Observations 3: Data Assimilation of Water Vapour Observations at NWP Centres

OUTLINE:

- Data Assimilation
    - A simple analogy: data fitting
    - 4D-Var
    - The observation operator : RT modelling

- Review of Radiative Transfer
    - MW
        - Clear sky RT: weighting functions
        - Spectroscopy (v_o,S, F)
        - Line-by-Line to fast RT models
        - Scattering RT
        - Summary
    - IR
        - IR *vs* MW

Variational assimilation: A simple analogy - data fitting

- Given some measurements, **y(x)**, find the best model fit for model **f(x,c)** by adjusting coefficients in model (**c**) to achieve a 'best' fit:

- Define a cost, **J**, that measures misfit of model to measurements *eg* RMS of y-f(x,c)

- Minimise the cost wrt c

- Involves computing the gradient of J wrt c

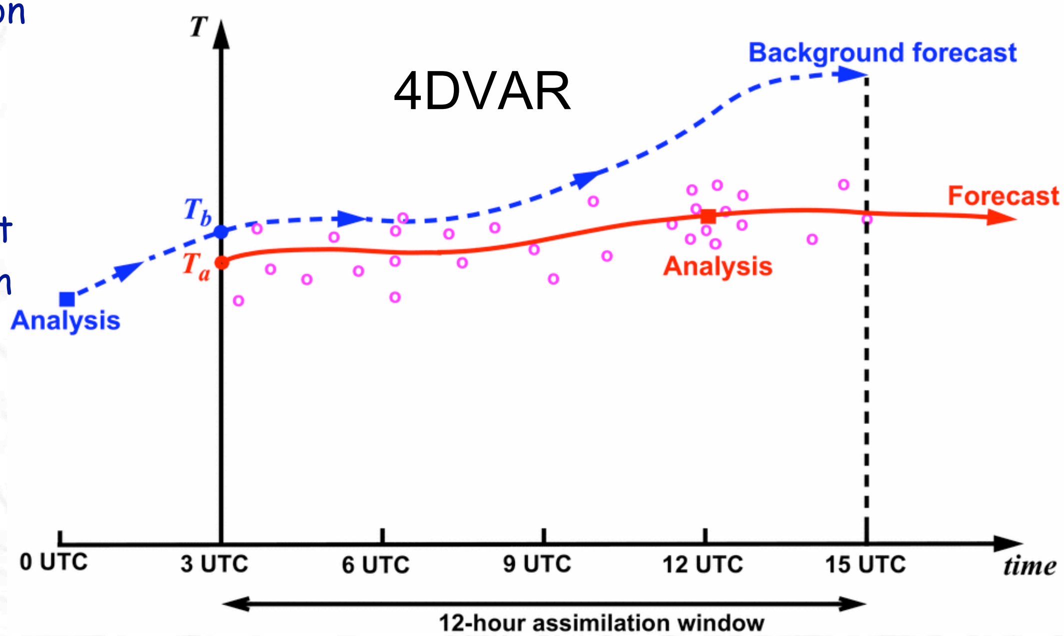
- With prior knowlege of c ,eg previous estimates of c_0 with uncertainties $U(c_0)$, we can modify the cost to include two terms : misfit to model + misfit to prior estimates, something like :

$$J(c) = \frac{(c - c_0)^2}{u(c_0)^2} + \frac{(y - f(x,c))^2}{u(y)^2}$$

Data Assimilation: 4D-Var

Data assimilation combines information from

- Observations
- A short-range "background" forecast that carries forward the information extracted from prior observations
- Error statistics
- Dynamical and physical relationships



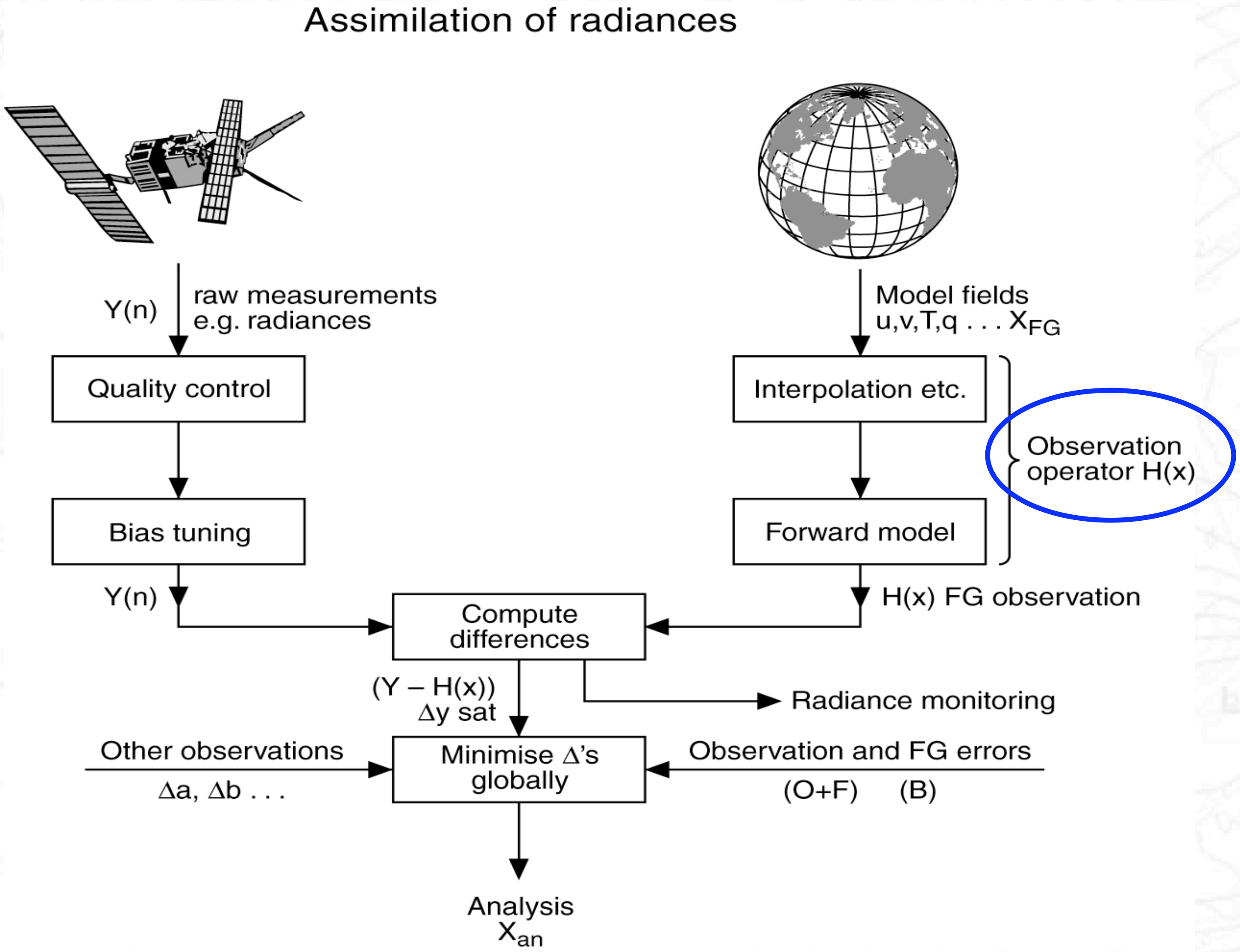
This produces the "most probable" atmospheric state (maximum-likelihood estimate)***

