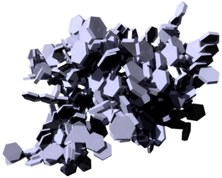
Considerations for radiative transfer observation operators in data assimilation

Patrick Eriksson

Department of Space, Earth and Environment
Chalmers University of Technology,
Gothenburg, Sweden

patrick.eriksson@chalmers.se



Special thanks to: the ARTS team (mainly Hamburg and Chalmers Uni.)
Vasileios Barlakas (Chalmers)
Alan Geer (ECMWF)

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Outline

1. Background and motivation
2. Basics and clear-sky
3. Microwave all-sky radiative transfer

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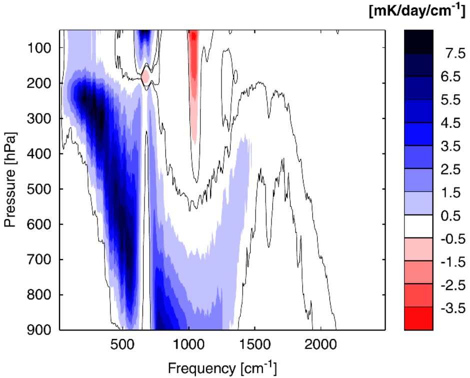
My background, ICI, AWS and ARTS

- Involved in the upcoming ICI and AWS missions
  - both going into the sub-mm range ($>$ 300 GHz)
  - both to be launched in about 3 years
- Did my PhD on Odin/SMR
  - a limb sounder
  - did the first satellite-based sub-mm observations
- Atmospheric Radiative Transfer Simulator (ARTS)
  - started and maintained together with Stefan Buehler (Uni. Hamburg)
  - main strength is microwaves, IR covered, moving towards optical
  - an example on reference forward model

Radiative transfer (RT) in NWP

- Calculation of radiative fluxes
  - heating by solar radiation
  - cooling by outgoing radiation ⇒
  - broadband calculations
  - the full radiation field must be determined



Buehler et al, JQSRT, 2006

- Data assimilation (DA)
  - mapping the model state (x) to the observation (y) ⇒
  - only top-of-the-atmosphere values required,
  - but Jacobian (or adjoint) needed ⇒
  - handled by the "forward model",
  - part of the observation operator

$$y = F(x, b)$$

$$J = \frac{dF}{dx}$$

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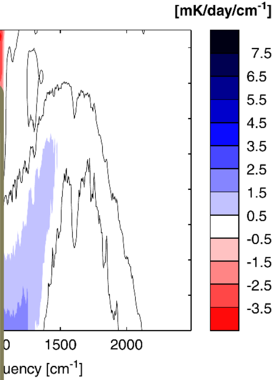
Radiative transfer (RT) in NWP



Buehler et al, JQSRT, 2006

Lack of consistency!

- Inside observation operator
  - mainly between wavelength regions
- Between flux calculations and DA
  - different scattering solvers applied for same region

<u>Mainly matter of treatment of clouds and precip</u>

- hydrometeor types can be ignored
- assumed size distribution differs
- assumed shape differs
- and e.g. implied fall speed not consistent

Observation operator: overall considerations

- Efficiency
  - i.e. low calculation burden
- Accuracy
  - errors in observation operator as important as instrumental errors
  - the combined "observation error" is:

$$\Delta y = \frac{dF}{db}\Delta b + \epsilon$$

    where all RT modelling errors are assigned to b and ϵ is the instrumental error
  - Examples on RT modelling error sources
    - spectroscopic data
    - simplified physics
  - (semi-)systematic errors can be handled by bias correction
    - but simulation errors tend to be state dependent!
- Limit to forecast model not fixed!

