Karlsruhe Institute of Technology

Max-Planck-Institut für Meteorologie

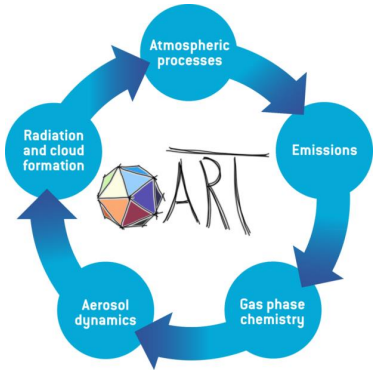
DKRZ DEUTSCHES KLIMARECHENZENTRUM

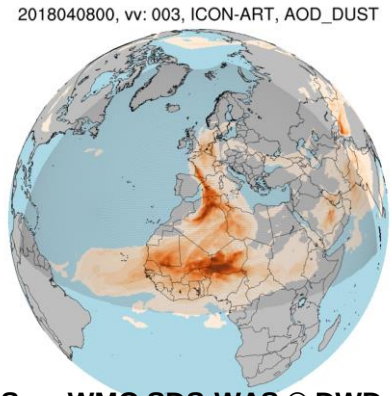
Deutscher Wetterdienst
Wetter und Klima aus einer Hand

DWD

ICON-ART

Training Course 2023





See: WMO SDS-WAS © DWD

Instructors

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Group leader, IMK-TRO, KIT

- Julia Bruckert

Research Associate, IMK-TRO, KIT

- Lisa Muth

Research Associate, IMK-TRO, KIT

Please note that you can use web browser (preferably Chrome) or PC client or Apps to join this meeting.

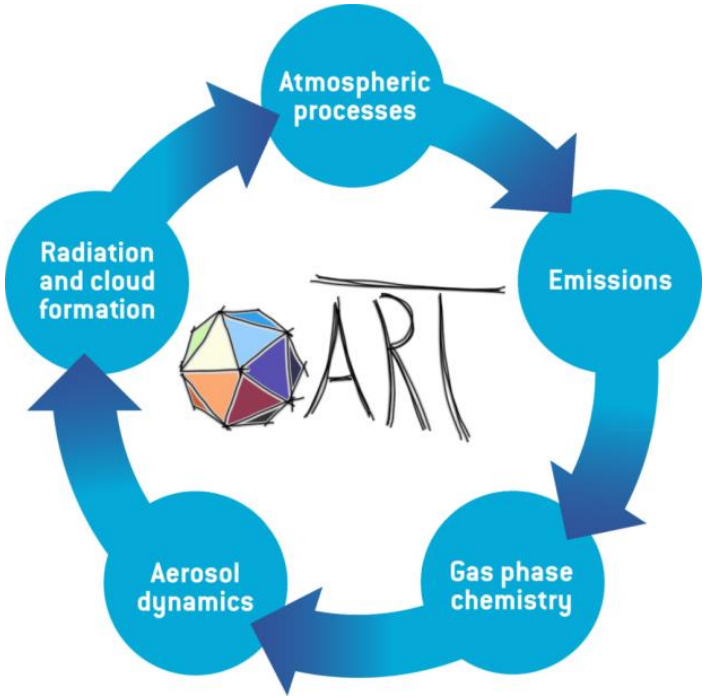
During the course, you will get an account to access the DKRZ supercomputer Levante. Please ONLY use this account, regardless whether you have another account on Levante.

You will need a laptop or PC with Linux terminal for login and the exercises.

Part 1: Introduction to the ICON-ART – technical aspects

Ali Hoshyaripour and the IMK-TRO ARTists

ICON-ART



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

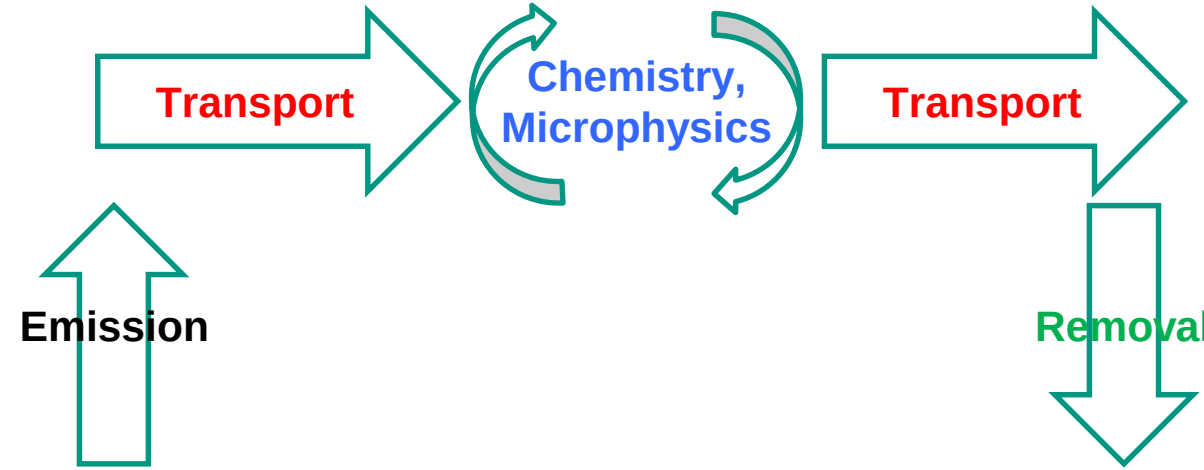
Rieger et al. (2015), Weimer et al. (2017)

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

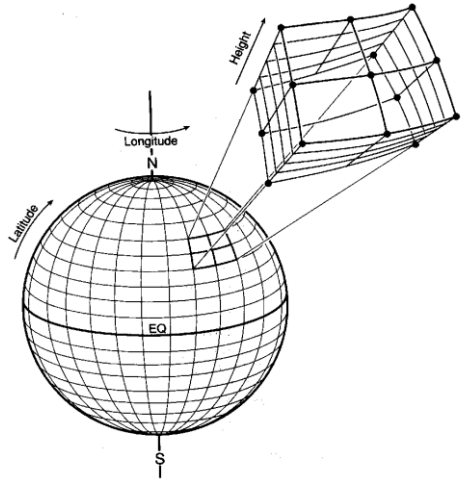
Atmospheric composition models

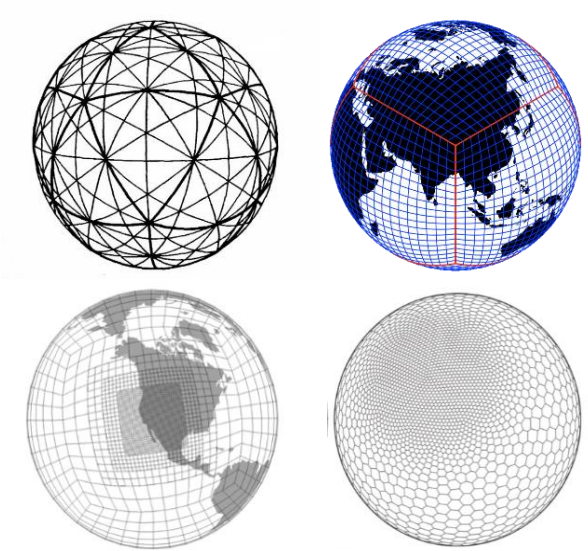


$$\frac{\partial \rho_i}{\partial t} = \left[\frac{\partial \rho_i}{\partial t}\right]_{adv} + \left[\frac{\partial \rho_i}{\partial t}\right]_{mix} + \left[\frac{\partial \rho_i}{\partial t}\right]_{conv} + \left[\frac{\partial \rho_i}{\partial t}\right]_{scav} + \left[\frac{\partial \rho_i}{\partial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

Modelling atmospheric composition

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





Source: D. Jacob

Emissions treated in ART

Continuity Equation for gases

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

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

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

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}).

Chemistry

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

- 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 ordinary differential equations, one for each species in the mechanism.