***if background and observation errors are Gaussian, unbiased, uncorrelated with each other; all error covariances are correctly specified; model errors are negligible within the 12-h analysis window

$$\mathbf{J}(\mathbf{x}) = \underbrace{(\mathbf{x}_b - \mathbf{x})^T \mathbf{B}^{-1} (\mathbf{x}_b - \mathbf{x})}_{\text{background constraint}} + \underbrace{[\mathbf{y} - \mathbf{h}(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y} - \mathbf{h}(\mathbf{x})]}_{\text{observation constraint}}$$

$$\mathbf{h}(\mathbf{x}) = \mathbf{h}[\grave{I}\ (\mathbf{x})]$$ simulates the observations

Radiance Assimilation



Scattering in the MW:
Why MW radiometers see through clouds and IR radiometers don't !

- Importance of scattering governed by size parameter: x=2πr/_.
- Mie scattering important for x ~ 1 or greater.
- For water clouds, r~10_m, MW _'s ~2-6 mm, -> $x \sim 10^{-2}$ -> water clouds appear as homogeneous absorbers/emitters,
  - -> scattering unimportant.
- For ice, rain or snow, r~1-10mm, x~1
  - -> scattering important.

Scattering:
size parameter for clouds / hydrometeors

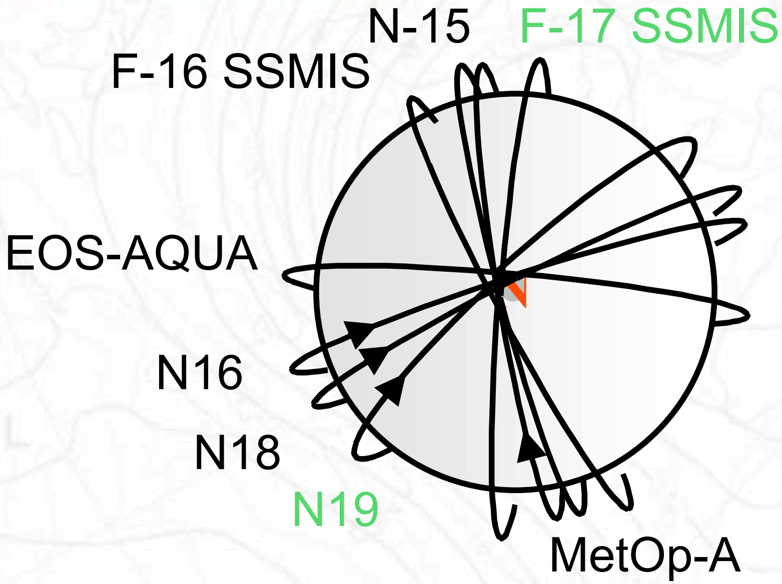
	Size (a)	Size parameter λ=0.5 μm	Size parameter λ=10 μm	Size parameter λ=1 cm
Aerosol	1 μm	1.26×10^{1}	6.3×10^{-1}	6.3×10^{-4}
Water droplet	10 μm	1.26×10^{2}	6.3×10^{0}	6.3×10^{-3}
Ice crystal	100 μm	1.26×10^{3}	6.3×10^{1}	6.3×10^{-2}
Raindrop	1 mm	1.26×10^{4}	6.3×10^{2}	6.3×10^{-1}
Snowflake	1 cm	1.26×10^{5}	6.3×10^{3}	6.3×10^{0}

Rayleigh | Mie | G. Optics

(Adapted from Liou, *An introduction to atmospheric radiation*, 2002. Table 5.1)

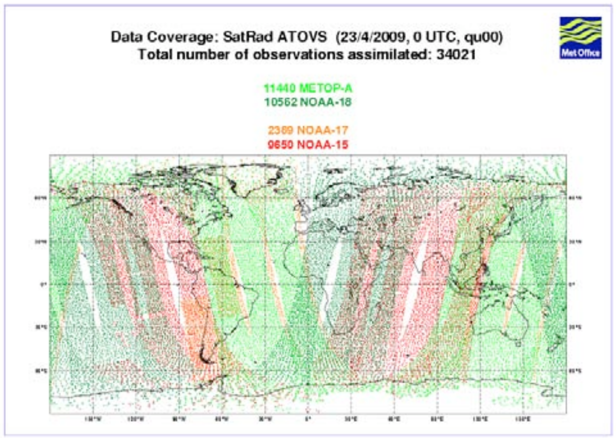
A. Bodas-Salcedo

Microwave Sounders in operational systems

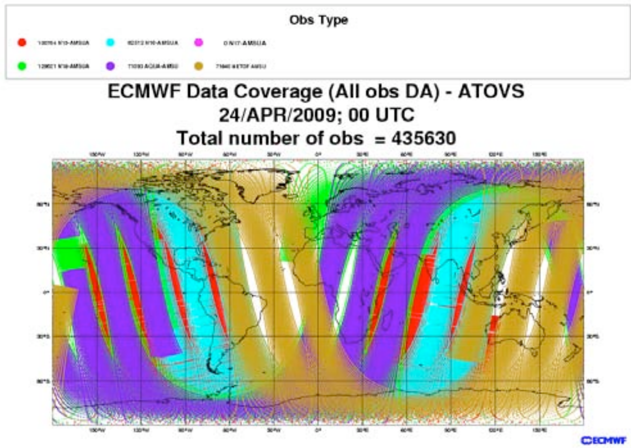


- T information from 50-60 GHz O_2 absorption

- Q information from 183 GHz H_2O absorption, and window channels at (19, 22, 37, 89 and 150 GHz)



