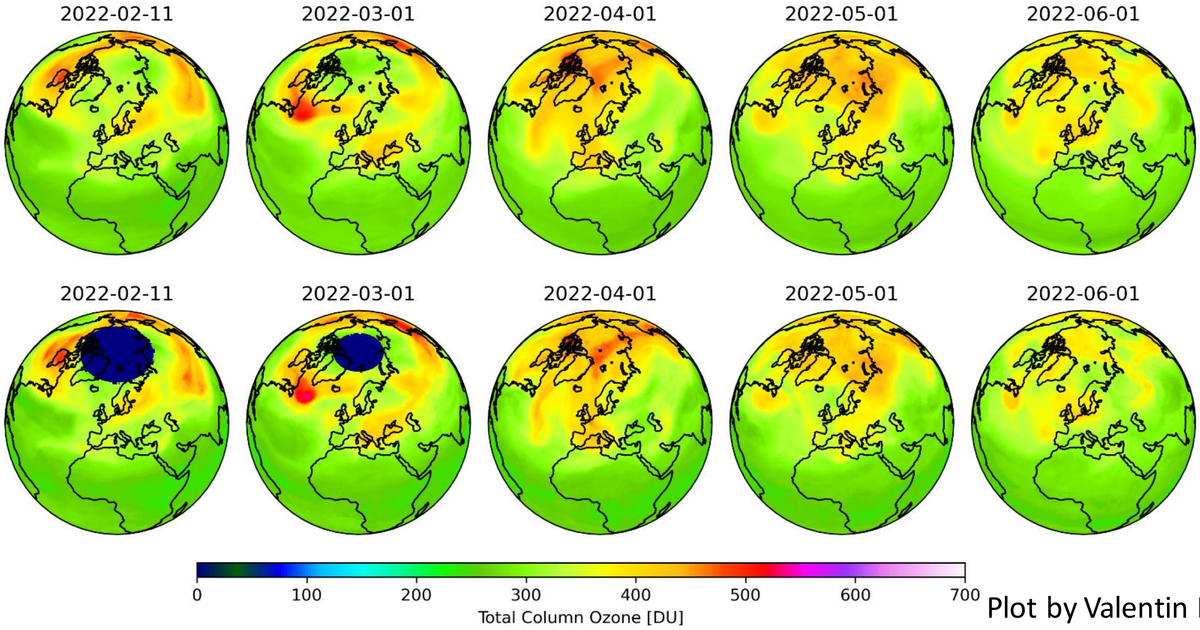
- Different schemes
  - Linoz: ozone
  - SimNOy: N2O
  - OH (included in the Aerosol experiment)
- Useful for fast simulations with good accuracy

```
<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

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

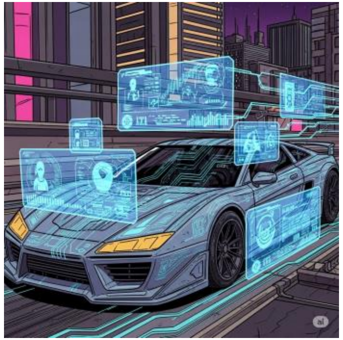


ICON-ART Linoz

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

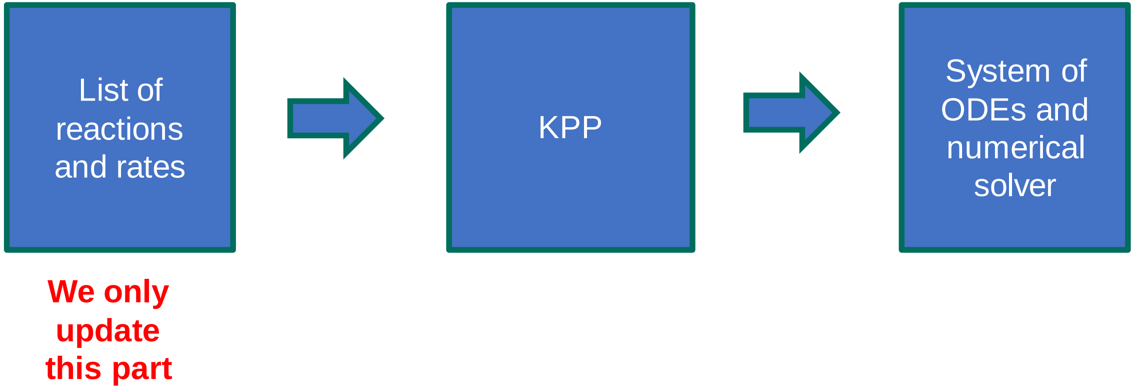
- MECCA based
- Needs pre-processing
- Can be very complex
- Most accurate
- You can easily achieve slowdowns of factor 100 or more of your simulations
- Best suited for short simulations or only local areas (Tutorial Experiment 2: Air Quality)

```
<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

type of data

ICON grid

Optional

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


Biomass burning


Volcanic


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:**	GFAS data	ART_BCF

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

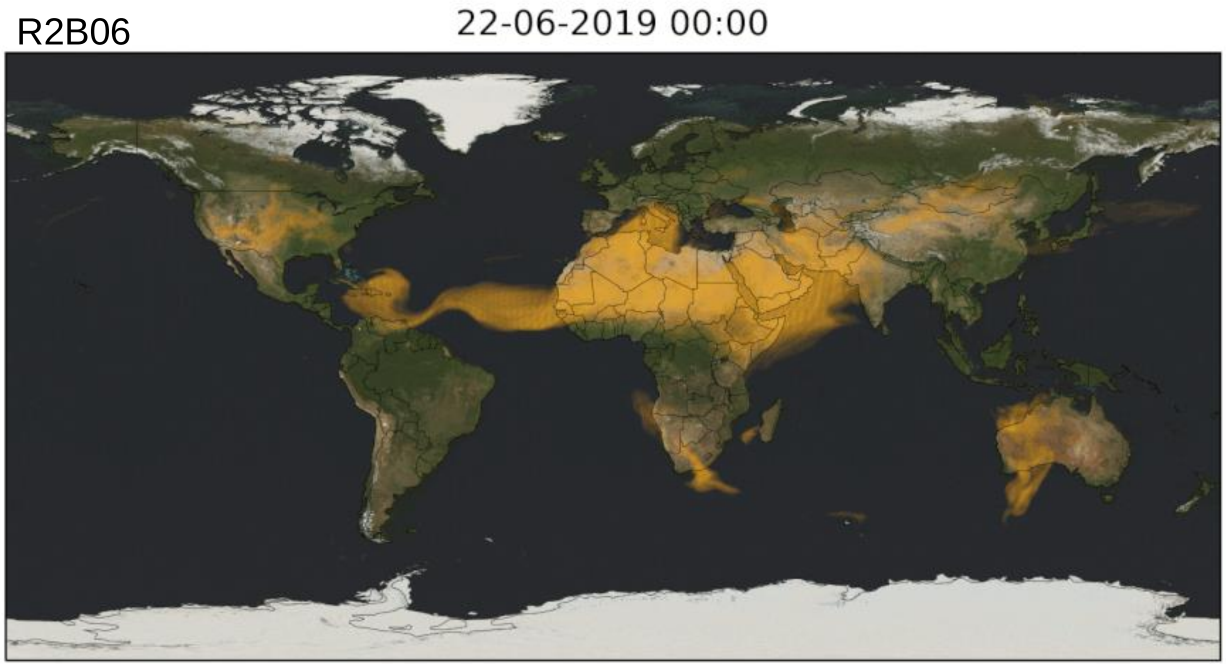
Part 2: Primary aerosols

Ali Hoshyaripour (KIT), Julia Bruckert (KIT)