Source: Brasseur and Jacob 2017

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)

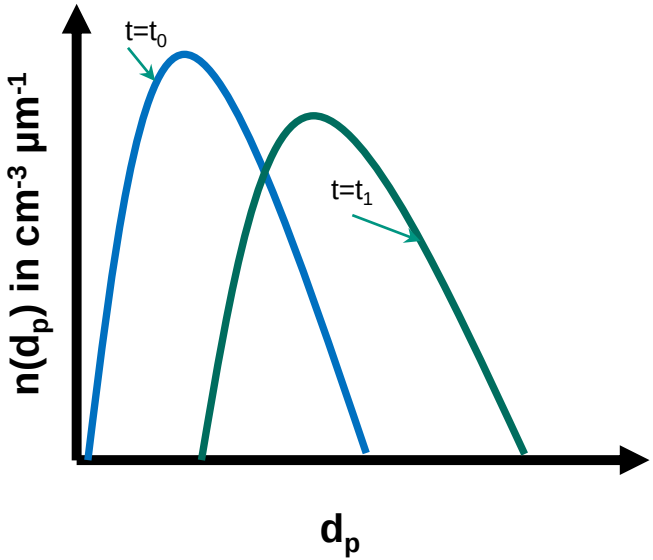
We only update this part

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.



Continuity Equation for aerosols number conc.

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

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.

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

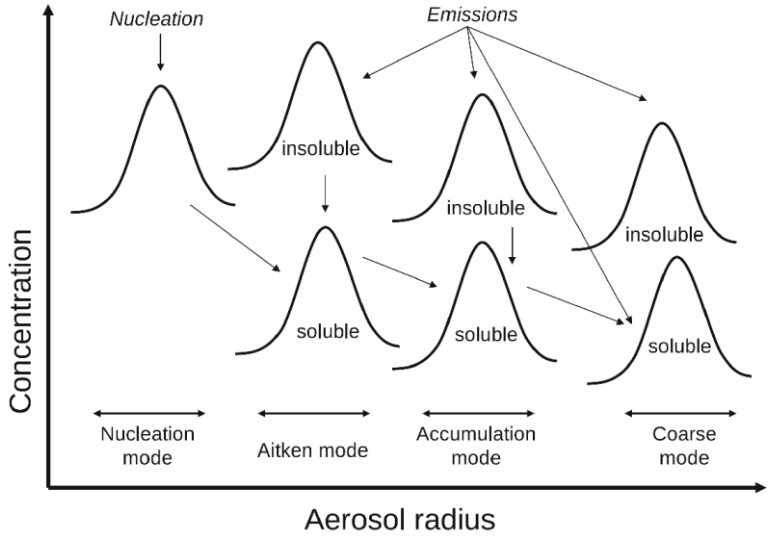
$$+ R_{emisv} + R_{depv} + R_{sedv} + R_{washv} + R_{nucv} + R_{coagv}$$

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

$R_{c/ev}$ = 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

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

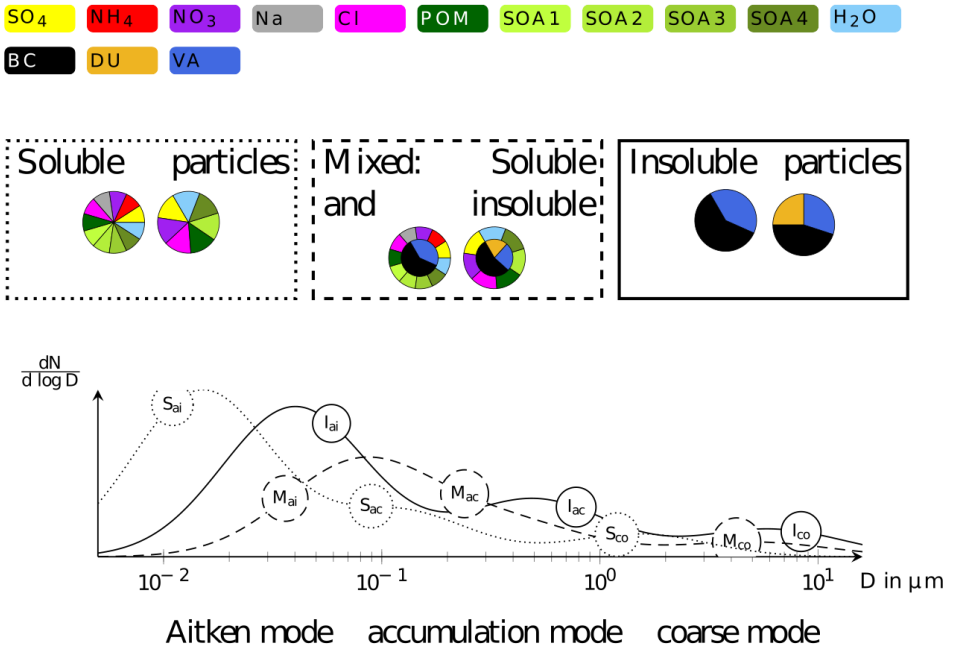
Aerosol Dynamics (AERODYN) in ICON-ART

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

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

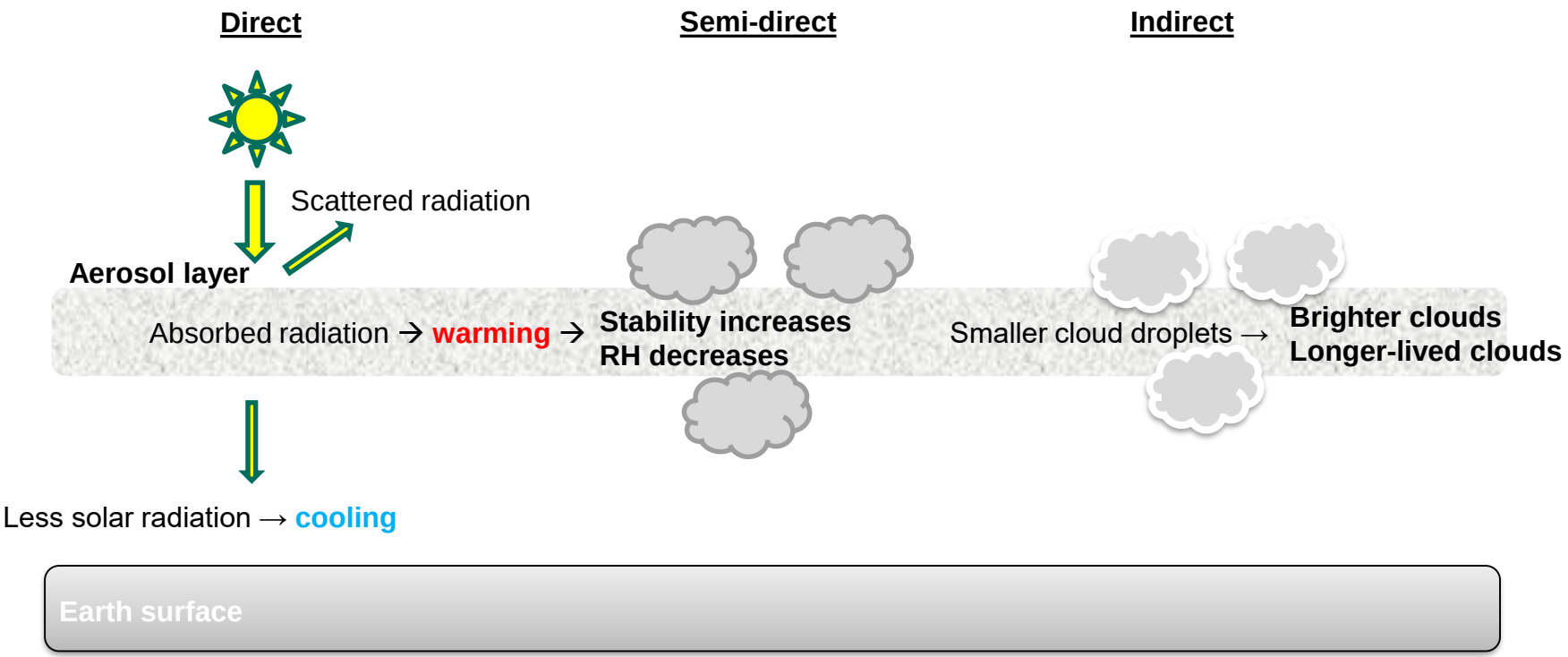
$$\frac{\partial}{\partial t} M_{3,i} = -\mathrm{Ca}_{3,ij} + \mathrm{Co}_{3,i} + \mathrm{Nu}_3,$$