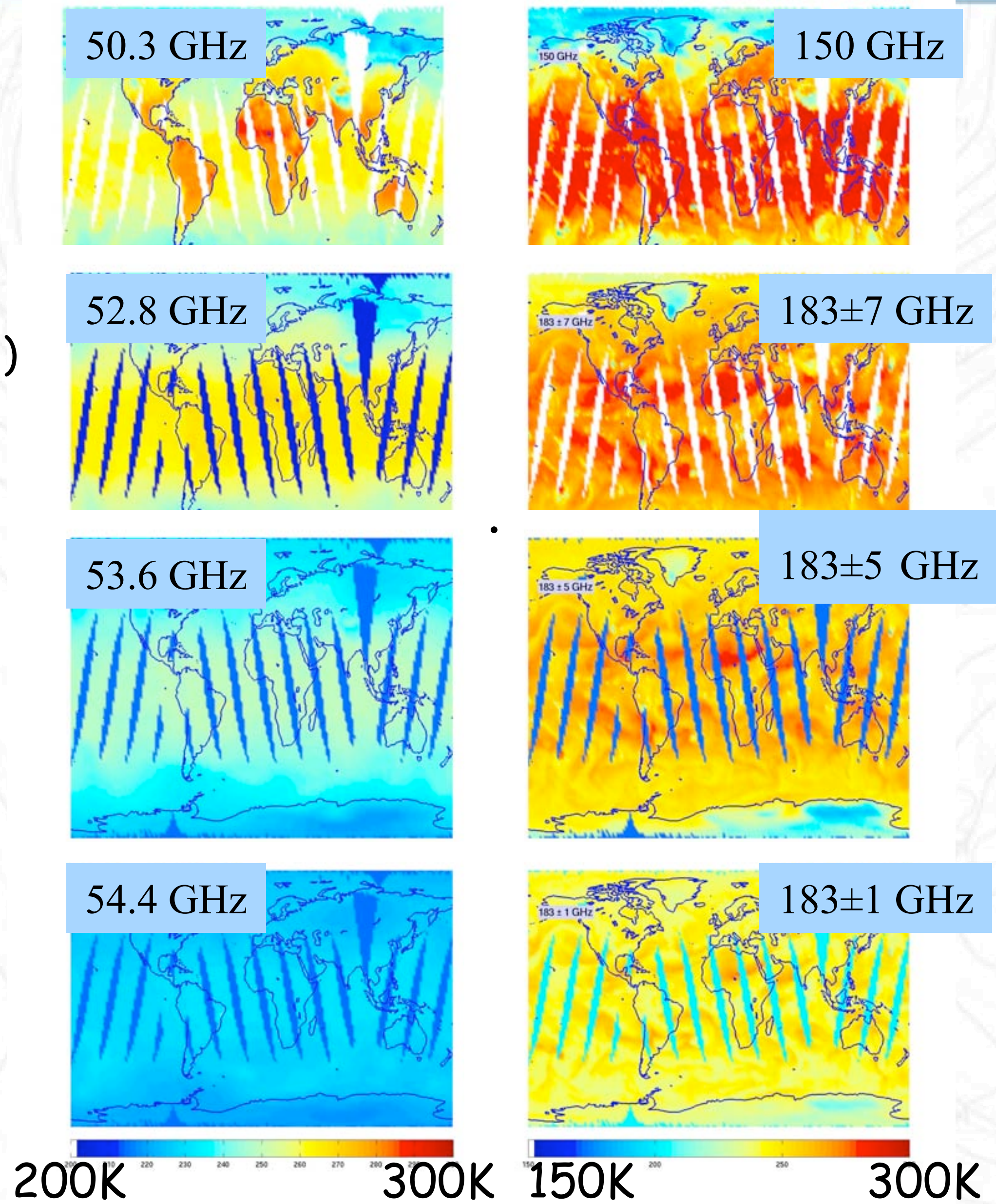
Met Office



ECMWF

Microwave data: some examples of measured radiances

Brightness Temperature measurements obtained over ~12 hours by (F-16 SSMIS)