Empa Materials Science and Technology

Multi-aerosol simulations

R2B06



Mineral Dust

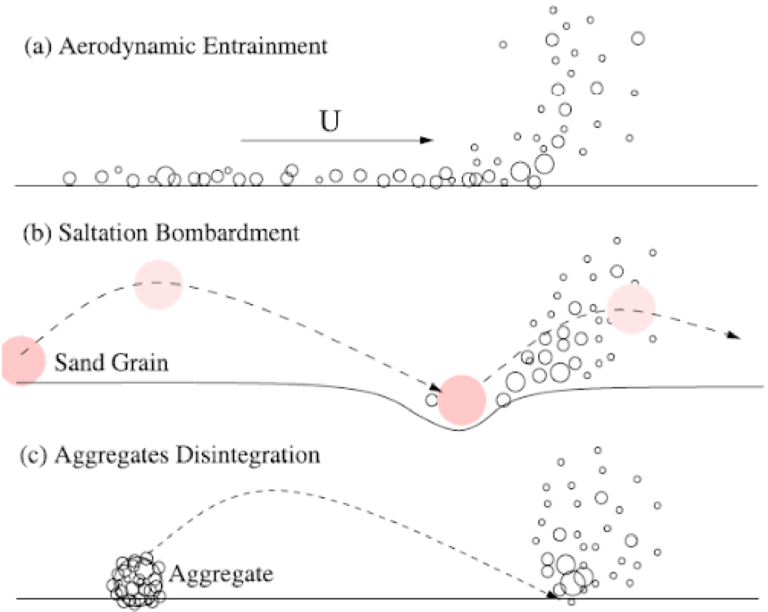
Sea Salt

Biomass Burning Aerosols

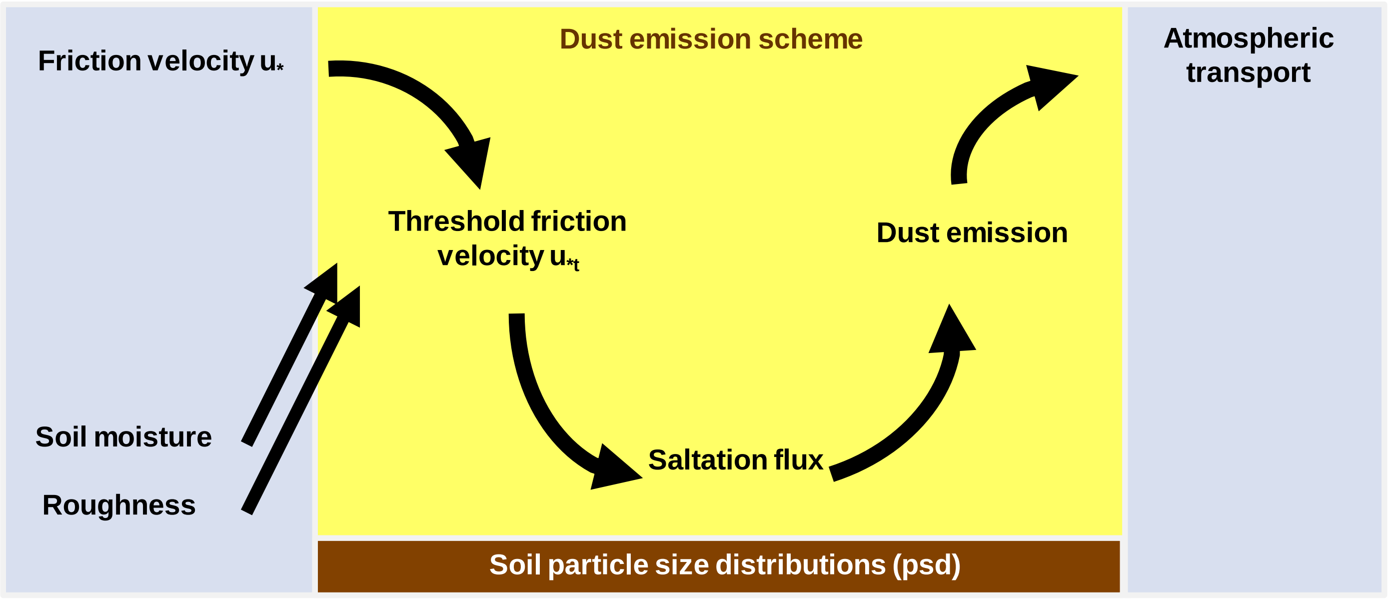
Anika Rohde

Mineral dust: emission mechanisms

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



Mineral dust: implementation in ICON-ART



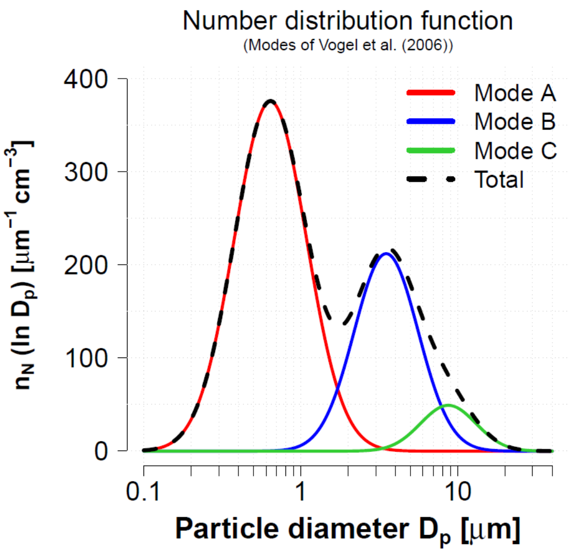
Rieger 2016, Vogel et al., 2006, Hoose, 2005

Mineral dust: implementation in ICON-ART

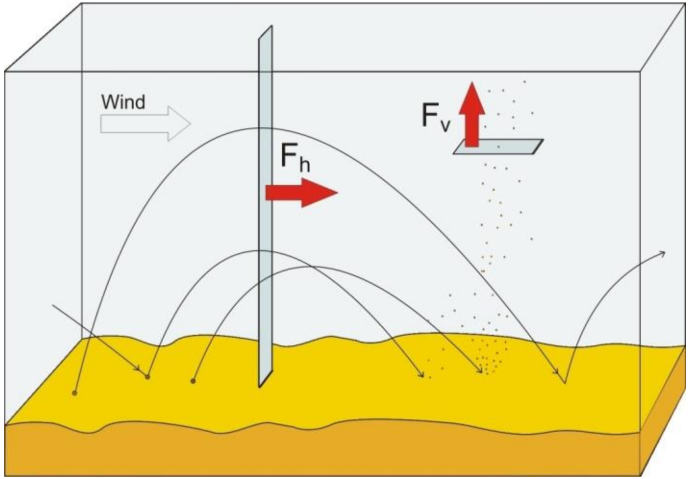
- **Input:**
  - friction velocity
  - soil moisture
  - vegetation cover + land use data
  - soil type (Harmonized World Soil Database, HWSD (2012))
  - soil particle size distributions (Shao et al., 2010)