- the ISORROPIA II for gas–aerosol partitioning



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

Aerosol effects on the atmosphere



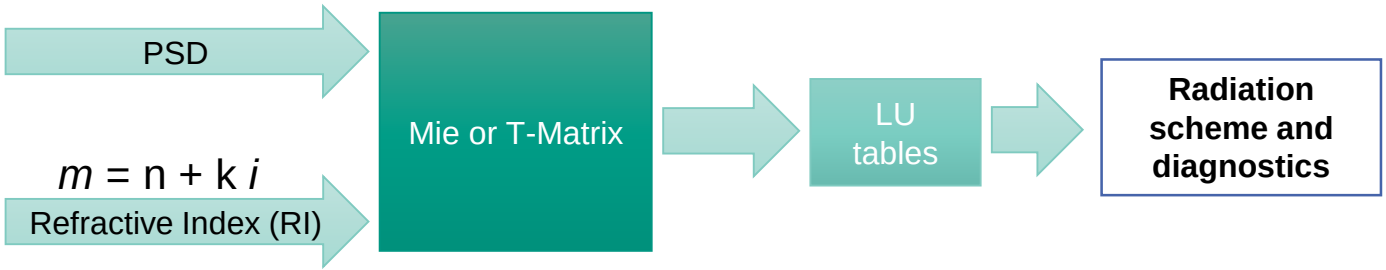
Aerosol optical properties in ICON-ART

- 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*



What do I need for an ICON-ART simulation

- Everything that you need for ICON simulation (grid, external parameters, initial conditions etc)
  - **ART namelist and run_nml switches**
  - **Input data:** provide the input parameters/values that are required for a simulation → Depend on application
  - **XML files:** provide additional information about the ART parameters → Depend on application (see 2nd part)

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

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'
```

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), 5 (from file)	IGX
Aerosol	iart_init_aero	0 (cold start), 5 (from file)	IAE

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

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.

ART - Directories

- **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

Part 2: Introduction to XML files

Julia Bruckert and the IMK-TRO ARTists

XML Files

- Extensible Markup Language (XML)
- Human- **and** machine-readable format

```
<modes>
  <aerosol id="asha">
    <kind type="char">2mom</kind>
    <d_gn type="real">1.190E-6</d_gn>
    <sigma_g type="real">1.410E+0</sigma_g>
    <rho type="real">2.600E+3</rho>
  </aerosol>
</modes>
```

Why do we need XML files?

ART – Tracers

Sea Salt
Mineral Dust
Volcanic Ash
Chemical Species
…

Different for every run

→ **XML files**

Xml files

1. **Chemtracer for chemical species and passive tracers**
2. **MECCA chemistry tracer→ will be automatically generated**

3. **Aerosol tracers**
4. **Aerosol modes**
5. **Coagulation**

6. Chemistry emission
7. **Aerosol emission**
8. **Point source**

9. Diagnostics
10. Mie, Meng

See examples in icon-kit/externals/art/runctrl_examples/xml_ctrl/

tracers_chemtracer.xml

```
<tracers>
   <chemtracer id="testtr" full="FALSE" chemtr="TRUE" >
      <tag001 type="char">chemtr</tag001>
      <mol_weight type="real">1.190E-6</mol_weight>
      <transport type=„char">stdchem</transport>
      <unit type="char">mol mol-1</unit>
      <c_solve type="char">passive</c_solve>
   </chemtracer>
   <chemtracer id="TRCH4" full="FALSE" chemtr="TRUE" >
..
   </chemtracer>
</tracers>
```

Passive tracer: no chemical depletion

tracers_chemtracer.xml

```
<tracers>
   <chemtracer id="testtr" full="FALSE" chemtr="TRUE" >
..
   </chemtracer>
   <chemtracer id="TRCH4" full="FALSE" chemtr="TRUE" >
      <tag001 type="char">chemtr</tag001>
      <mol_weight type="real">1.190E-6</mol_weight>
      <lifetime type="real">1.410E+0</lifetime>
      <transport type=„char">stdchem</transport>
      <unit type="char">mol mol-1</unit>
      <c_solve type="char">OH</c_solve>
      <products type="char">TRCO</products>
   </chemtracer>
</tracers>
```

Depletion by OH (OH-concentration is parameterized)

tracers_mecca.xml

Will be generated automatically (see MECCA-Experiment on Friday)!

```
<tracers checksum="ba2cb9611f43db61cc172b2d9d1e30f9">
  <meccatracer id="O2_1D" full="TRUE" chemtr="FALSE">
    <tag001 type="char">full</tag001>
    <mol_weight type="real">32.0E-3</mol_weight>
    <transport type="char">stdaero</transport>
    <number type="int"> 1 </number>
    <iconv type="int">1</iconv>
    <iturb type="int">1</iturb>
    <init_mode type="int">0</init_mode>
    <init_name type="char">O2_1D</init_name>
    <unit type="char">mol mol-1</unit>
    <c_solve type="char">mecca</c_solve>
  </meccatracer>
...
</tracers>
```

Do not change the order of tracers in the MECCA xml !!

Tags in chemtracer and mecca xml

Bold: always required

tag	type	options	description
c_solve	character	param, lt, cold, OH, linoz, simnoy, passive	solving mechanism/strategy
emissions		anthropogenic, biogenic, biomassBurning	usage see in tracers_chemtracer_amip.xml*
htop_proc	real	in m	top height for processes
iconv	integer	0 (off), 1 (on)	transport by convection (default=1)
initc	character	file	initialize from Input file
init_mode	integer	0 (off), 1 (on)	initialize tracer
init_name	character		name of tracer in initialization file
iturb	integer	0 (off), 1 (on)	transport by turbulence (default=1)
latbc	character	file	read data for LBC
lfeedback	integer	0 (off), 1 (on)	child → parent feedback in nested simulations (default=0)
lifetime	real	in s	value for lifetime
mol_weight	real	in kg/mol	value for molar weight
products	character	name of tracer	name of resulting tracer after depletion
tag001,...	character		name of tag to be added to tracer name
transport	character	stdaero, stdchem, ..., off	choice of transport template
unit	character	e.g., mol mol-1	unit of tracer

* in icon-kit/externals/art/runctrl_examples/xml_ctrl/

tracers_aerosol.xml

```
<tracers>
  <aerosol id="nmb">
    <moment type="int">0</moment>
    <mode type="char">insol_acc,insol_coa,giant</mode>
    <unit type="char">kg-1</unit>
    <transport type="char">stdaero</transport>
  </aerosol>
  <aerosol id="ash">
    <moment type="int">3</moment>
    <mode type="char">insol_acc,insol_coa,giant</mode>
    <sol type="real">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">stdaero</transport>
  </aerosol>
</tracers>
```

Tags in aerotracer xml

Bold: always required

tag	type	options	description
htop_proc	real	in m	top height for processes
initc	character	file	initialize from Input file
inucl	integer	0 (off), 1 (on)	H2SO4 nucleation for so4 tracer (default=1); 1 for so4_sol_ait, 0 for other so4 tracer)
label	character	e.g., dusta	allows to name tracers individually
latbc	character	file	read data for LBC
lfeedback	integer	0 (off), 1 (on)	child → parent feedback in nested simulations (default=0)
mode	character	insol_acc, mixed_acc,..	indicates in which modes the tracer occurs
mol_weight	real	in kg/mol	value for molar weight
moment	integer	0, 3	zeroth (number) or third (mass) moment
rho	real	in g/m3	density of tracer, not needed for zeroth moment
sol	integer	0 (no), 1 (yes)	indicates whether the tracer is soluble or not
transport	character	stdaero, stdchem, ..., off	choice of transport template
unit	character	e.g., mug kg-1, kg-1	unit of tracer

Grib information in aerotracer and chemtracer xml

- productDefinitionTemplate
- constituentType
- discipline
- parameterCategory
- parameterNumber
- bitsPerValue
- typeOfDistributionFunction
- numberOfModeOfDistribution
- modeNumber
- numberOfDistributionFunctionParameters
- localInformationNumber
- scaledValueOfDistributionFunctionParameter_1
- scaleFactorOfDistributionFunctionParameter_1
- scaledValueOfDistributionFunctionParameter_2
- scaleFactorOfDistributionFunctionParameter_2

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>
```

Initialization of modes with median diameter and standard deviation
≠ emission distribution !!!