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Example: all-sky assimilation of microwave humidity channels

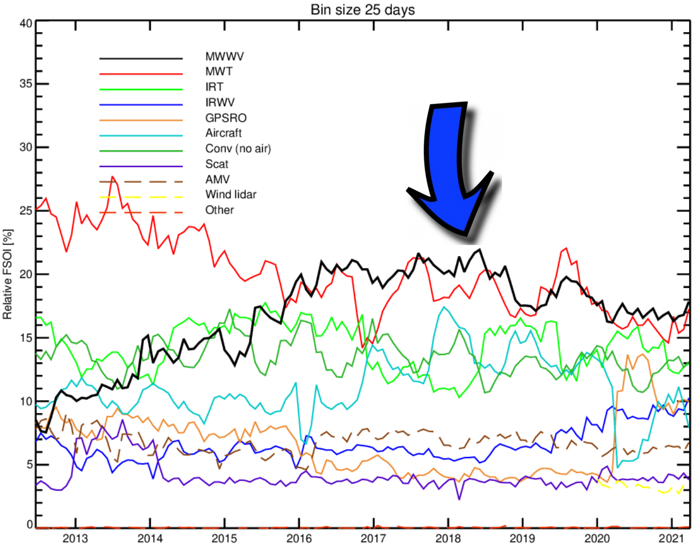

Figure provided by Alan Geer

<u>Done</u>

- Moving from clear-sky to all-sky DA
  - and more data assimilated
- Improvements of RTTOV

<u>Future</u>

- Updates of RTTOV in the pipeline
- More observations
  - existing not used
  - more channels
  - new bands (229/240GHz + sub-mm)

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RTTOV

- RTTOV is the European DA forward model
  - Saunders et al., GMD, 2018
- Developed and maintained by NWP SAF
- Several RT solvers
  - including RTTOV-SCATT for microwave all-sky
- Data part of the package
  - gas transmittances
  - surface emissivities
  - particle scattering data
  - ...
- Fast, only 0.5% of total DA time
  - more time in RTTOV-SCATT than "clear-sky"!
- RTTOV = Radiative Transfer for TOVS
  - TOVS = TIROS Operational Vertical Sounder
    - TIROS = Television InfraRed Observation Satellite

nidity channels

ing from clear-sky
l-sky DA
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Trio 1: sources to radiation

Wavelength/frequency limits reflect scope of RTTOV

- Solar radiation
  - 0.4 - 15 μm
  - AVHRR, SEVIRI, MODIS . . .

- Thermal/telluric emission (from atmosphere and surface)
  - IR: 2 - 20 μm
  - microwaves: 10 - 190 GHz (30 - 1.6 mm)
  - being added: 190 - 750 GHz (1.6 - 0.4 mm)
  - instruments: HIRS, IASI, AMSU, SSMIS . . .

- Active sensors
  - lidar (Aeolous)
  - radar (CloudSat)
  - GNSS radio occultation (GRAS, COSMIC, . . .)

Trio 2: main physical mechanisms

- Absorption
  - by molecules and particles
  - basically always a concern
    - one exception is RO

- Emission
  - insignificant for optical and active observations
  - in general coupled to absorption (LTE)

- Scattering
  - optical: molecules, aerosols and hydrometeors
  - IR: aerosols, hydrometeors
  - microwaves: large ($>\sim 100\mu$m) hydrometeors
  - the surface is also scattering/reflecting

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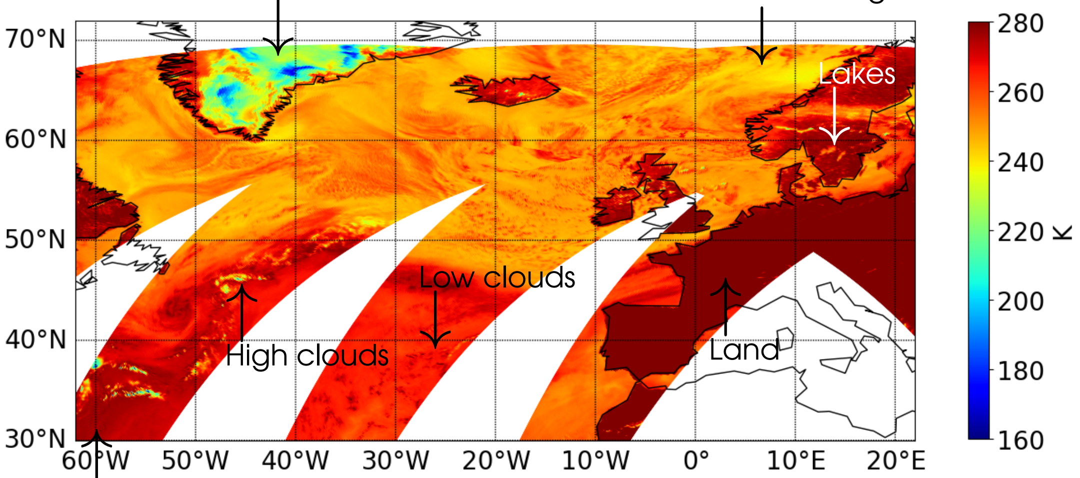
Trio 3: geometries