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

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



Mineral dust emission in ICON-ART



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

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

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

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

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

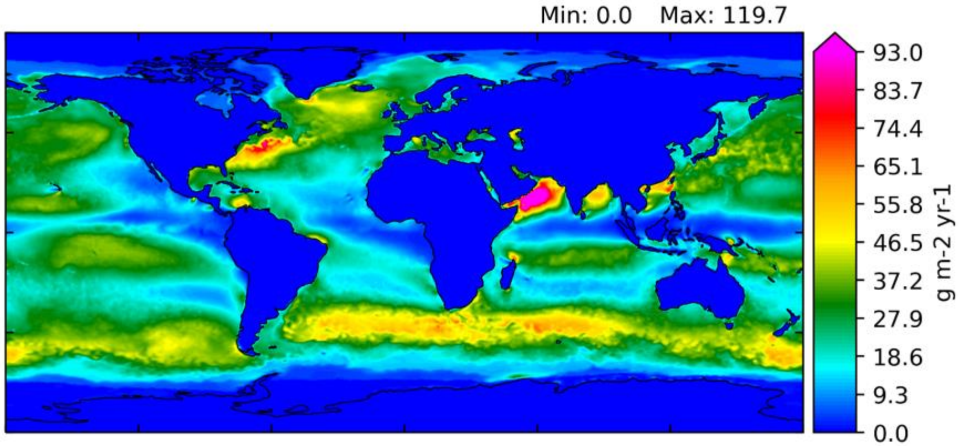
Vogel et al., 2006, Hoose, 2005

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

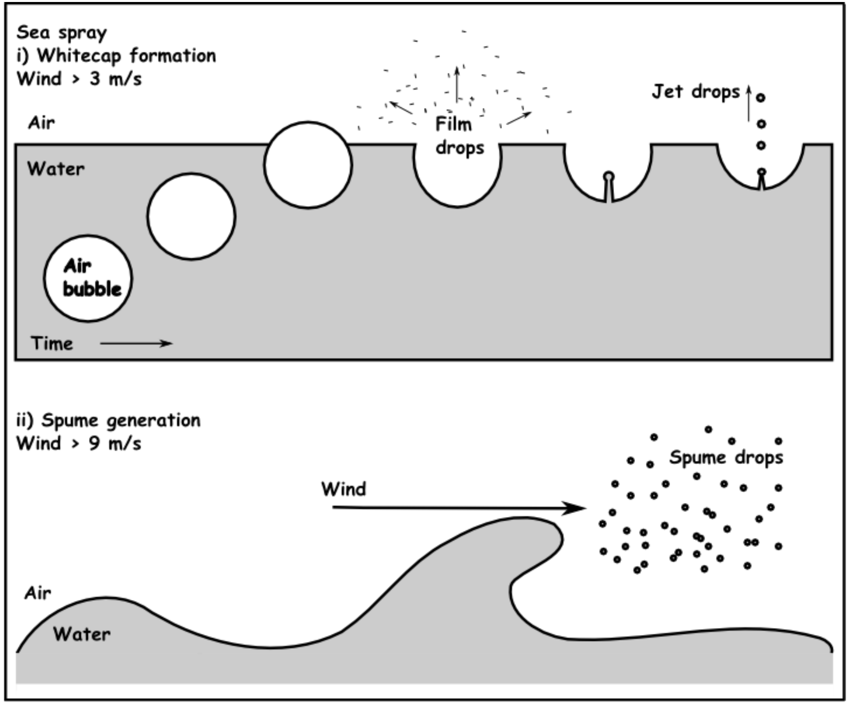


Emission of sea salt

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 emission in ICON-ART

$$\frac{dF(D_p,U_{10},T)}{dD_p} = T_w \cdot \left(235 \cdot U_{10}^{3.5} \exp\left(-0.55\left(\ln\left(\frac{D_p}{0.1}\right)\right)^2\right) + 0.2 \cdot U_{10}^{3.5} \exp\left(-1.5\left(\ln\left(\frac{D_p}{3}\right)\right)^2\right) + 6.8 \times 10^{-3} \cdot U_{10}^{3} \exp\left(-1\left(\ln\left(\frac{D_p}{30}\right)\right)^2\right)\right).$$

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

Grythe et al. 2014

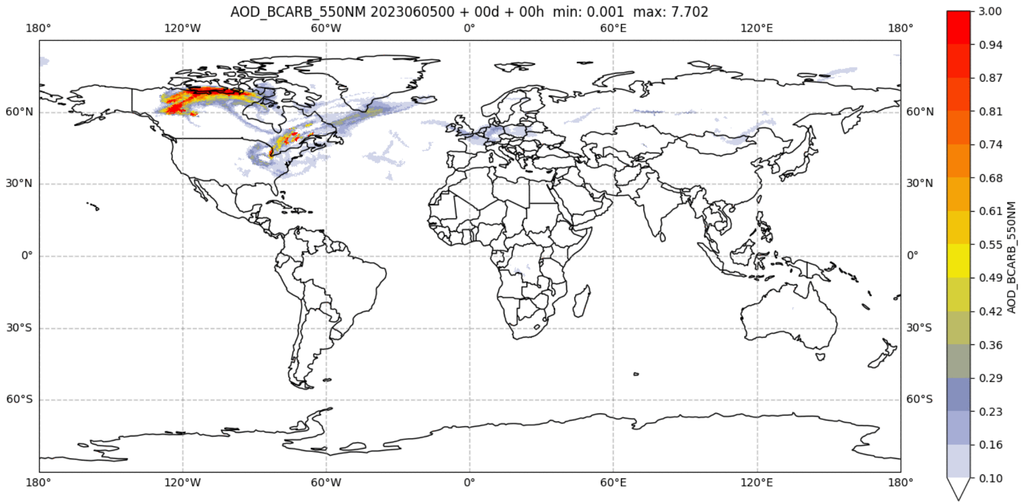
Biomass burning emissions

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

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

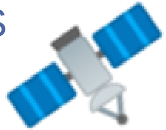
- In ICON-ART we use one biomass-burning aerosol mode with d = 150 nm and sigma = 2

PermaStrom@DWD



Biomass burning emissions in ICON-ART

GFAS



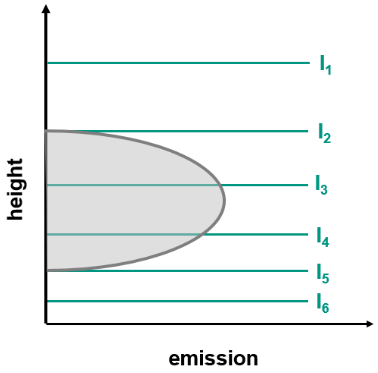
Kaiser et al., 2009

Emission rate:

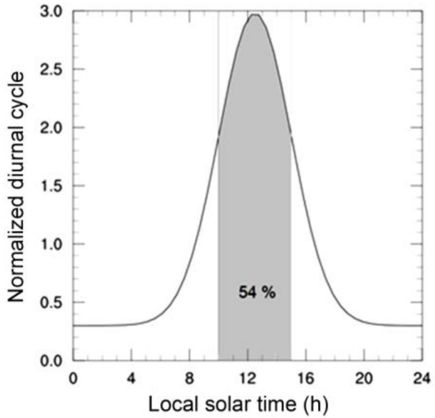
$$E(z) = M \cdot W_{emiss}(z) \cdot c_{emiss}$$

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

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

ICON-ART

EXP 1: Primary aerosols

Julia Bruckert (KIT)