Activation of aerosol dynamical processes

Tags in modes xml

Bold: always required

tag	type	options	description
condensation	integer	0 (off), 1 (on)	condensation of H2SO4 on this mode?
d_gn	real	in m	value for the initial median diameter of the number distribution
dissfac_mean	real		dissociation factor (needed with ikoehler=1)
icoag	integer	0 (off), 1 (on)	mode involved in coagulation? If 1 for any mode, then provide coagulate.xml
ikoehler	integer	0 (off), 1 (on)	Activation via Köhler theory (warm clouds), needs dissfac_mean tag
kind	character	1mom or 2mom	1-moment or 2-moment description of distribution
sigma_g	real		standard deviation of the distribution
shift2larger	character	e.g., sol_acc	Name of larger mode to be shifted to, when diameter threshold (shift_diam) exceeded
shift2mixed	character	e.g., mixed_acc	Name of mixed mode to be shifted to, when soluble mass threshold of 5% exceeded
shift_diam	real	in m	diameter threshold for shift2larger

coagulate.xml

```
<coagulate>
   <smallmode id="insol_acc">
      <nmodes type="int">4</nmodes>
      <bigmode id="insol_acc" type="char">insol_acc</bigmode>
      <bigmode id="mixed_acc" type="char">mixed_acc</bigmode>
      <bigmode id="insol_coa" type="char">insol_coa</bigmode>
      <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
   </smallmode>
…
   <smallmode id="insol_coa">
      <nmodes type="int">2</nmodes>
      <bigmode id="insol_coa" type="char">insol_coa</bigmode>
      <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
   </smallmode>
</coagulate>
```

insol_acc can coagulate with 4 partner modes

Coagulation of insol_acc with mixed_acc forms mixed_acc

aero_emiss.xml (emission mapping to modes)

```
<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">1.5e-6</d_g3_1>
    <sigma_g_1 type="real">1.7</sigma_g_1>
    <d_g0_2 type="real">3.454e-6</d_g0_2>
    <d_g3_2 type="real">6.7e-6</d_g3_2>
    <sigma_g_2 type="real">1.6</sigma_g_2>
    <d_g0_3 type="real">8.672e-6</d_g0_3>
    <d_g3_3 type="real">1.42e-6</d_g3_3>
    <sigma_g_3 type="real">1.5</sigma_g_3>
    <rho type="real">2.65e3</rho>
    <substances type="char">dust</substances>
  </routine>
</emiss>
```

Mode A

Mode B

Mode C

Median diameter number distribution

Median diameter mass distribution

Standard deviation

Tags in aerosol emission xml

Bold:
always required

routine options: volc, volc_fplume, dust, biomass_burn, seas_smith, seas_monahan, seas_martensson

tag	type	options	description
nmodes	integer		number of emission modes
d_g0_*	real		median diameter of number distribution of mode * (e.g., d_g0_1, d_g0_2, d_g0_3)
d_g3_*	real		median diameter of mass distribution of mode * (e.g., d_g3_1, d_g3_2, d_g3_3)
rho	real	in kg/m3	particle density (same for all modes)
sigma_g_*	real		standard deviation of mode *
substance	character	ash, dust, na, cl, soot	emitted substance

XML files for AERODYN

${ARTDIR}/runctrl_examples/xml_ctrl/:

- **tracers_aerosol.xml**
- **modes.xml**
- **emission.xml**
- **coagulate.xml**

XML files can determine whether or not AERODYN processes are accounted for. This means, we can still have simulations of externally mixed aerosols (**no AERODYN**).

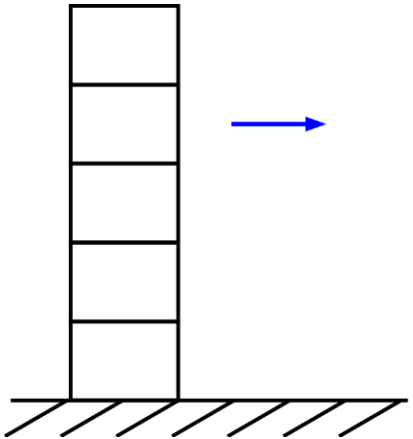
Others

- Point Source xml
- Diagnostics xml example: icon-kit/externals/art/runctrl_examples/xml_ctrl/diagnostics_aerosol_with_grib2.xml

Point Source

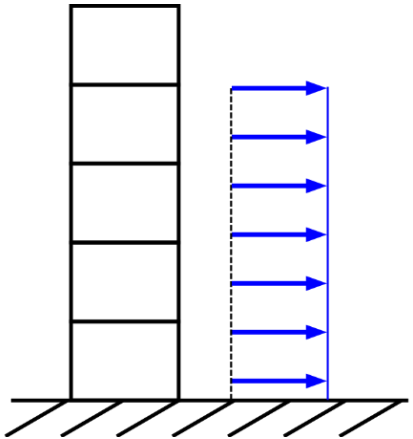
(A)

- **Emission in single point**



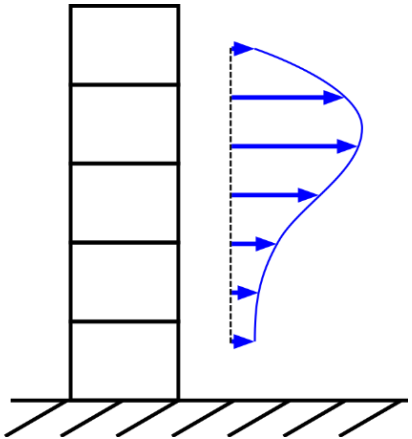
(B)

- **Emission with uniform profile**



(C)

- **Emission with user defined profile**



pntSrc.xml case (A)

```
<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)