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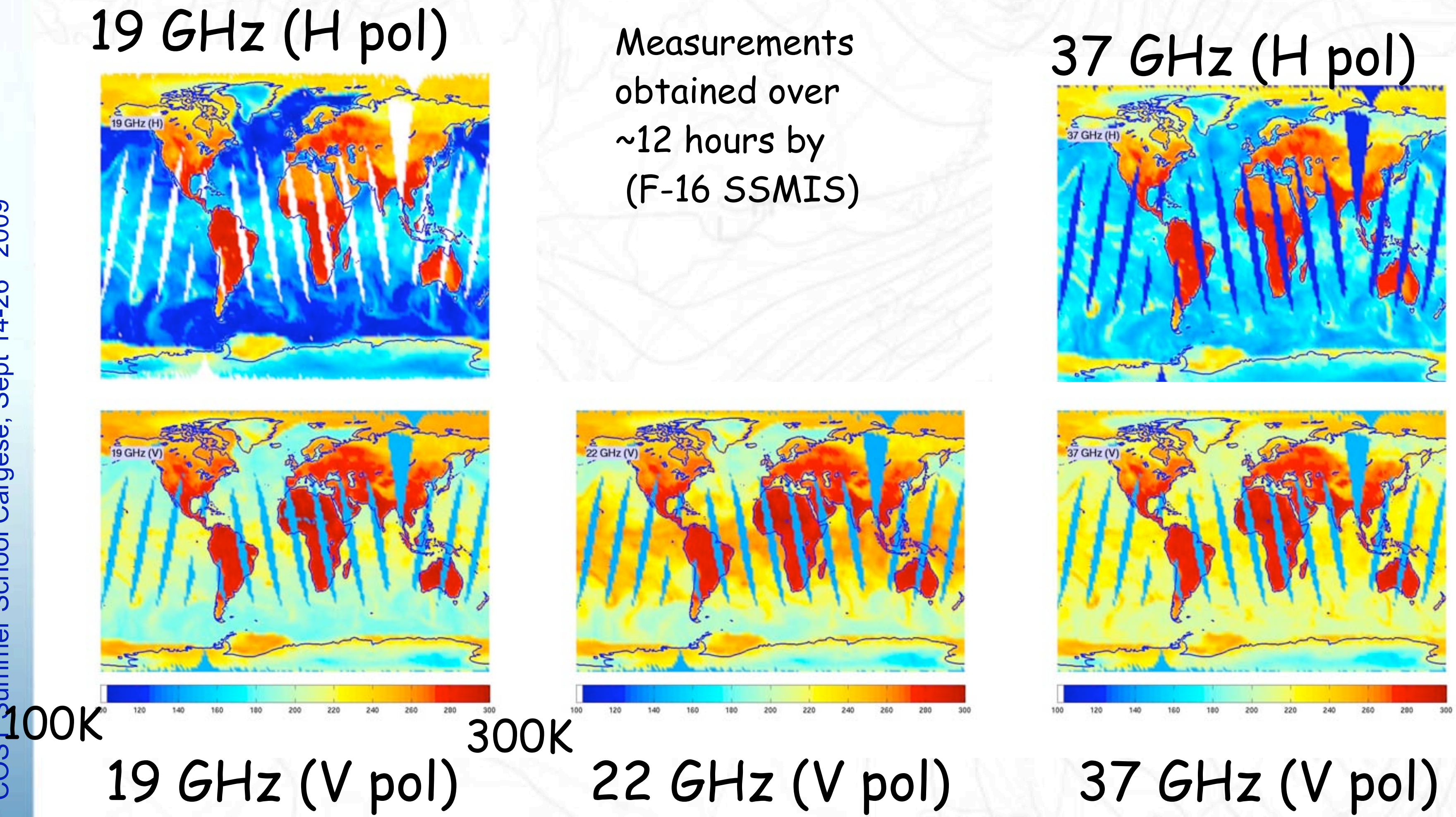
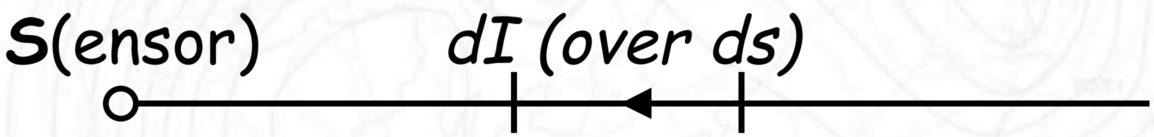


Recap: Radiative transfer equation in clear skies



Change in radiant intensity along a path is given by the sum of *source* and *loss* terms, in the clear sky case: emission and absorption, respectively:

$$dI_{emit} = \beta_a B \, ds \quad \text{(emission)}$$

$$dI_{abs} = -\beta_a I \, ds \quad \text{(absorption)}$$

Hence:

$$dI = dI_{emit} + dI_{abs}$$

$$= \beta_a (B-I) \, ds$$

and:

$$\boxed{dI/ds = \beta_a (B-I)}$$ (Schwarzschilds Equation)

Radiative transfer equation in clear skies

Introducing optical path:

$$\tau(s) = \int_s^S \beta_a(s')ds'$$

and noting:

$$\tau(S) = 0$$

$$d\tau = -\beta_a ds$$

$$\frac{dI}{d\tau} = I - B$$

use integrating factor $e^{-\tau}$:

$$e^{-\tau}\frac{dI}{d\tau} - Ie^{-\tau} = -Be^{-\tau}$$

$$\frac{d}{d\tau}\left[Ie^{-\tau}\right] = -Be^{-\tau}$$

$$\int_0^{\tau'} \frac{d}{d\tau}[Ie^{-\tau}]d\tau = -\int_0^{\tau'} Be^{-\tau}d\tau$$

$$\boxed{I(0) = I(\tau')e^{-\tau'} + \int_0^{\tau'} Be^{-\tau}d\tau}$$

after Petty (2006)

Radiative transfer equation in clear skies

$$I(0) = I(\tau')e^{-\tau'} + \int_0^{\tau'} Be^{-\tau} d\tau$$

Radiance at sensor

Integral of source function along path multiplied by transmission between sensor and each point

Radiance at start of path multiplied by path transmission

Radiative transfer equation in clear skies

Can write this in two other forms, firstly using:

$$t = e^{-\tau},$$

$$dt = -e^{-\tau} d\tau,$$

to get :

$$\boxed{I(0) = I(\tau')t(\tau') + \int_{t(\tau')}^{1} B dt.}$$

or using :