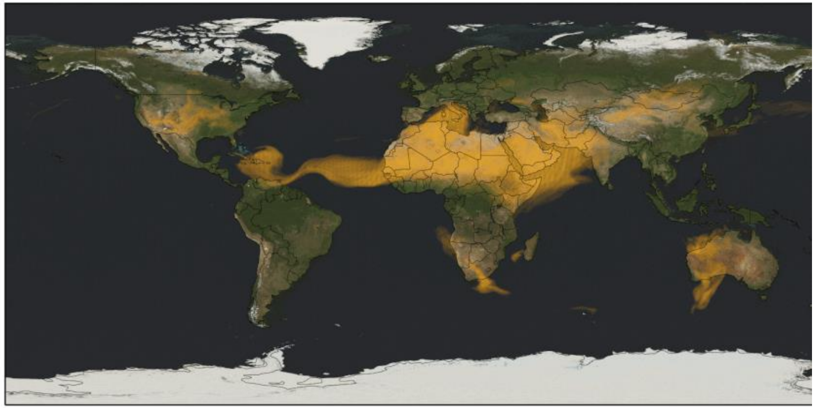
DKRZ Deutsches Klimarechenzentrum
KIT Karlsruher Institut für Technologie
natESM
Federal Ministry of Research, Technology and Space
Empa Materials Science and Technology

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

```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

```
<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

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)

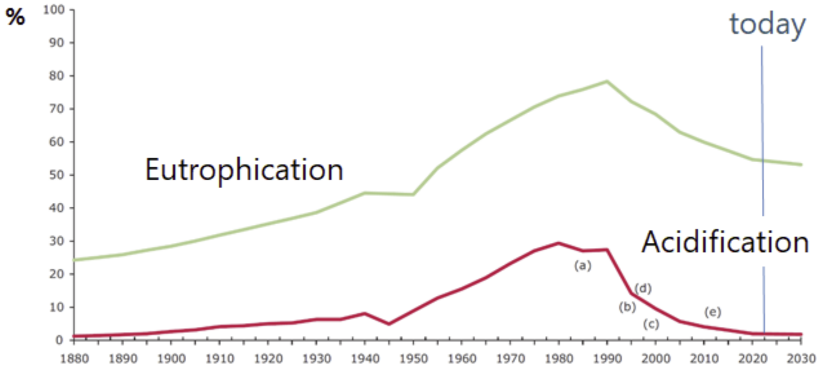
-health costs ~600 billion EUR in Europe in 2017 (OECD 2016)

54

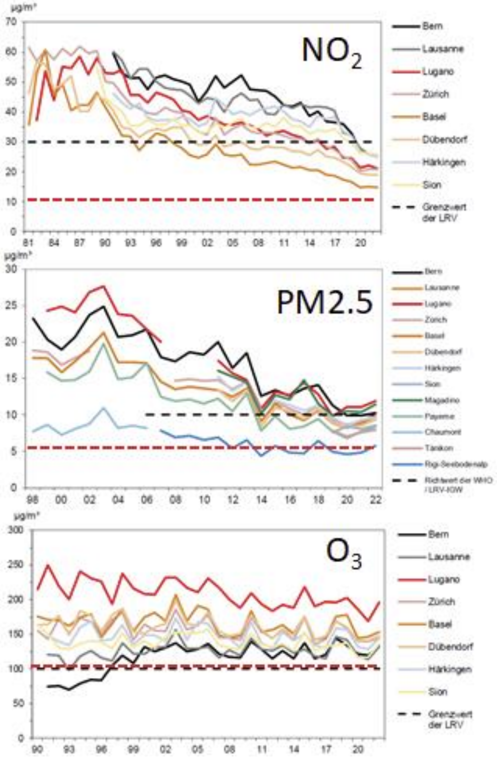
Air pollution trends

- 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



55

Primary versus secondary air pollutants

Primary air pollutants

- Directly produced and emitted at source
- Primary gases: Nitrogen oxides NO_x, sulfur dioxide SO_2, ammonia NH_3
- Primary particulate matter (PM) / primary aerosols:

  Natural: mineral dust, sea salt, pollen, biomass burning (BB) smoke, soot

  Anthropogenic: soot, primary organic aerosols (POA), abrasion particles

Secondary air pollutants

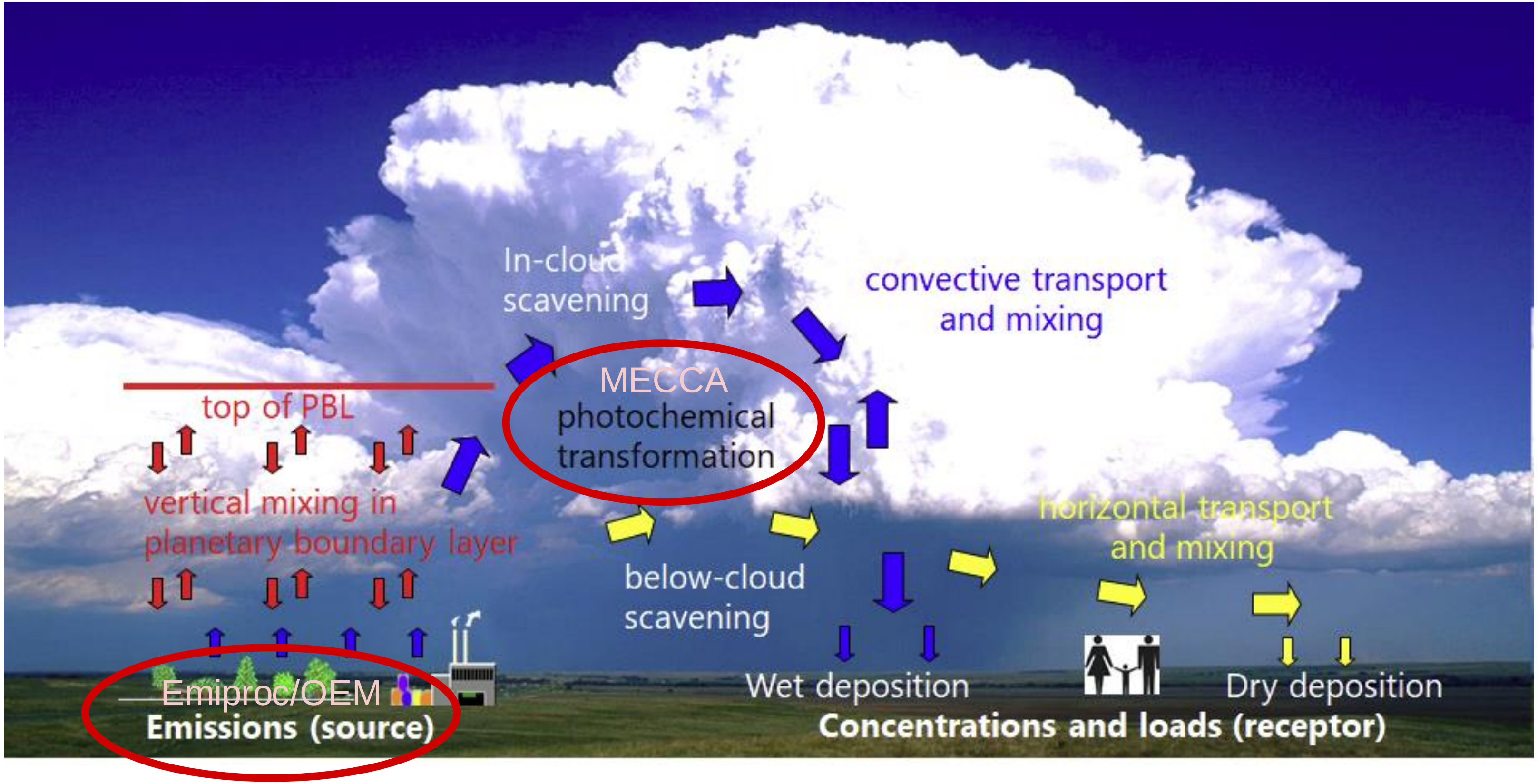
- Produced in atmosphere through photochemistry
- Secondary gases: Ozone O_3, nitric acid HNO_3, sulfuric acid H_2SO_4, PAN
- Secondary PM / secondary aerosols:

  Natural: secondary organic aerosols (SOA) from plant & BB emissions

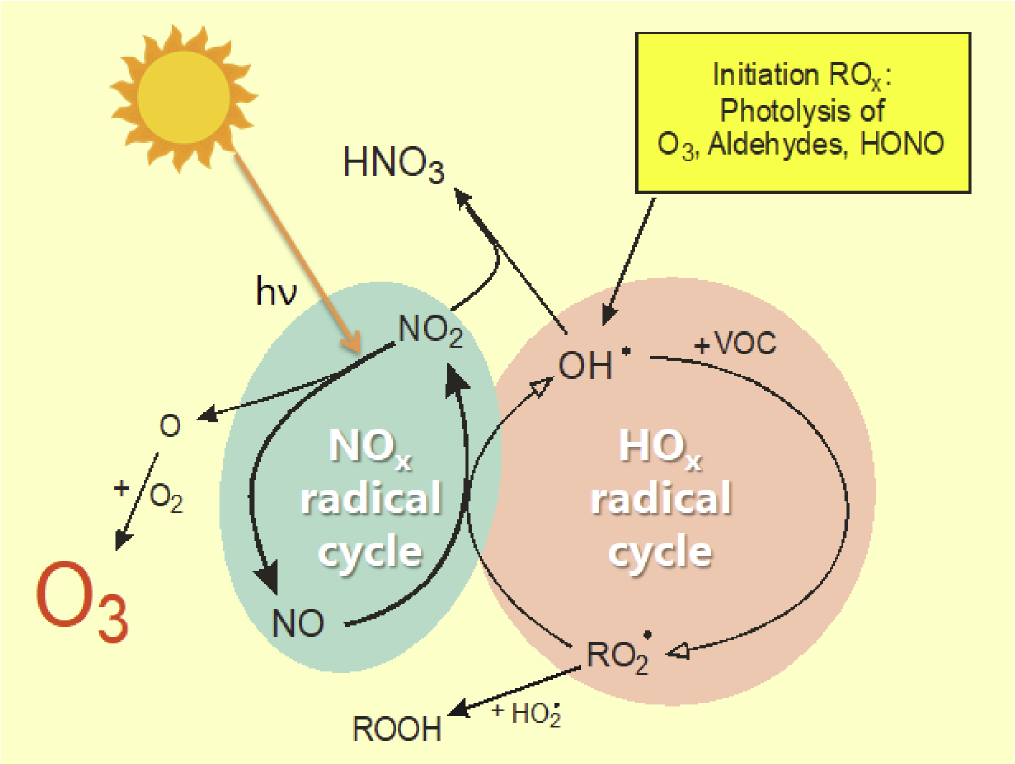
  Anthropogenic: secondary inorganic (SIA) and organic (SOA) aerosols

56

From emissions to concentrations to exposure



Schematic of photochemical ozone production

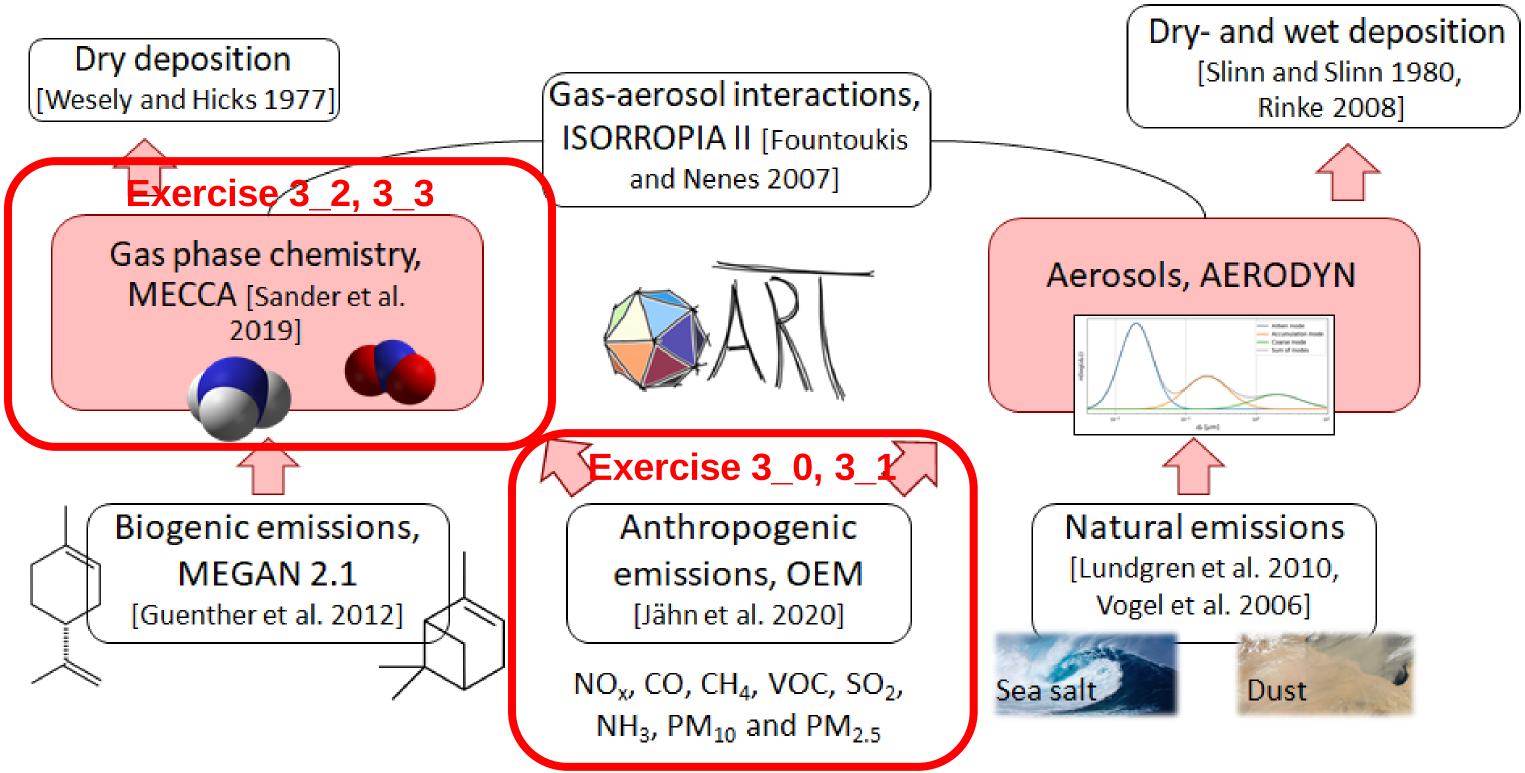


Production of O_3 requires presence of chemical precursors

- Nitrogen oxides (NO_X)
- Volatile organic compounds (VOCs) and CO

and coupling between NO_x and HO_x radical cycles

Full chemistry and aerosols in ICON-ART



Anthropogenic emissions in ICON-ART

Options

- **Point sources:** XML-file pntSrc.xml
  Source locations and their emission strengths
- **Offline files:** ART_ANT_iconR<n>B<k>-grid-yyyy-mm-dd-hh_<grid-num>.nc
  Reading of emissions from pre-processed files e.g. at 1h time steps
- **Online emissions:** *OEM module* (see next slides)
  Reading of emissions only at start, application of temporal and vertical profiles online during simulation