```
<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>
```

Tags in point source xml

Bold:
always required

tag	type	options	description
dg3_emiss	real	in m	median diameter of aerosol mass distribution
emiss_profile	character		anti-derivative of emission profile
endTime	character		end time of emission (default=9999-12-31T00:00:00)
height	real	in m	emission height
height_bot	real	in m	bottom height
lat	real	in degree	latitude
lon	real	in degree	longitude
sigma_emiss	real		standard deviation of aerosol distribution
startTime	character		start time of emission (default=1582-10-15T00:00:00)
source_strength	real		emission source strength
substance	character	e.g., TRSO2	substance nme from tracer xml
unit	character	e.g., kg s-1	unit of source strength

Part 3: Configuration and Installation

Julia Bruckert and the IMK-TRO ARTists

Levante

Three different storage spaces on Levante

- Home: to store shell setup files, source codes, scripts, and important files (24GB)
- Work: project space shared between all users of a project
- Scratch: 15TB, data deleted after 2 weeks

Compile the ICON-ART Code

- **Login on Jupyterhub on Levante (login data on next slide):**
  https://jupyterhub.dkrz.de/hub/home
- **Open new terminal and go to the directory with the ICON-ART Code**

  cd icon-kit
- **Configure and compile the code in icon-kit/** :

  ./config/dkrz/levante.intel --enable-art --enable-ecrad

  make –j 8

Part 4: Exercises

Julia Bruckert and the IMK-TRO ARTists

Exercise 1
Simulation of a Volcanic Eruption

Objectives:
How to introduce a point source
How to introduce externally and internally mixed aerosols

Exercise 1.1:

- Simulation of the last Raikoke eruption in June 2019 with externally mixed aerosols
- Open Exp1-1.ipynb in ~/Volcano/ and follow the instructions
- Plot the results with the provided Python script

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

Exercise 1.2:

- Repeat the simulation of the last Raikoke eruption in June 2019 with internally mixed aerosols
- Open Exp1-2.ipynb in ~/Volcano/ and follow the instructions
- Plot the results and discuss the differences to the previous simulation

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

Exercise 2

1. **Emission and transport of mineral dust**
2. **Interactions of mineral dust with radiation**

Objectives:

How to introduce aerosol tracers and modes

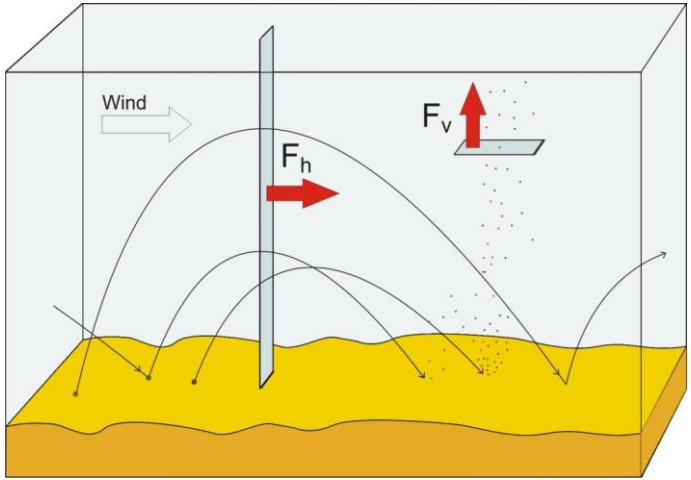
How to introduce online emissions

How to activate interactions in namelist

Mineral dust emission

iart_dust = 1

Requires external parameters. These are read from an external Soil Type dataset.



Mode	dg in µm	σ
1	1.7	1.5
2	6.7	1.6
3	14.2	1.7

Rieger et al (2015), Vogel et al. (2006)

External data for mineral dust simulation

Table 3.3.: External input parameters necessary for the mineral dust emission scheme.

Parameter	Description
fr_hcla	Fraction of soil type **Heavy Clay** in grid cell (without dimension).
fr_silc	Fraction of soil type **Silty Clay** in grid cell (without dimension).
fr_lcla	Fraction of soil type **Light Clay** in grid cell (without dimension).
fr_sicl	Fraction of soil type **Silty Clay Loam** in grid cell (without dimension).
fr_cloa	Fraction of soil type **Clay Loam** in grid cell (without dimension).
fr_silt	Fraction of soil type **Silt** in grid cell (without dimension).
fr_silo	Fraction of soil type **Silt Loam** in grid cell (without dimension).
fr_scla	Fraction of soil type **Sandy Clay** in grid cell (without dimension).
fr_loam	Fraction of soil type **Loam** in grid cell (without dimension).
fr_sclo	Fraction of soil type **Sandy Clay Loam** in grid cell (without dimension).
fr_sloa	Fraction of soil type **Sandy Loam** in grid cell (without dimension).
fr_lsan	Fraction of soil type **Loamy Sand** in grid cell (without dimension).
fr_sand	Fraction of soil type **Sand** in grid cell (without dimension).
fr_udef	Fraction of **Undefined** soil type in grid cell (without dimension).

Exercise 2.1.: Steps

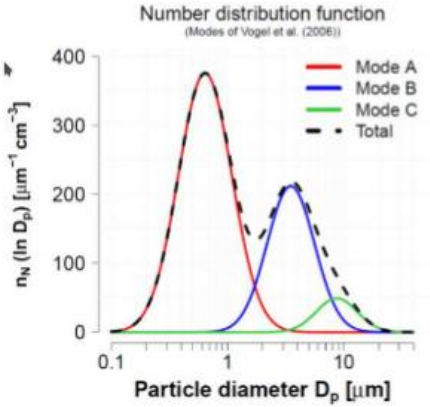
- Open Exp02.ipynb in ~/Dust/ and follow the instructions
- Plot the results with the provided Python script

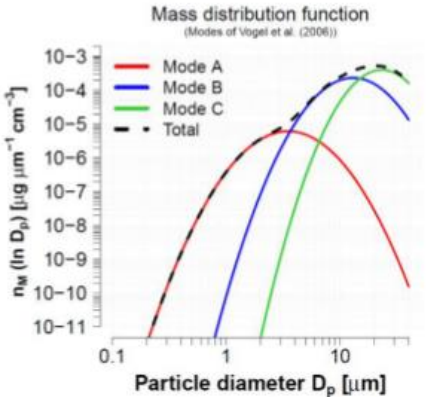
```
&art_nml
      lart_aerosol              = .TRUE.                    ! activate treatment of aerosols
      iart_dust                 = 1                         ! activate dust emission
      iart_init_aerosol         = 5                         ! Initialization from file
      cart_aerosol_xml          = '<path to tracer xml>'
      cart_modes_xml            = '<path to modes xml>'
      cart_diagnostics_xml      = '<path to diagnostics xml>'     ! necessary to write emission to output
      cart_input_folder         = '<path to external data for mineral dust and aerosol initialization file>'
/
```

aero_emiss.xml

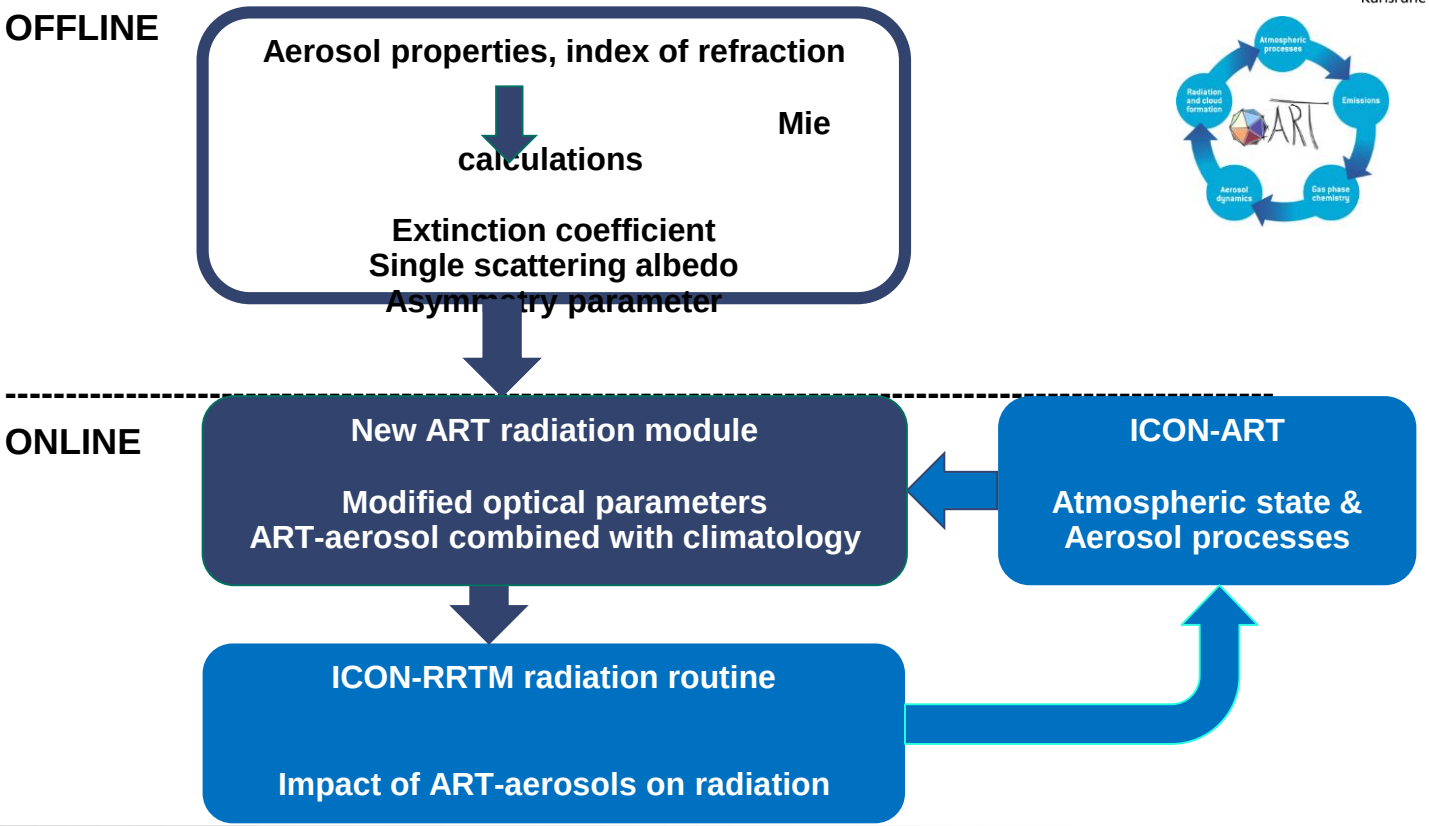
```
<emiss>
 <routine id="dust">
   <nmodes type="int">3</nmodes>
   <d_g0_1 type="real">???</d_g0_1>
   <d_g3_1 type="real">???</d_g3_1>
   <sigma_g_1 type="real">???</sigma_g_1>
   <d_g0_2 type="real">???</d_g0_2>
   <d_g3_2 type="real">???</d_g3_2>
   <sigma_g_2 type="real">???</sigma_g_2>
   <d_g0_3 type="real">???</d_g0_3>
   <d_g3_3 type="real">???</d_g3_3>
   <sigma_g_3 type="real">???</sigma_g_3>
   <rho type="real">???</rho>
   <substances type="char">dust</substances>
 </routine>
</emiss>
```

Mode	Mean diameter (µm) number distribution	Mean diameter (µm) mass distribution	Standard deviation
A	0.64	1.5	1.7
B	3.5	6.7	1.6
C	8.7	14.2	1.5





ICON-ART – Mineral dust radiative effect



Rieger et al (2017), Gasch et al. (2017)

Exercise 2.2.: Steps

- Simulation with a feedback of mineral dust concentration on radiation budget. The provided runfile is set in a way that aerosol radiation interaction is not active. In order to activate the radiation feedback, set iart_ari=1 in art_nml and irad_aero=9 in radiation_nml (change the name of the output folder first!) and repeat the simulation
- Plot the results with the provided Python script and discuss the differences

Exercise 2
Atmospheric chemistry modeling using MECCA

Objectives:
How to generate a chemical mechanism
How to simulate with chemistry

MECCA

- Module Efficiently Calculating the Chemistry of the Atmosphere
- Chemistry module that contains a comprehensive chemical mechanism and allows to create an own chemistry mechanism
- Uses the Kinetic PreProcessor (KPP) by Adrian Sandu and Rolf Sander for the numerical integration

- Detailed description is given in ~/MECCA-chemistry/caaba_3.0/mecca/kpp/doc/kpp_UserManual.pdf for KPP only and ~/MECCA-chemistry/caaba_3.0/manual/caaba_mecca_manual.pdf (chapter 7)

MECCA equation file (comprehensive mechanism)

- ~/MECCA-chemistry/caaba_3.0/mecca/gas.eqn