- Downward
- Upward
- Limb sounding

Example observation

GMI 89 GHz, V-pol



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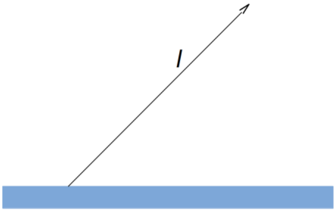
The simplest case: “IR clear sky”

<u>Assumptions</u>

- Solar radiation can be neglected
- Atmospheric scattering can be neglected
- Surface acts as a blackbody

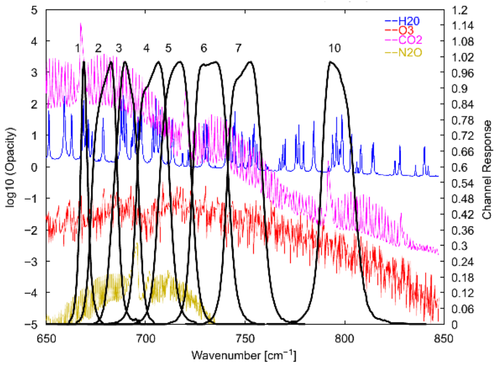


- *B*: Planck function
  - analytical expression
- T_s: surface skin temperature
- *T*: atmospheric temperature
  - temperatures given by forecast model
- *k*: absorption per length unit
  - main challenge for this case
  - RTTOV provides “look-up tables” of layer optical thicknesses ($k\Delta l$)

$$y = B(T_s)e^{-\int_0^L k(l)dl} + \int_0^L B(T(l))k(l)e^{-\int_l^L k(l')dl'}dl$$

Calculation and representation of layer optical thicknesses

- Monochromatic values per gas obtained by combining
  - line-by-line calculations
  - empirical "continuum" terms
- These values are weighted with channel response
  - for efficiency, only one RT calculation per channel
- Main errors/approximations:
  - Data compressed to lookup-table
  - RT only exact for monochromatic calculations
  - Non-perfect spectroscopic data
    - line mixing, speed-dependent line shape, . . .
- Systematic errors $\sim$ 1 K
- Random errors $<$ 0.1 K



Buehler et al, JQSRT, 2010

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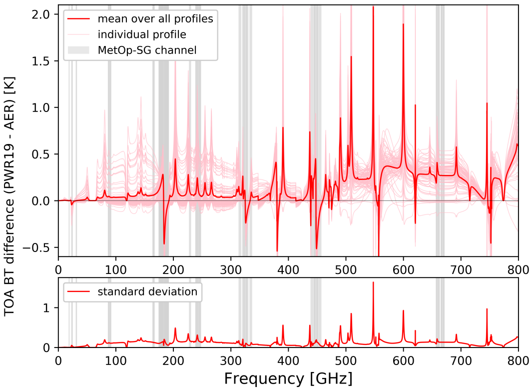
A present challenge: entering a poorly charted region

- RTTOV not valid above ∼300 GHz
  - ozone is ignored
  - weaker H_2O not included
  - accuracy of absorption models?
- Existing sub-mm observations
  - three limb sounders
    - SMR and MLS active
  - some airborne measurements
    - only ISMAR active
  - ground-based only from high altitudes
    - mainly astronomy sites
- RTTOV is being extended
  - by UK Met Office ⇒

PWR19 vs. AER H_2O absorption models

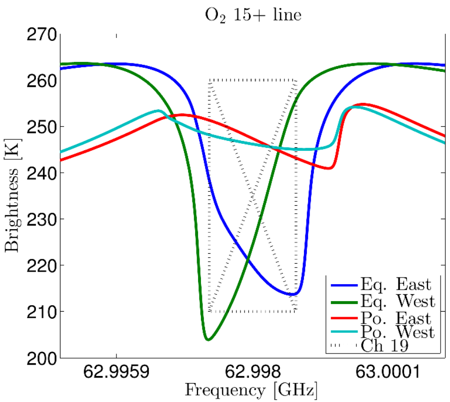


Work and figure by Emma Turner, UK Met Office

Complications occurring in the mesosphere

Examples on non-standard physics

- Zeeman effect
  - affects microwave oxygen transitions
  - causes polarised absorption/emission
  - radiances depend on polarisation and viewing direction
  - magnitude?
  - RTTOV: Zeeman effect parameterised
    - no clear overall bias
    - but semi-random errors up to 6 K