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

61

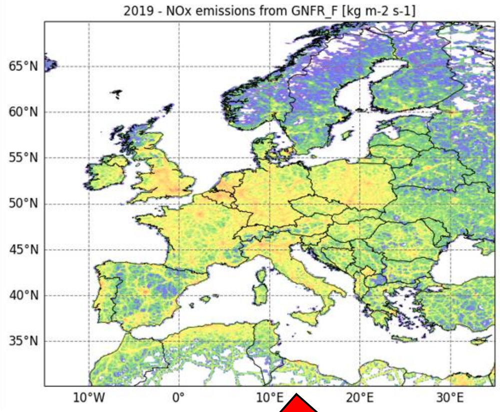
Online emissions module OEM

- 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
  - **dayofweek.nc, hourofday.nc, monthofyear.nc**: temporal profiles per species, sector and country
  - **hourofyear.nc**: alternative temporal profiles
  - **vertical_profiles.nc**: vertical profiles per species and sector

emiproc emission pre-processor

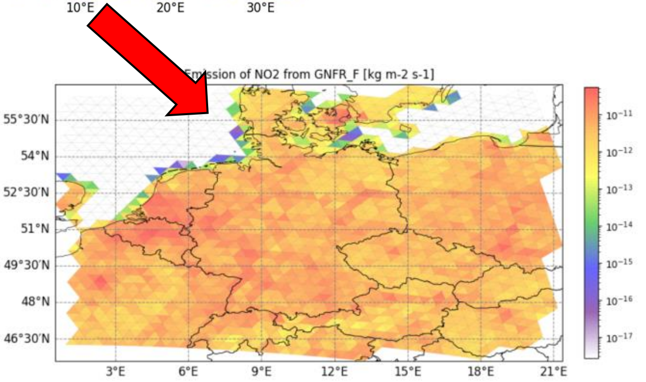
- Open source python package (https://github.com/C2SM-RCM/emiproc)
- Features:
    - Inventories: TNO, EDGAR, GFAS, ..
    - Models: ICON, COSMO, (WRF), ..
    - Conservative remapping
    - Merging of inventories
    - Source-sector specific temporal and vertical emission profiles
    - Speciation of NO_x and VOC
    - Creates all inputs files required by OEM



TNO-CAMS regular grid

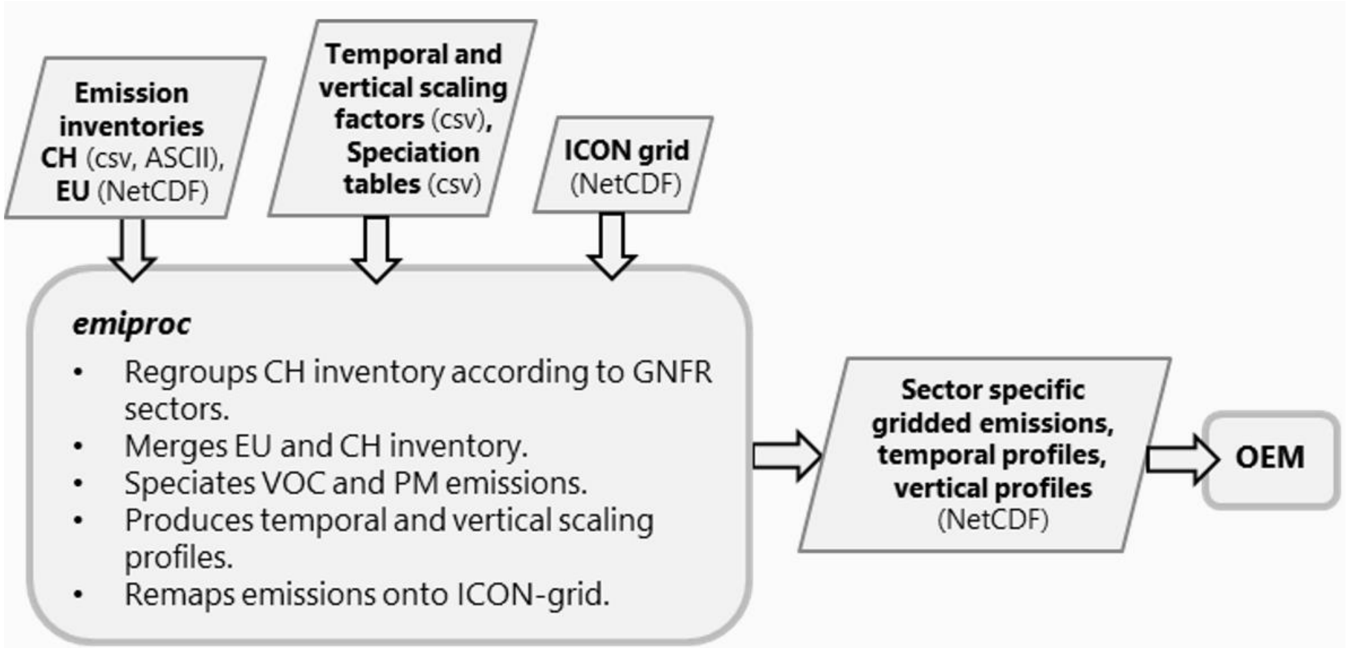
Traffic NO_x emissions

ICON triangular grid. Traffic NO_2 emissions



emiproc emission pre-processor

Example for preparing emissions for simulation over Switzerland



64

Using OEM tracers in ICON-ART

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'
/
```

Using OEM tracers in ICON-ART

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_type = emis: makes NH3 an OEM emis. tracer

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

Emission categories contributing to NH3

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
- Quite 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)

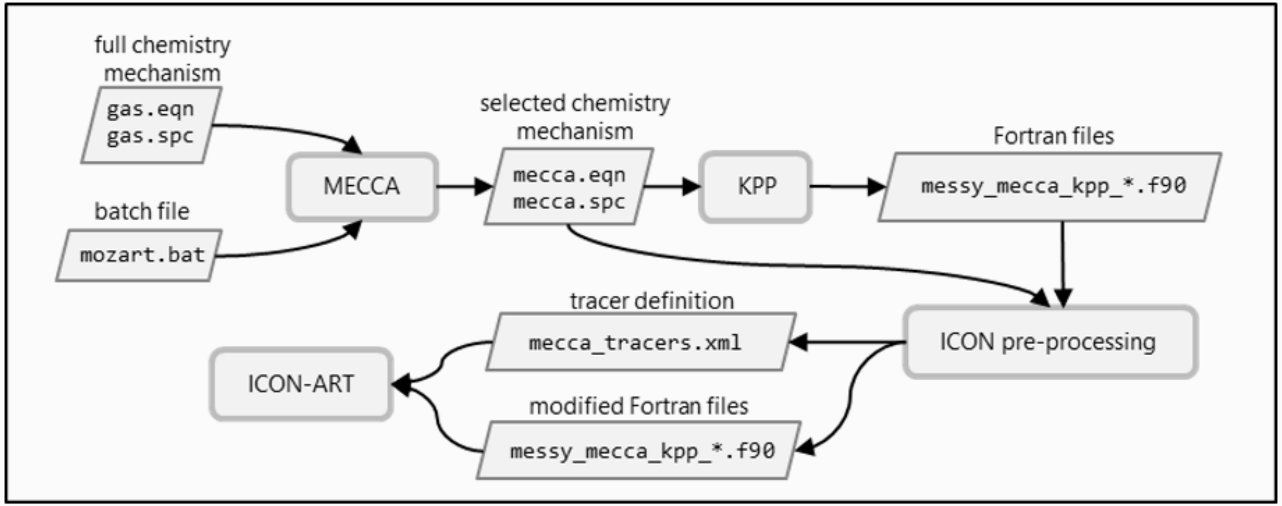
L. K. Emmons[1], S. Walters[1], P. G. Hess[1,*], J.-F. Lamarque[1], G. G. Pfister[1], D. Fillmore[1,**], C. Granier[2,3], A. Guenther[1], D. Kinnison[1], T. Laepple[1,***], J. Orlando[1], X. Tie[1], G. Tyndall[1], C. Wiedinmyer[1], S. L. Baughcum[4], and S. Kloster[5,*]

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
```