```
#EQUATIONS

{<G1nnn> ------------------------------ O ------------------------}

// O only (#G10nn)
<G1000>  O2   + O1D    = O3P + O2 : {%StTrG} 3.3E-11{§1.1}*EXP(55./temp); {&1945}
<G1001>  O2   + O3P {+M} = O3     : {%StTrG} 6.E-34{§1.1}*((temp/300.)**(-2.4))*cair; {&1945}
<G1002>  O3   + O1D    = 2 O2     : {%StG}   1.2E-10{§1.2}; {&&1945}
<G1003>  O3   + O3P    = 2 O2     : {%StG}   8.E-12{§1.15}*EXP(-2060./temp); {&1945}

{<G2nnn> ------------------------------ H ------------------------}{@\myhline}

// H + O (#G21nn)
<G2100>  H+ O2 {+M}  = HO2        : {%StTrG} k_3rd(temp,cair,4.4E-32,1.3,4.7E-11,0.2,0.6){§1.3}; {&1945}
<G2101>  H+ O3       = OH + O2    : {%StG}   1.4E-10{§1.1}*EXP(-470./temp); {&1945}
…
```

MECCA replacement file for small changes

- ~/MECCA-Chemistry/caaba_3.0/mecca/rpl/example.rpl

```
// here, reaction G4110 is replaced by a modified reaction:
#REPLACE <G4110>
<a> CO + OH = HO2 + CO2 : {%StTrG} 1.57E-13 + cair*3.54E-33; {&1628}
#ENDREPLACE

…

// add a new reaction:
#REPLACE <>
<G9876JD> XYZ + OH = RO2 + H2O : {%StG} 1.57E-13; {&&}
#ENDREPLACE

// to delete a reaction, specify an empty replacement:
#REPLACE <G4200>
#ENDREPLACE
…
```

MECCA batch file to create the mechanism

- ~/MECCA-Chemistry/caaba_3.0/mecca/batch/simple.bat

```
set apn                 = 0             # number of aerosol phases [0...99, default=0]
set gaseqnfile    = gas.eqn
set rplfile             =               # no replacements
set wanted              = "Tr && G && \!C && \!Cl && \!Fl && \!Br && \!I && \!Hg && \!Het"
set mcfct               = n             # Monte-Carlo factor?
set diagtracfile    =                   # diagnostic tracers?
set rxnrates            = n             # calculate accumulated reaction rates?
set tagdbl              = n             # tagging, doubling, both, none ??
set kppoption           = k             # k=kpp, 4=kp4, q=quit
set integr              = rosenbrock_posdef # integrator
set decomp              = n             # remove indirect indexing
set latex               = n             # latex list of reactions
set graphviz            = n             # graphviz plots?
set deltmp              = y             # delete temporary xmecca files?
```

Exercise 2

- Open Exp03.ipynb in ~/MECCA-chemistry
- Follow the instructions to create the mechanism and to perform an ICON-ART simulation
- Plot the results with the provided python script

Help!

99,99% of the times, code is not the problem! So if you face an error, please take the following steps (priority):

1- Look at ICON and ART documentation

2- Check (double-check!) your namelist, XML and data files

3- check icon-art.kit.edu → userguid

4- Contact us!

Appendix 2:
ART Namelist parameters

General variables

```
cart_input_folder             !< Absolute Path to ART source code

iart_init_aero           !< Initialization of aerosol species

iart_init_gas            !< Initialization of gaseous species

lart_diag_out                 !< Enable output of diagnostic fields

lart_pntSrc                   !< Enables point sources

lart_emiss_turbdiff           !< Switch if emissions should be included as surface flux
condition

cart_io_suffix           !< user given suffix instead of automatically generated grid number

                              !  in ICON-ART input filename convention:

                              !  ART_iconR<n>B<kk>-grid-<yyyy-mm-dd-hh>_<grid_suffix>.nc
```

Atmospheric Chemistry

```
lart_chem                    !< Main switch to enable chemistry

lart_chemtracer              !< Switch for parametrised chemtracers

lart_mecca                   !< Switch for MECCA chemistry

lart_psc                     !< Switch for computation of PSCs

cart_vortex_init_date    !< Date of vortex initialization

cheminit_file(max_dom)   !< Path to chemical initialization file

cart_cheminit_coord          !< Path to chemical initialization coordinate file

cart_cheminit_type           !< Type of chemical initialization coordinate file
```

Paths and filenames of XML configuration