Larsson et al, AMT, 2016

- Non-LTE
  - RTTOV applies a correction for the CO_2 band around 4.3 μm
  - correction up to 10 K
  - accuracy?

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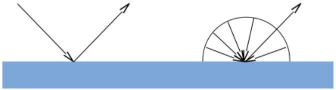
Complications due to surface scattering/reflections

- Surface emissivity poorly constrained by forecast model
  - can be estimated by model parameters for water
  - for other surfaces “atlases” applied
  - or must be retrieved from observations
- Specular, Lambertian or in between?
  - lambertian normally assumed at short wavelengths
  - specular normally assumed at microwaves
  - less critical for IR as high surface emissivity
- Also down-welling radiation needs to be determined
  - by selecting a representative angle, only one extra clear-sky calculation could suffice



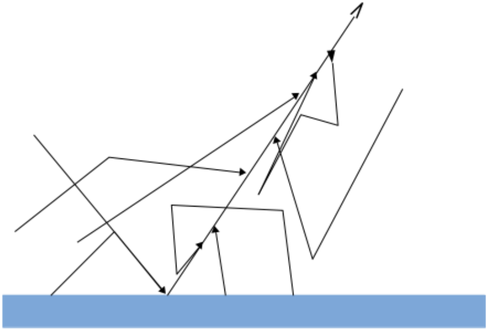
- More in talks by
  - Catherine Prigent, Wed
  - Alan Geer, Fri

Outline

Main complications, 1

The complete radiation field must be determined

- The RT problem is not confined to one or a few directions
- Strongly increased calculation burden
- DA requires simplifications



RTTOV-SCATT

- Scattering source term determined by Delta-Eddingtion (2-stream)
  - followed by pencil-beam integration along line-of-sight
- Accuracy reevaluated by comparison to a reference model (ARTS)
  - mean systematic/random error $< 2/1$ K (at significant scattering)
    - compensating errors!
  - just about 10% of total error assumed for DA
  - but errors above 10 K occur and larger errors to be expected for sub-mm
  - more in Barlakas et al., to be submitted

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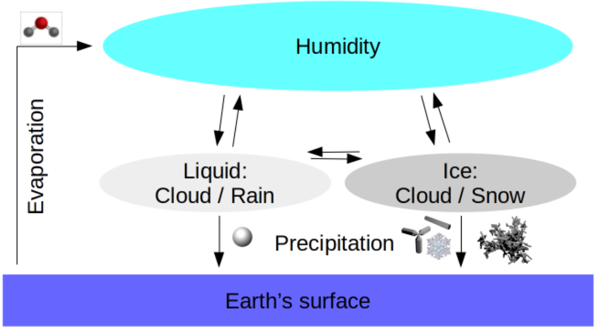
Main complications, 2

Size, shape and orientation of particles matter

- Scattering not proportional to particle mass
  - we need to assume a particle size distribution (PSD)
- Two particles with same mass scatter differently if shape differs
  - we need at least to assume the "habit"
- Change orientation of a non-spherical particle and RT properties change
  - at least select between totally or azimuthally random orientation (TRO/ARO)



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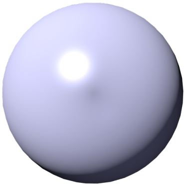
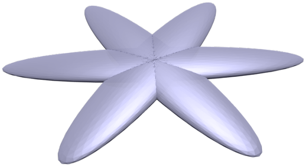
“Snow” in RTTOV-SCATT
Default habits

V8 (2006)



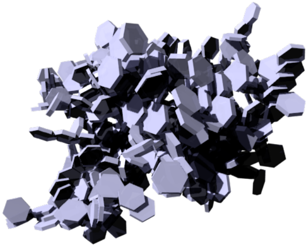
Soft sphere approximation

V11 (2013)