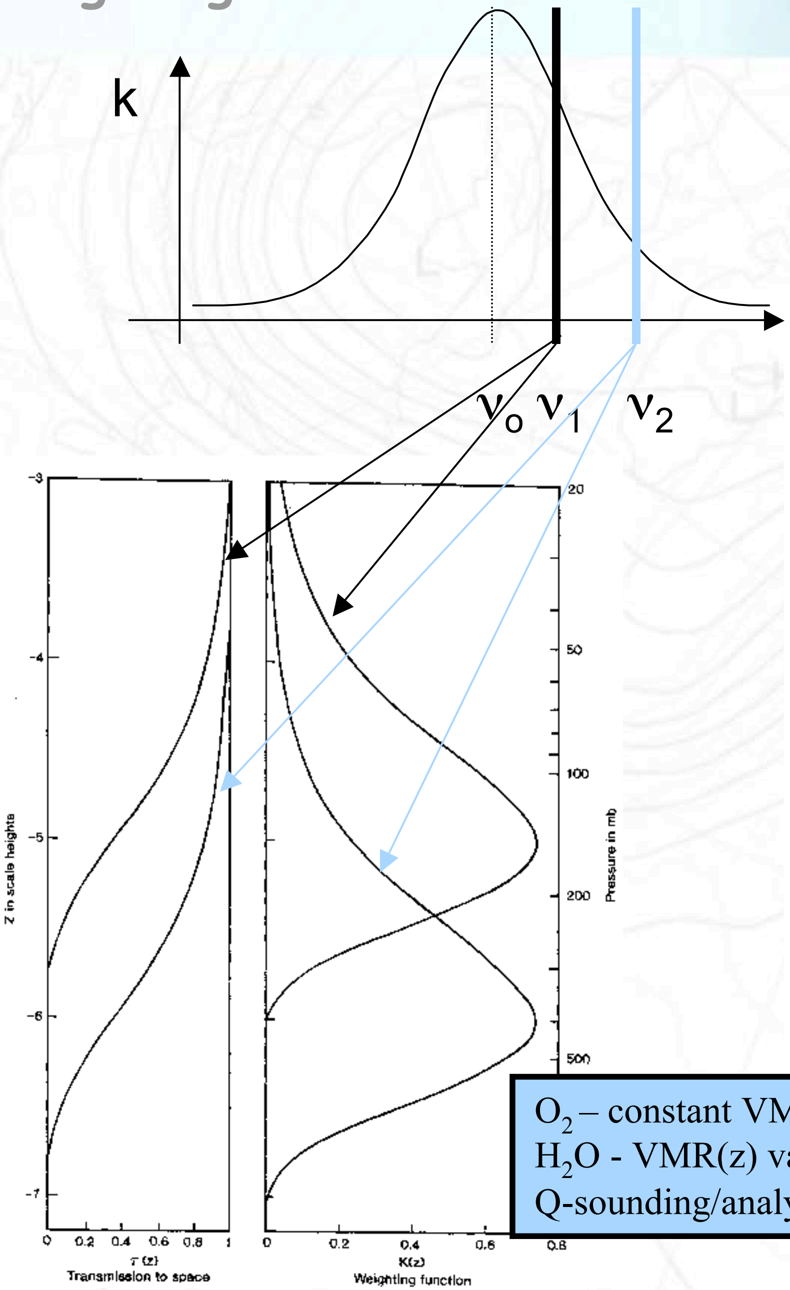
$$dt = \frac{dt}{ds} ds$$

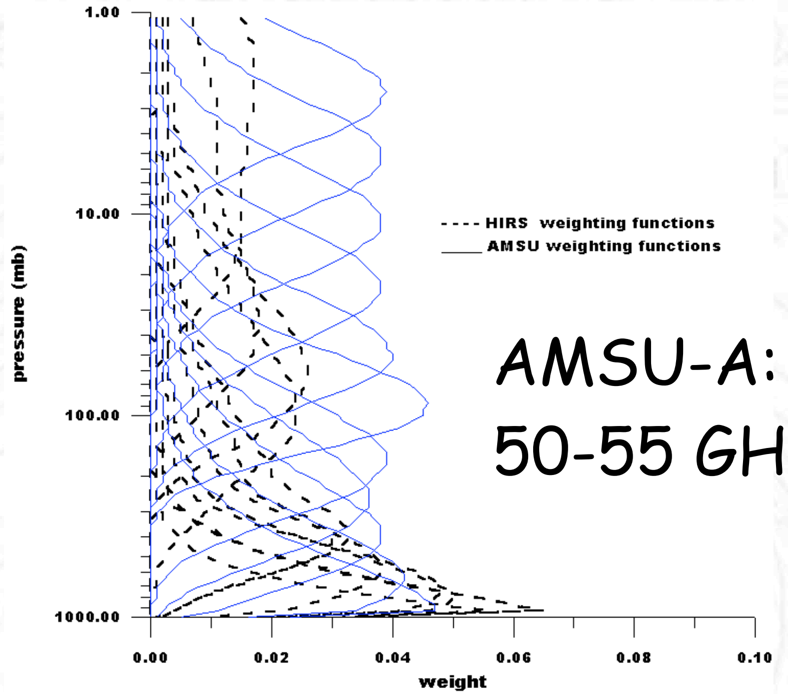
to get :