```
cart_chemtracer_xml          !< Path to XML file for parametrised chemtracers

cart_mecca_xml               !< Path to XML file for MECCA tracers

cart_aerosol_xml             !< Path to XML file for aerosol tracers

cart_modes_xml               !< Path to XML file for modes

cart_pntSrc_xml              !< Path to XML file for point sources

cart_diagnostics_xml         !< Path to XML file for aerosol diagnostics (GRIB2 meta
data)

cart_emiss_xml_file          !< path and file name of the xml files for emission metadata

cart_ext_data_xml            !< Path to XML file for metadata of datasets

                             !  that can prescribe tracers
```

Atmospheric Aerosol

```
lart_aerosol                !< Main switch for the treatment of atmospheric aerosol
iart_seasalt                !< Treatment of sea salt aerosol,
iart_dust                   !< Treatment of mineral dust aerosol
iart_anthro                 !< Treatment of anthropogenic aerosol
iart_fire                   !< Treatment of wildfire aerosol
iart_volcano                !< Treatment of volcanic ash aerosol
iart_nonsph                 !< Treatment of nonspherical particles
iart_pollen                 !< Treatment of pollen
iart_radioact               !< Treatment of radioactive particles
cart_volcano_file           !< Absolute path + filename of input file for volcanoes
cart_radioact_file          !< Absolute path + filename of input file for radioactive
```

Feedback processes

```
iart_aci_warm                !< Nucleation of aerosol to cloud droplets

iart_aci_cold                !< Nucleation of aerosol to cloud ice

iart_ari                     !< Direct interaction of aerosol with radiation
```

References

- ICON tutorial 2019 https://code.mpimet.mpg.de/attachments/download/19568/ICON_tutorial_2019.pdf
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Karlsruhe Institute of Technology

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DKRZ DEUTSCHES KLIMARECHENZENTRUM

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

How to use AERODYN?

Aerodyn - Tracers XML

```
<tracers>
  <aerosol id="nmb">
    <moment type="int">0</moment>
    <mode type="char">insol_acc,insol_coa,sol_acc,sol_coa,mixed_acc,mixed_coa,giant</mode>
    <unit type="char">kg-1</unit>
    <transport type="char">stdaero</transport>
  </aerosol>
  <aerosol id="dust">
    <moment type="int">3</moment>
    <mode type="char">insol_acc,insol_coa,mixed_acc,mixed_coa</mode>
    <sol type="real">1.0</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">stdaero</transport>
  </aerosol>
```

```
  <aerosol id="na">
    <moment type="int">3</moment>
    <mode type="char">sol_acc,sol_coa,mixed_acc,mixed_coa</mode>
    <sol type="real">1.</sol>
    <mol_weight type="real">22.9898E-3</mol_weight>
    <rho type="real">2.2E+3</rho>
    <unit type="char">mug kg-1</unit>
    <transport type="char">stdaero</transport>
  </aerosol>
  <aerosol id="cl">
    <moment type="int">3</moment>
    <mode type="char">sol_acc,sol_coa,mixed_acc,mixed_coa</mode>
    <sol type="real">1.</sol>
    <mol_weight type="real">35.453E-3</mol_weight>
    <rho type="real">2.2E+3</rho>
    <unit type="char">mug kg-1</unit>
    <transport type="char">stdaero</transport>
  </aerosol>
  <aerosol id="seas">
    <moment type="int">3</moment>
    <mode type="char">giant</mode>
    <sol type="real">1.0</sol>
    <mol_weight type="real">58.44E-3</mol_weight>
    <rho type="real">2.2E+3</rho>
    <unit type="char">mug kg-1</unit>
    <transport type="char">stdaero</transport>
  </aerosol>
<tracers>
```

Aerodyn - Modes XML

```
<modes>
  <aerosol id="sol_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">1</icoag>
  </aerosol>
  <aerosol id="insol_acc">
                <kind type="char">2mom</kind>
                <d_gn type="real">6.00E-7</d_gn>
                <sigma_g type="real">1.700E+0</sigma_g>
                <condensation type="int">0</condensation>
                <shift2mixed type="char">mixed_acc</shift2mixed>
                <icoag type="int">1</icoag>
  </aerosol>
  <aerosol id="mixed_acc">
                <kind type="char">2mom</kind>
                <d_gn type="real">6.00E-7</d_gn>
                <sigma_g type="real">1.700E+0</sigma_g>
                <condensation type="int">0</condensation>
                <icoag type="int">1</icoag>
  </aerosol>
  <aerosol id="sol_coa">
                <kind type="char">2mom</kind>
                <d_gn type="real">2.0E-6</d_gn>
                <sigma_g type="real">2.2</sigma_g>
                <condensation type="int">0</condensation>
                <icoag type="int">1</icoag>
  </aerosol>
  <aerosol id="insol_coa">
                <kind type="char">2mom</kind>
                <d_gn type="real">2.0E-6</d_gn>
                <sigma_g type="real">2.2</sigma_g>
                <condensation type="int">0</condensation>
                <shift2mixed type="char">mixed_coa</shift2mixed>
                <icoag type="int">1</icoag>
  </aerosol>
  <aerosol id="mixed_coa">
                <kind type="char">2mom</kind>
                <d_gn type="real">2.0E-6</d_gn>
                <sigma_g type="real">2.2</sigma_g>
                <condensation type="int">0</condensation>
                <icoag type="int">1</icoag>
  </aerosol>
  <aerosol id="giant">
                <kind type="char">2mom</kind>
                <d_gn type="real">1.200E-5</d_gn>
                <sigma_g type="real">2.0</sigma_g>
                <condensation type="int">0</condensation>
                <icoag type="int">0</icoag>
  </aerosol>
</modes>
```

Aerodyn - Emissions XML

Automated mapping to mode

```
<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>
    <d_g0_2 type="real">3.454E-6</d_g0_2>
    <d_g3_2 type="real">6.700E-6</d_g3_2>
    <sigma_g_2 type="real">1.600E+0</sigma_g_2>
    <d_g0_3 type="real">8.672E-6</d_g0_3>
    <d_g3_3 type="real">1.420E-5</d_g3_3>
    <sigma_g_3 type="real">1.500E+0</sigma_g_3>
    <rho type="real">2.650E3</rho>
    <substances type="char">dust</substances>
  </routine>
  <routine id="seas_martensson">
    <nmodes type="int">1</nmodes>
    <d_g0_1 type="real">0.200E-6</d_g0_1>
    <d_g3_1 type="real">0.690E-6</d_g3_1>
    <sigma_g_1 type="real">1.900E+0</sigma_g_1>
    <rho type="real">2.2E3</rho>
    <substances type="char">na,cl</substances>
  </routine>
  <routine id="seas_monahan">
    <nmodes type="int">1</nmodes>
    <d_g0_1 type="real">2.000E-6</d_g0_1>
    <d_g3_1 type="real">8.500E-6</d_g3_1>
    <sigma_g_1 type="real">2.000E+0</sigma_g_1>
    <rho type="real">2.2E3</rho>
    <substances type="char">na,cl</substances>
  </routine>
  <routine id="seas_smith">
    <nmodes type="int">1</nmodes>
    <d_g0_1 type="real">1.200E-5</d_g0_1>
    <d_g3_1 type="real">2.793E-5</d_g3_1>
    <sigma_g_1 type="real">1.700E+0</sigma_g_1>
    <rho type="real">2.2E3</rho>
    <substances type="char">seas</substances>
  </routine>
</emiss>
```

Aerodyn - Coagulate XML