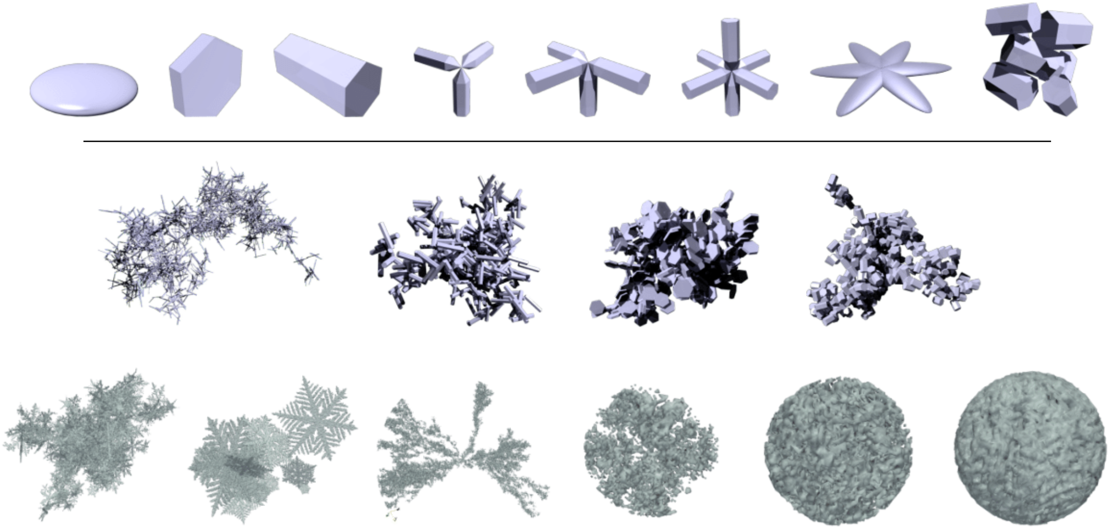
Liu database

V13 (2020)



ARTS database

The ARTS database of ice hydrometeor scattering properties



The ARTS database of ice hydrometeor scattering properties

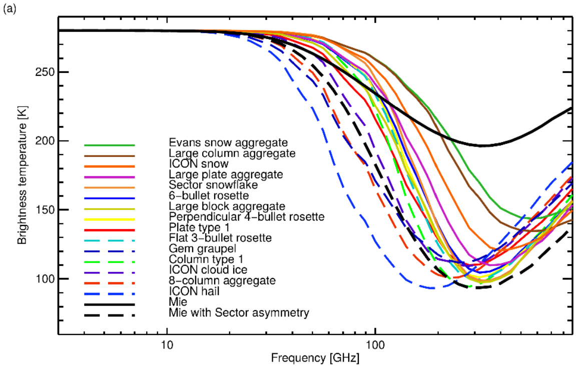
Summary:

- 34 habits for totally random orientation (TRO)
  - Eriksson et al., ESSD, 2018
- Each habit: ≥30 sizes
  - first general database having realistic aggregate habits
- 3 temperatures per habit
- 1 - 886 GHz
- In RTTOV v13, these ARTS data default for all hydrometeor types
  - thus RTTOV-SCATT is prepared for ICI
- Two habits for azimuthally random orientation (ARO) added
  - Brath et al., AMT, 2020

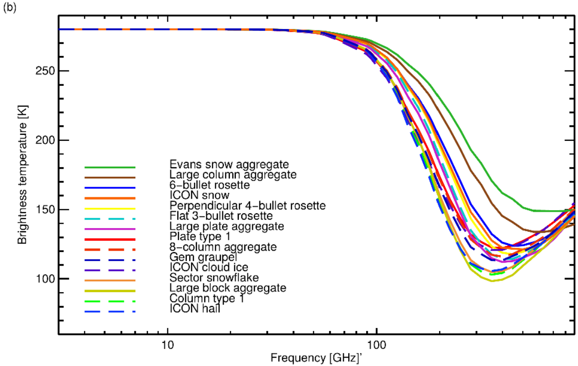
Example on impact of habit and PSD

Not independent contributions

PSD = F07t



PSD = MH97



- For details see Geer et al., GMDD
  - describing hydrometeor set-ups in RTTOV-SCATT V13