$$\boxed{I(S) = I(s_0)t(s_0) + \int_{s_0}^{S} B(s) \frac{dt(s)}{ds} ds}$$

Weighting function

Weighting functions

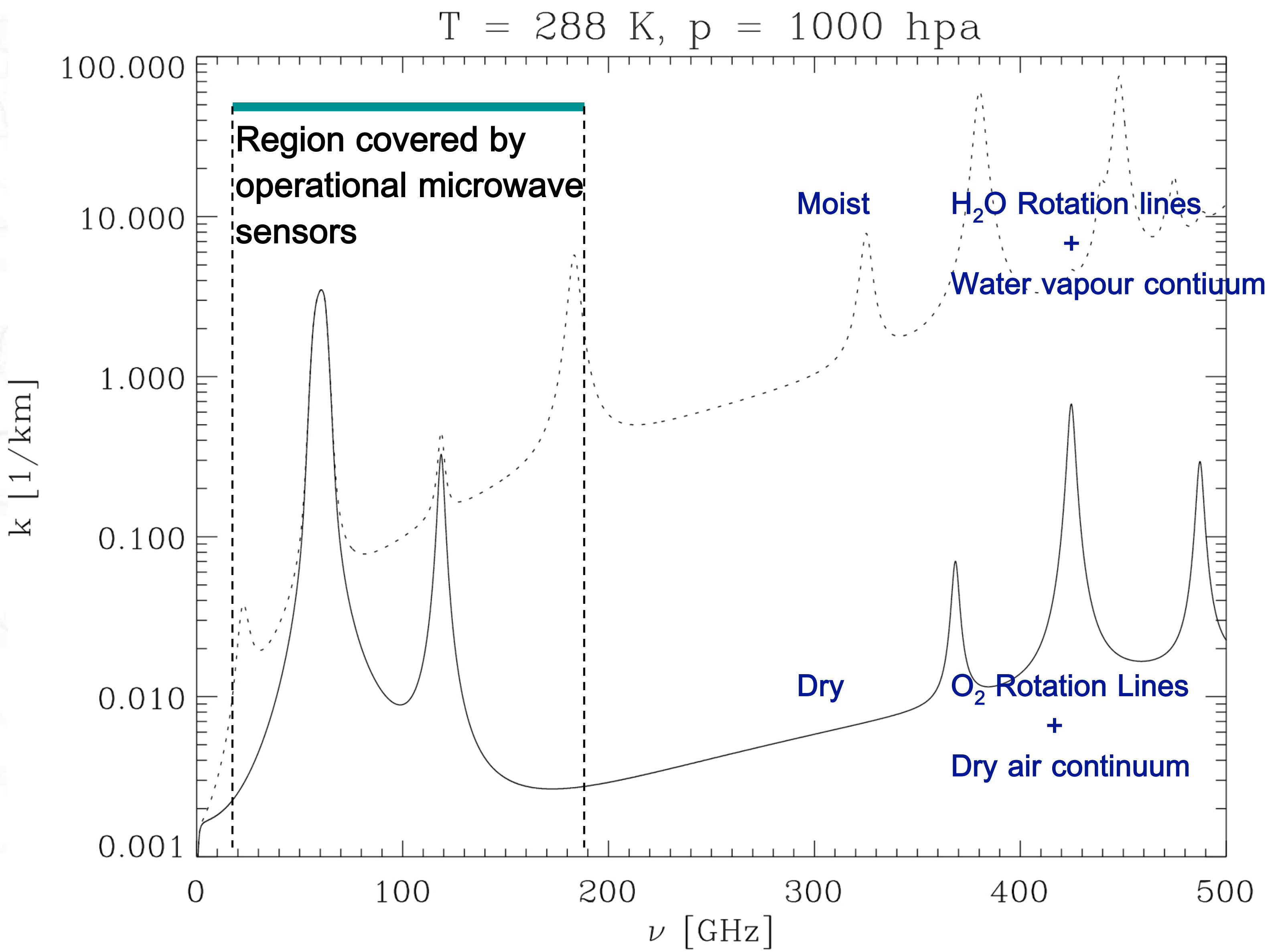




AMSU-A:
50-55 GHz

O_2 – constant VMR(z) → weighting function fixed. T-sounding 'linear'
H_2O - VMR(z) variable → weighting function is state dependent.
Q-sounding/analysis problem is NON LINEAR

The Microwave Spectrum



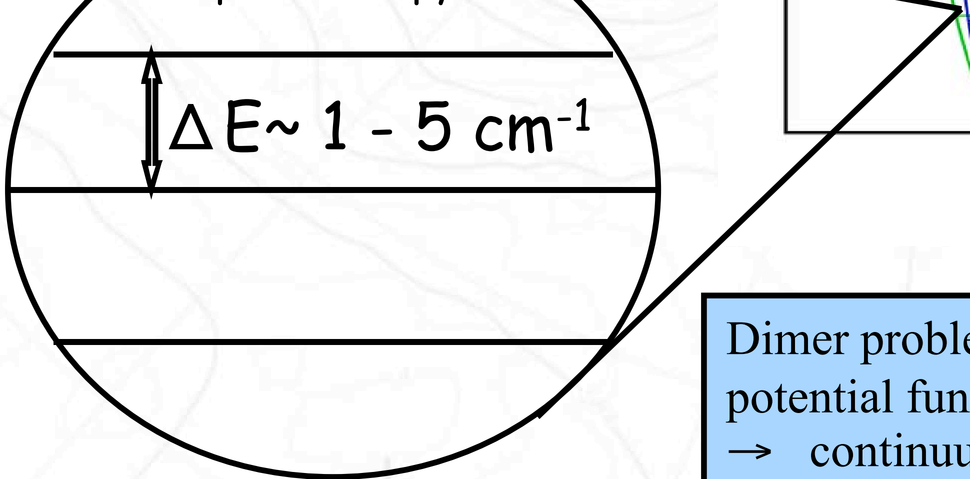
The Role of Water Vapour in the Climate System, COST Summer School Cargese, Sept 14-26th 2009

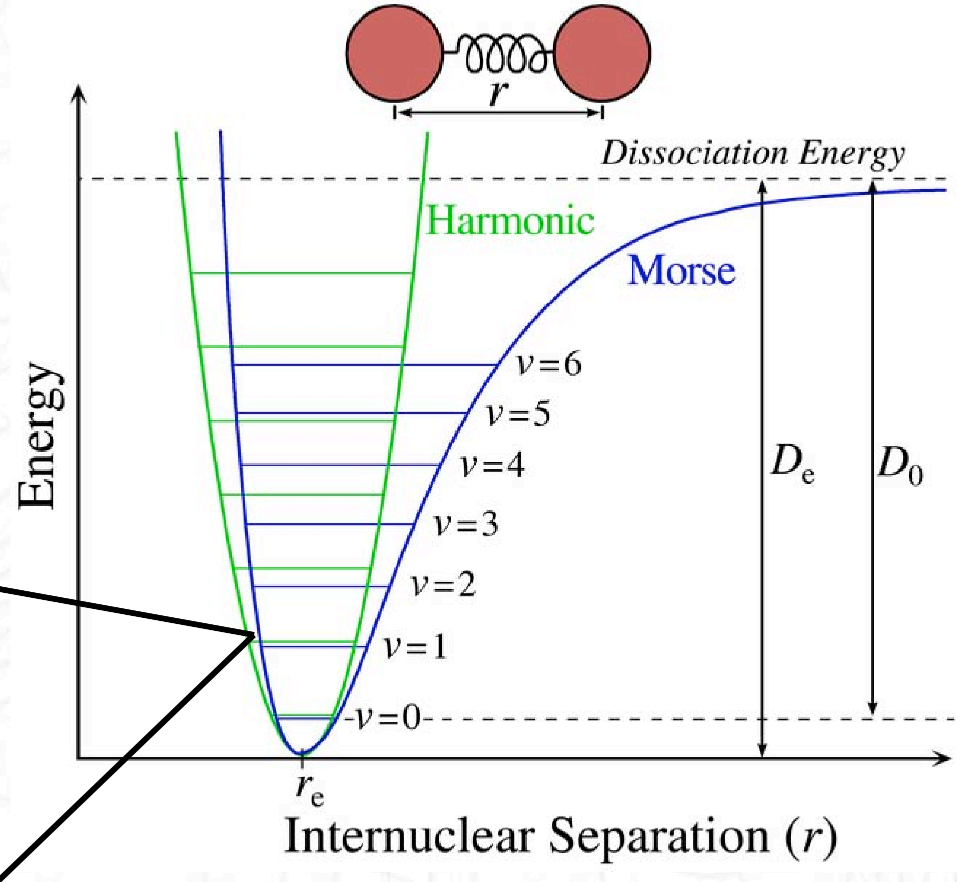
Vibrational-Rotational (IR) / Rotational Spectroscopy (MW)

Microwave absorption lines are normally due to rotational transitions.