68

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)

69

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>
<transport type="char">hadv52aero</transport>
<number type="int"> 45 </number>
<unit type="char">mol mol-1</unit>
<iconv type="int">1</iconv>
<iturb type="int">1</iturb>
<c_solve type="char">mecca</c_solve>
<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>
```


70

Using MECCA tracers in ICON-ART

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

71

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

ICON-ART

EXP 2: Air quality

Corinna Keller (EMPA)

Empa
Materials Science and Technology

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

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

DKRZ KIT Empa natESM

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

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

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'
/
```


77

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 4: Secondary aerosols

Ali Hoshyaripour (KIT), Julia Bruckert (KIT)

Empa
Materials Science and Technology

Continuity Equation for aerosols

Continuity equation for particle <u>number</u> concentration

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

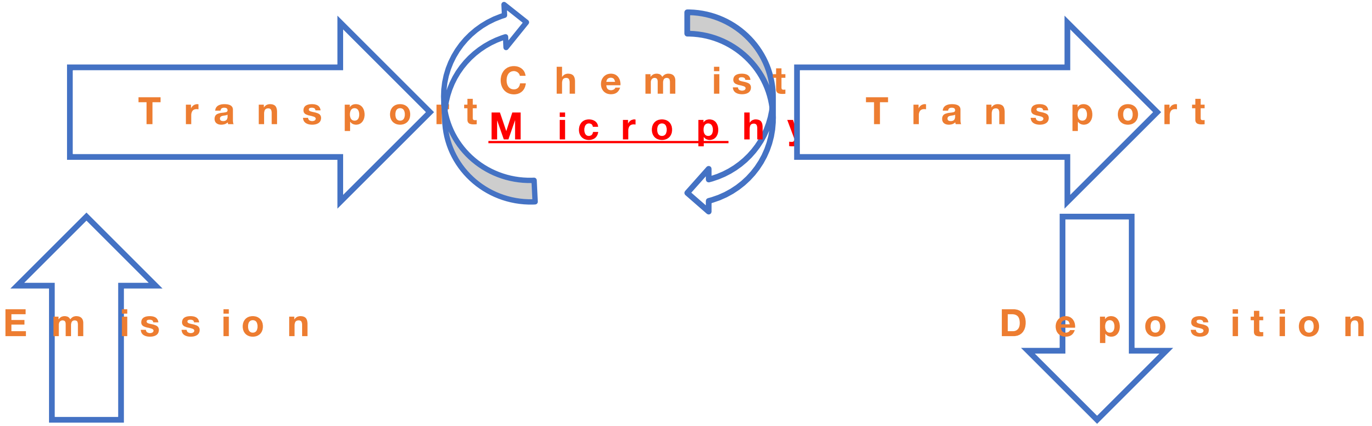
Continuity equation for particle <u>volume</u> concentration