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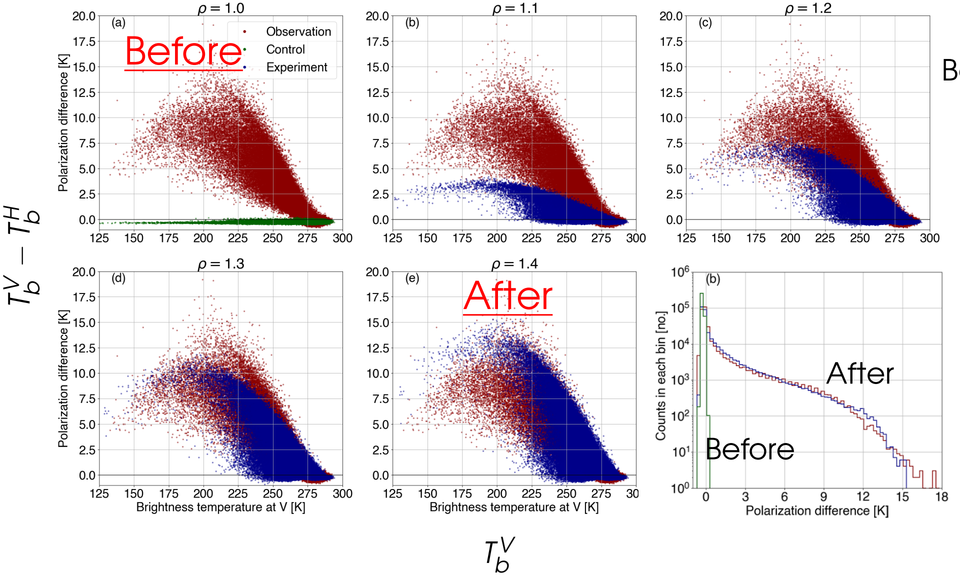
Approximation of particle orientation introduced

So far only conically scanners, here tested on GMI 166 GHz V and H

▸ Background in extra slides



Barlakas et al., AMT, 2021

$$\rho = \frac{\tau_H}{\tau_V}$$

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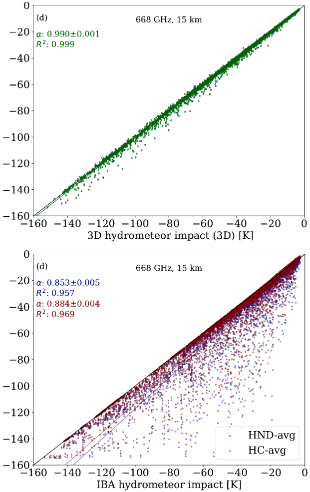
3D and beam filling

- Have been studied for precipitation
- Here more recent results for > 175 GHz
  - with similar conclusions
- Full 3D calculations can be avoided ⇒
  - relatively small, random error
- but requires good representation of cloud structures inside footprint
- Ignoring “beam-filling” can result in large, one-sided, errors ⇒
  - for ICI, particularly in the tropics
- If footprint decreased
  - beam-filling error ↘
  - 3D error ↗
- Impact inside observation operators?

Simulations of ICI@668 GHz
Deviations from diagonal = error



Barlakas and Eriksson, RS, 2020

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Outlook (with focus on RTTOV-SCATT)

Official plans for RTTOV at `nwp-saf.eumetsat.int/site/software/rttov/future-plans`

Short term

- RTTOV-SCATT v13 become operational in cycle 48r1 (2022)

  ▸ Summary of changes in extra slides

- Extend ARO approximation of oriented particles to cross-track and radar

Long term

- Improve representation of beam filling
- Add melting particles
- Increased consistency with other RT calculations
- Testing sub-mm in practice
- Handling V and H polarisation in parallel
- Support atmospheric models also providing mean size
- Use machine learning?
- ...