Differences in rotational energy levels are small in comparison to :

- Vibrational levels ($\Delta E \sim 100\text{–}5000 cm^{-1}$)
  - (IR spectroscopy)
- Electronic states ($\Delta E \sim 10{,}000 cm^{-1}$)
  - UV/VIS spectroscopy





Dimer problem – not a true bound state.
potential function shallow - levels very close
→ continuum-like absorption ?

Broadening of atmospheric absorption / emission lines

For most absorption / emission lines in the earths atmosphere, two broadening mechanisms are important:

- Pressure (collisional) broadening (*)
- Doppler broadening

If both are important (eg in IR) the line shape is given by the convolution of both – the Voigt line shape

ν_0, S, F

Line strengths (S)

See Rothman *et al* 1987

$$S_{if}(T) = \frac{8\pi^3}{3hc}\upsilon_{if}\underbrace{\left[1-\exp(-c_2\upsilon_{if}/T)\right]}_{\text{Spontaneous emission term}}\frac{\overbrace{g_i}^{\text{Nuclear spin degeneracy}}\overbrace{I_a}^{\text{Isotopic abundance}}}{\underbrace{Q(T)}_{\text{partition function}}}\times\underbrace{\exp(-c_2E_i/T)}_{\text{Boltzmann factor for ground state with energy } E_i}\mathbf{R}_{if}.10^{-36}$$

where : $\mathbf{R}_{if} = |\langle i|M|f\rangle|^2$ - transition dipole matrix element
= 0 if no change in dipole moment involved in transition from i to j

Note : S(T)

obtained through measurement, and available through published spectroscopic databases (eg HITRAN..)

Pressure Broadening (F)

Lorentz line shape omits this factor

$$f(\nu_0,\nu) = \frac{1}{\pi}\frac{\nu}{\nu_0}\left[\frac{\gamma}{(\nu_0-\nu)^2+\gamma^2}+\frac{\gamma}{(\nu_0+\nu)^2+\gamma^2}\right]$$

$$\cong \frac{1}{\pi}\left[\frac{\gamma}{(\nu_0-\nu)^2+\gamma^2}\right]$$

Van Vleck and Weisskopf (1945)

Approximation valid near line centre at most microwave frequencies and higher

$$\gamma = \frac{1}{2\pi\tau}$$

mean time between collisions

$$FWHM = 2\gamma$$

$$\gamma = \gamma_0(T)p$$

Pressure broadening coefficient is obtained through measurement and is available from spectroscopic databases

$\gamma_0 \sim$ 1-3 GHz. atm^{-1}

who cares ?
eg .22 GHz line widths

Doppler Broadening (F)

$$g(\nu,\nu_0) = \sqrt{\frac{mc^2}{2\pi kT\nu_0^{\ 2}}}\exp\left(-\frac{mc^2(\nu-\nu_0)^2}{2kT\nu_0}\right)$$

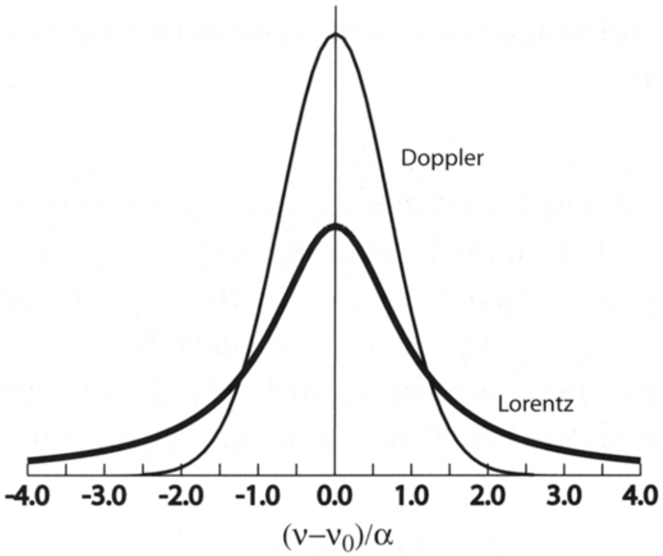
Due to Doppler shift resulting from relative motion between observer and abs/emitting molecule

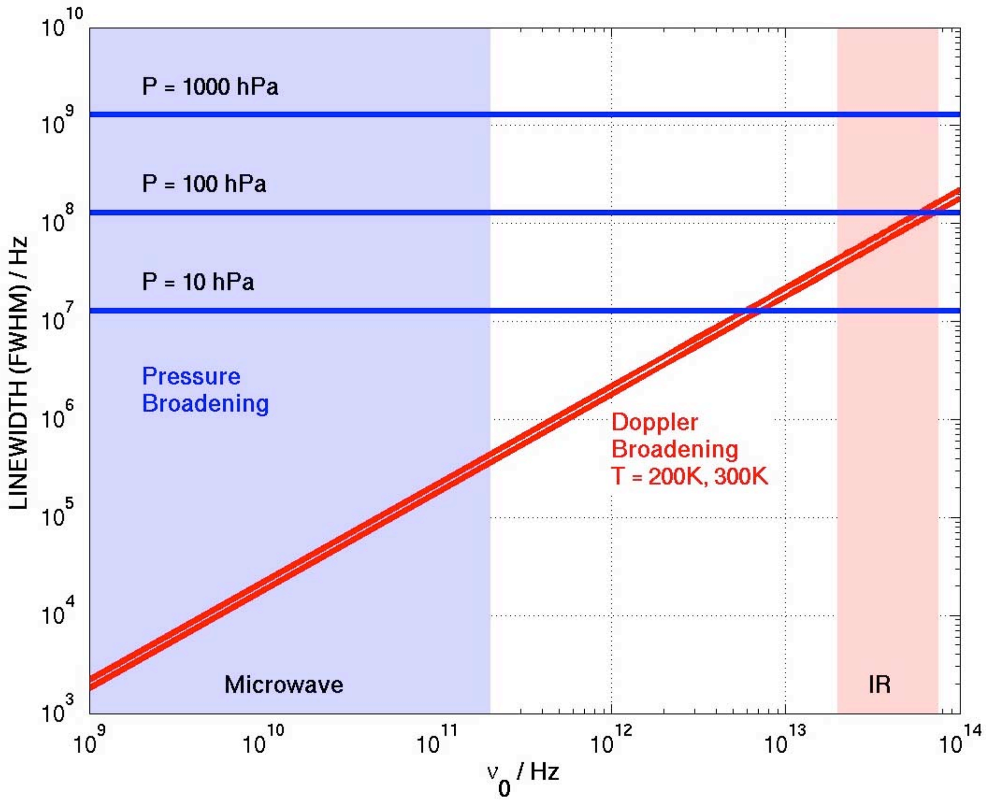
$$\sigma = \sqrt{\frac{kT}{mc^2}}\nu_0$$