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

Source: Jacobson 2005

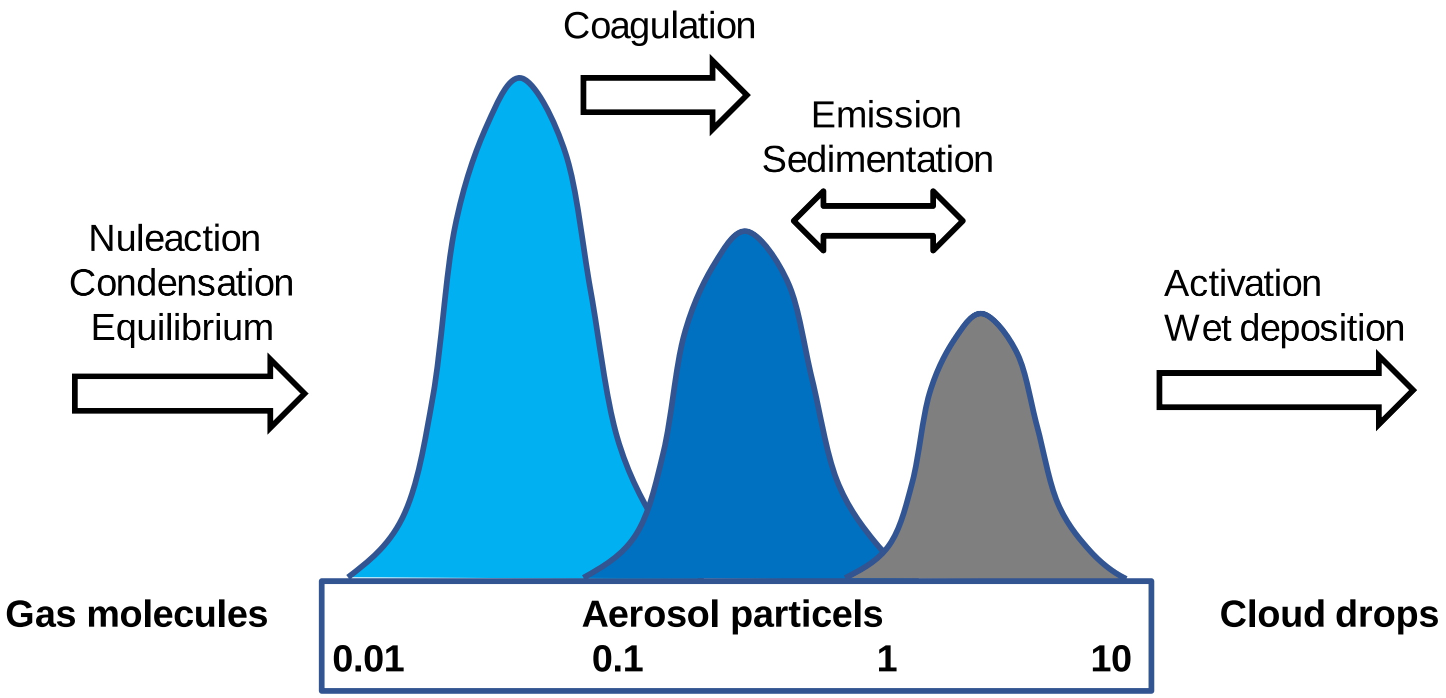
Aerosol microphysics

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



80

Aerosol microphysical processes



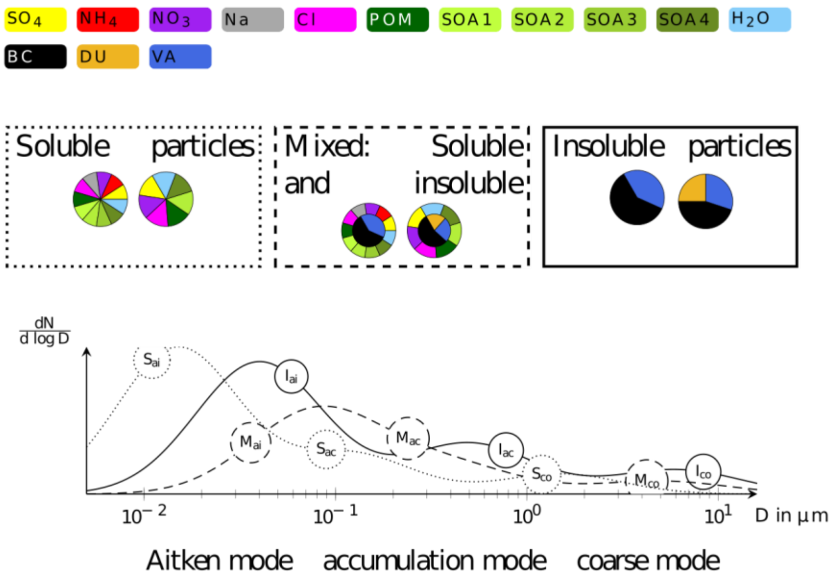
Aerosol modes and processes in ART

ICON-ART

- Simulating the evolution of aerosol physicochemical properties due to aerosol microphysics at an affordable computational cost.
- The modal approach is a promising compromise.
- Prognostic equations for the number density and the mass concentration (only microphysics terms):

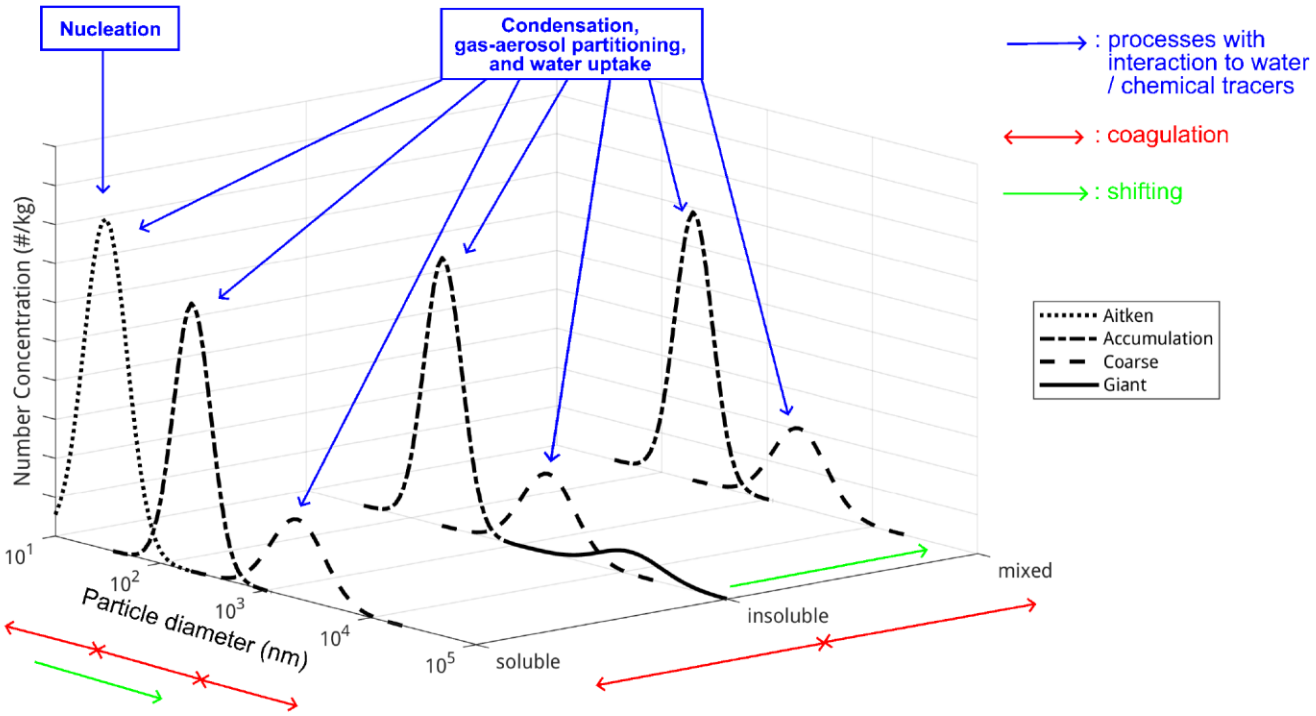
$$\frac{\partial}{\partial t} M_{0,i} = -\mathrm{Ca}_{0,ii} - \mathrm{Ca}_{0,ij} + \mathrm{Nu}_0,$$

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



Muser, Hoshyaripour et al. 2020

Aerosol modes and processes in ART



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

EXP 3: Secondary aerosols

Julia Bruckert (KIT)

Empa
Materials Science and Technology

Emission and aerosol aging after the Raikoke 2019 eruption

Objectives:

How to use the point source for emissions

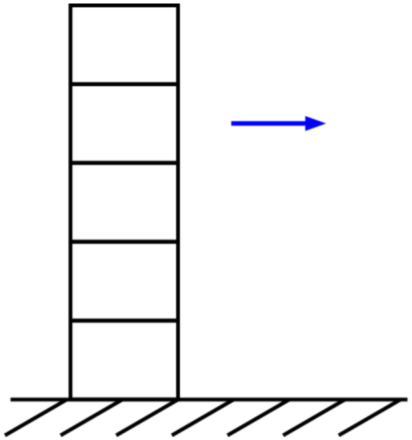
How to activate aerosol dynamical processes (nucleation, condensation, coagulation)

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

Point Source

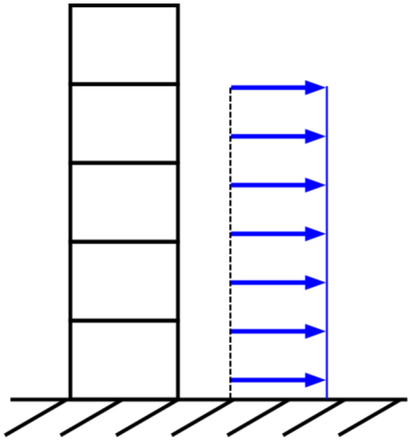
(A)

- **Emission in single point**



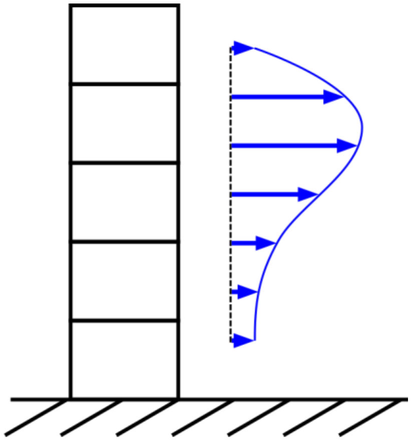
(B)

- **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([zstar])</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

```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	soluble	/	/

- 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)

96