```
<coagulate>
  <smallmode id="sol_acc">
    <nmodes type="int">6</nmodes>
    <bigmode id="sol_acc" type="char">sol_acc</bigmode>
    <bigmode id="insol_acc" type="char">mixed_acc</bigmode>
    <bigmode id="mixed_acc" type="char">mixed_acc</bigmode>
    <bigmode id="sol_coa" type="char">sol_coa</bigmode>
    <bigmode id="insol_coa" type="char">mixed_coa</bigmode>
    <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
  </smallmode>
  <smallmode id="insol_acc">
    <nmodes type="int">5</nmodes>
    <bigmode id="insol_acc" type="char">insol_acc</bigmode>
    <bigmode id="mixed_acc" type="char">mixed_acc</bigmode>
    <bigmode id="sol_coa" type="char">mixed_coa</bigmode>
    <bigmode id="insol_coa" type="char">insol_coa</bigmode>
    <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
  </smallmode>
  <smallmode id="mixed_acc">
    <nmodes type="int">4</nmodes>
    <bigmode id="mixed_acc" type="char">mixed_acc</bigmode>
    <bigmode id="sol_coa" type="char">mixed_coa</bigmode>
    <bigmode id="insol_coa" type="char">mixed_coa</bigmode>
    <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
  </smallmode>
  <smallmode id="sol_coa">
    <nmodes type="int">3</nmodes>
    <bigmode id="sol_coa" type="char">sol_coa</bigmode>
    <bigmode id="insol_coa" type="char">mixed_coa</bigmode>
    <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
  </smallmode>
  <smallmode id="insol_coa">
    <nmodes type="int">2</nmodes>
    <bigmode id="insol_coa" type="char">insol_coa</bigmode>
    <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
  </smallmode>
  <smallmode id="mixed_coa">
    <nmodes type="int">1</nmodes>
    <bigmode id="mixed_coa" type="char">mixed_coa</bigmode>
  </smallmode>
</coagulate>
```

Without aerosol microphysics - Tracers XML

```
<tracers>
  <aerosol id="dusta">
    <moment type="int">3</moment>
    <mode type="char">dusta</mode>
    <label type="char">dusta</label>
    <sol type="real">1.0</sol>
    <mol_weight type="real">50.00E-3</mol_weight>
    <rho type="real">2.650E3</rho>
    <unit type="char">mug kg-1</unit>
  </aerosol>
  <aerosol id="dusta0">
    <moment type="int">0</moment>
    <mode type="char">dusta</mode>
    <sol type="real">1.0</sol>
    <mol_weight type="real">50.00E-3</mol_weight>
    <rho type="real">2.650E3</rho>
    <unit type="char">kg-1</unit>
  </aerosol>
  …
```

Without aerosol microphysics - Modes XML

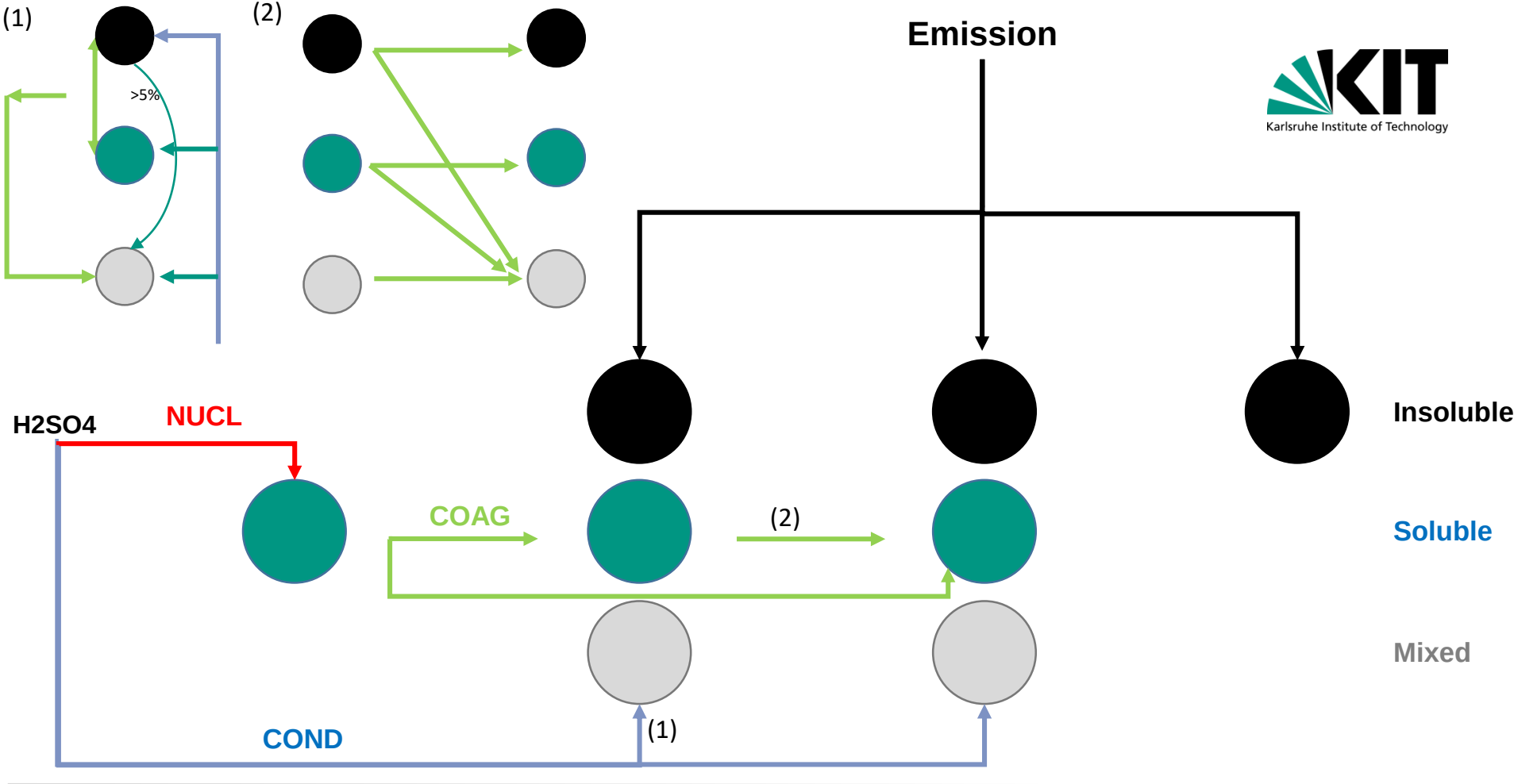
```
<modes>
  <aerosol id="dusta">
    <kind    type="char">2mom</kind>
    <d_gn    type="real">6.445E-7</d_gn>
    <d_gm    type="real">1.500E-6</d_gm>
    <sigma_g type="real">1.700E+0</sigma_g>
    <rho     type="real">2.650E+3</rho>
    <condensation type="int">0</condensation>
    <icoag type="int">0</icoag>
  </aerosol>
  <aerosol id="dustb">
    <kind    type="char">2mom</kind>
    <d_gn    type="real">3.454E-6</d_gn>
    <d_gm    type="real">6.700E-6</d_gm>
    <sigma_g type="real">1.600E+0</sigma_g>
    <rho     type="real">2.650E+3</rho>
    <condensation type="int">0</condensation>
    <icoag type="int">0</icoag>
  </aerosol>
  <aerosol id="dustc">
    <kind    type="char">2mom</kind>
    <d_gn    type="real">8.672E-6</d_gn>
    <d_gm    type="real">1.420E-5</d_gm>
    <sigma_g type="real">1.500E+0</sigma_g>
    <rho     type="real">2.650E+3</rho>
    <condensation type="int">0</condensation>
    <icoag type="int">0</icoag>
  </aerosol>
</modes>
```

Without aerosol microphysics - Emissions 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>
    <d_g0_2 type="real">3.454E-6</d_g0_2>
    <d_g3_2 type="real">6.700E-6</d_g3_2>
    <sigma_g_2 type="real">1.600E+0</sigma_g_2>
    <d_g0_3 type="real">8.672E-6</d_g0_3>
    <d_g3_3 type="real">1.420E-5</d_g3_3>
    <sigma_g_3 type="real">1.500E+0</sigma_g_3>
    <rho type="real">2.650E3</rho>
    <substances type="char">dusta,dustb,dustc</substances>
  </routine>
</emiss>
```

Processes occur in the following order:

1. ***Coagulation***
2. ***ISORROPIA***
3. ***Condensation***
4. ***Nucleation***
5. ***Shifting***
6. ***Washout***


(1)
(2)
>5%
Emission
H2SO4
NUCL
COAG
(2)
COND
(1)
Insoluble
Soluble
Mixed
Aitken
Accumulation
Coarse
Giant