Summary

- Continued development of RTTOV-SCATT (all-sky microwave)
  - improved data on ice hydrometeor scattering properties
  - approximation of oriented ice particles introduced
  - also radar supported
- There are still significant uncertainties
  - but considerably smaller than total DA uncertainty

- Sub-mm range will be introduced
  - RTTOV soon in good shape for ICI and AWS
  - preparing for ICI gives improvements already now!
- A main gap is consistency in treatment of clouds and precip:
  - inside DA, across the EM spectrum (more in talk by P. Chambon, Wed)
  - with calculation of fluxes
- In that process, several of present simulation errors should be tackled
  - but there will still be instrument/wavelength specific issues

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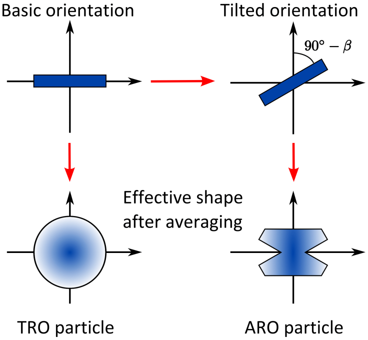
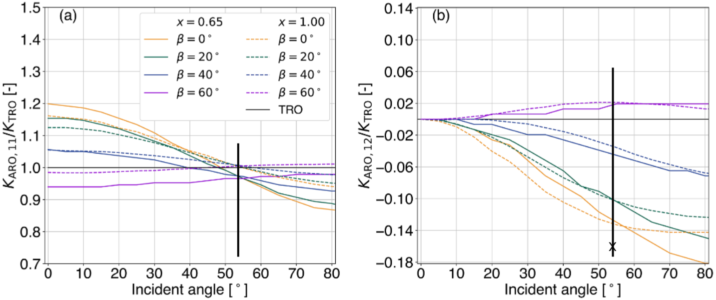
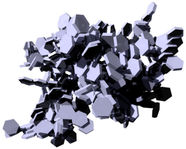
Extra slides

What about orientation?

- Azimuthally random orientation (ARO)
  - particles at an angle to the horizon
  - but no preference in azimuth
  - a distribution of "tilt angles" assumed
- Much more demanding in several ways
- ARTS database has been extended with two habits
  - Brath et al., AMT, 2020







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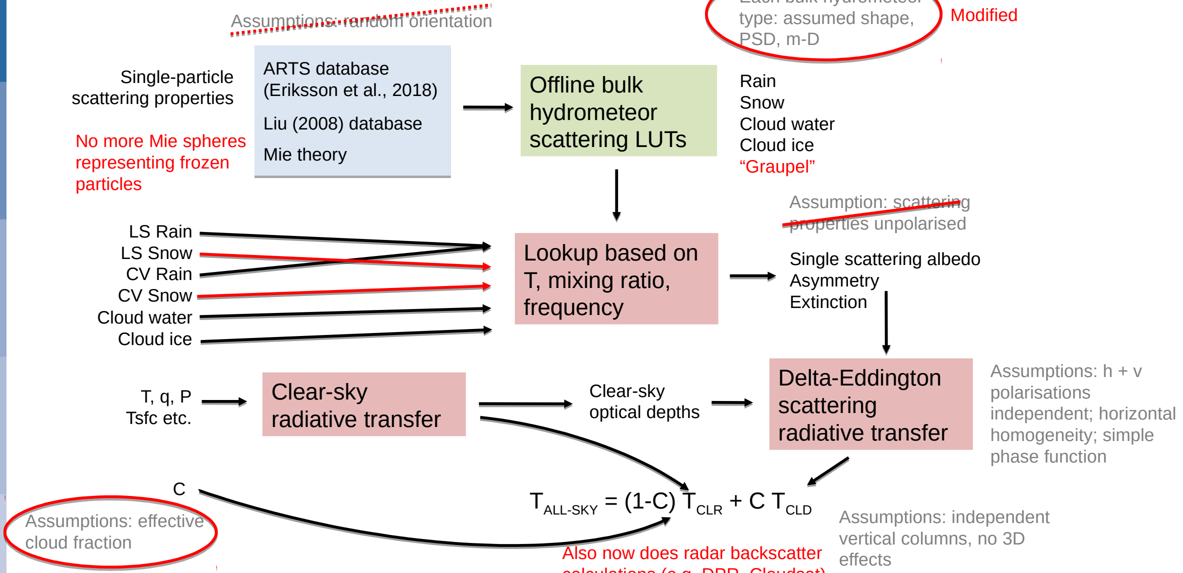
RTTOV-SCATT (v13.0)



For details see Geer et al., GMDD