$$FWHM = \sqrt{\frac{8kT\ln 2}{mc^2}}\nu_0$$

Note line widths scale linearly with frequency

Doppler vs Pressure Broadening : IR vs MW





Pressure broadening dominates in the MW, we can neglect Doppler broadening in <u>most</u> applications (not mesospheric sounding though)

Line-by-line to fast models (eg RTTOV)

- Use LbL to generate optical depths (_) in discrete layers, given inputs:
  - $\_{0}$, _, S_i - for each line in the spectral region of interest
  - P, T, q – for each layer, for a range of profiles (1000's)

- For each layer, find coefficients A, which solve (in a least squares sense) :

$$y = A.x$$

where (for a single frequency) :

y = vector of simulated optical depths (1×N)
x = matrix of predictors, constructed from p,T and q (M×N)
A= vector of coefficients (1×M)

(M = no of predictors, N = no. of profiles)

Fast Models: *eg* RTTOV

- For a given input profile (x), generate optical depths (tau) in each layer, using an expression of the form:

$$\tau = \sum_{i=1}^{n} a_i P_i$$

n = number of predictors, typically ~ 20
eg. T, q, T^2,….

- Predictors are simple functions of input profile
- Fast: ~1mS per profile
- K, TL, AD generated from 'direct' code
- Fast models now capable of :
  - Scattering calculations in MW & IR
    – allowing cloud/rain analysis
  - Modelling trace gas effects (eg CO_2, CO, CH_4, O_3, N_2O)

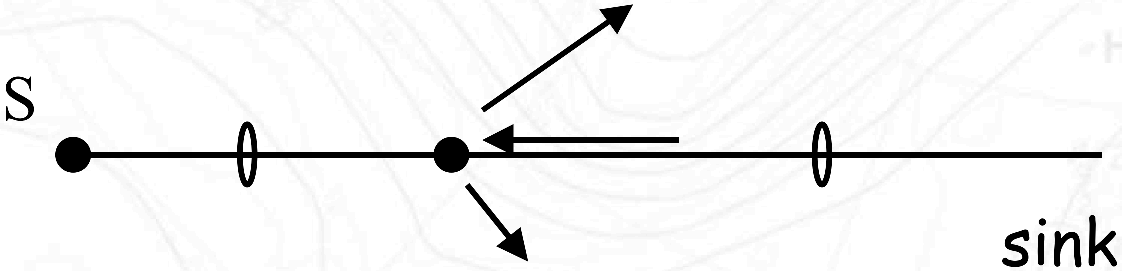
Fast RT models (*eg* RTTOV)

Version	Function	Input	Output
'Direct'	Forward calculation: generate T_B from profile (x)	· Profile (x) · Channel specifications · Observation geometry	Radiances, usually as brightness temperatures (T_B) for all channels.
K	Generate full Jacobian matrices (H)	[as for direct]	Arrays containing H (= dT_B/dx …) for all profile variables, and channels.
TL	Generate increments in radiance (_T_B) from increments in profile variables	[as for direct] + … increments in profile variables (_x)	Increments in radiances (_T_B)
AD	Generate gradients of cost wrt profile variables from gradients of cost wrt T_B.	[as for direct] + normalised departures: $R^{-1}.d$ $= R^{-1}(y-H(x_b))$ or $R^{-1}(y-H(x_b)-H\_x)$	Gradients of cost wrt Profile variables.

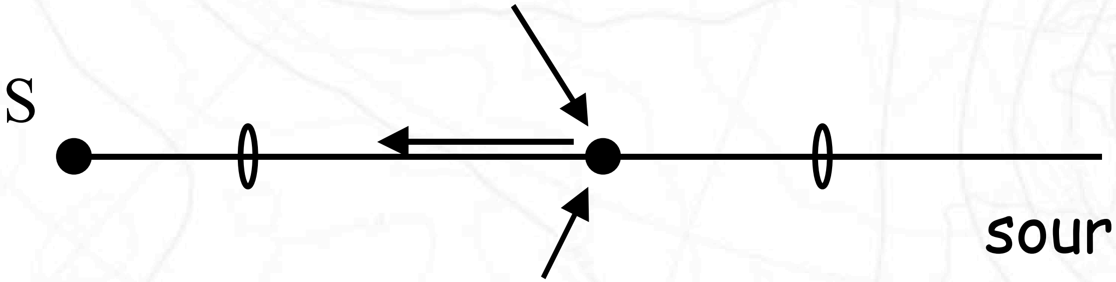
RT with scattering

Recall clear sky RT, where the change in radiant intensity along a path was given by the sum of sink (absorption) and source (emission) terms.

Scattering contributes to both sink and source terms:



sink: $dI_{ext} = -\beta_e I ds$



source: dI_{scat}

RT with scattering

$$dI = dI_{ext} + dI_{emit} + dI_{scat}$$

$$dI_{scat} = \frac{\beta_s}{4\pi}\int_{4\pi} p(\hat{\Omega}', \hat{\Omega}) I(\hat{\Omega}') d\omega' ds$$

$$\frac{1}{4\pi}\int_{4\pi} p(\hat{\Omega}', \hat{\Omega}) d\omega' = 1$$

normalised *phase* function, represents scattering from angles Ω' into view direction Ω

$$dI = -\beta_e I ds + \beta_a B ds + \frac{\beta_s}{4\pi}\int_{4\pi} p(\hat{\Omega}', \hat{\Omega}) I(\hat{\Omega}') d\omega' ds$$

then, dividing through by: $d\tau = -\beta_e ds$

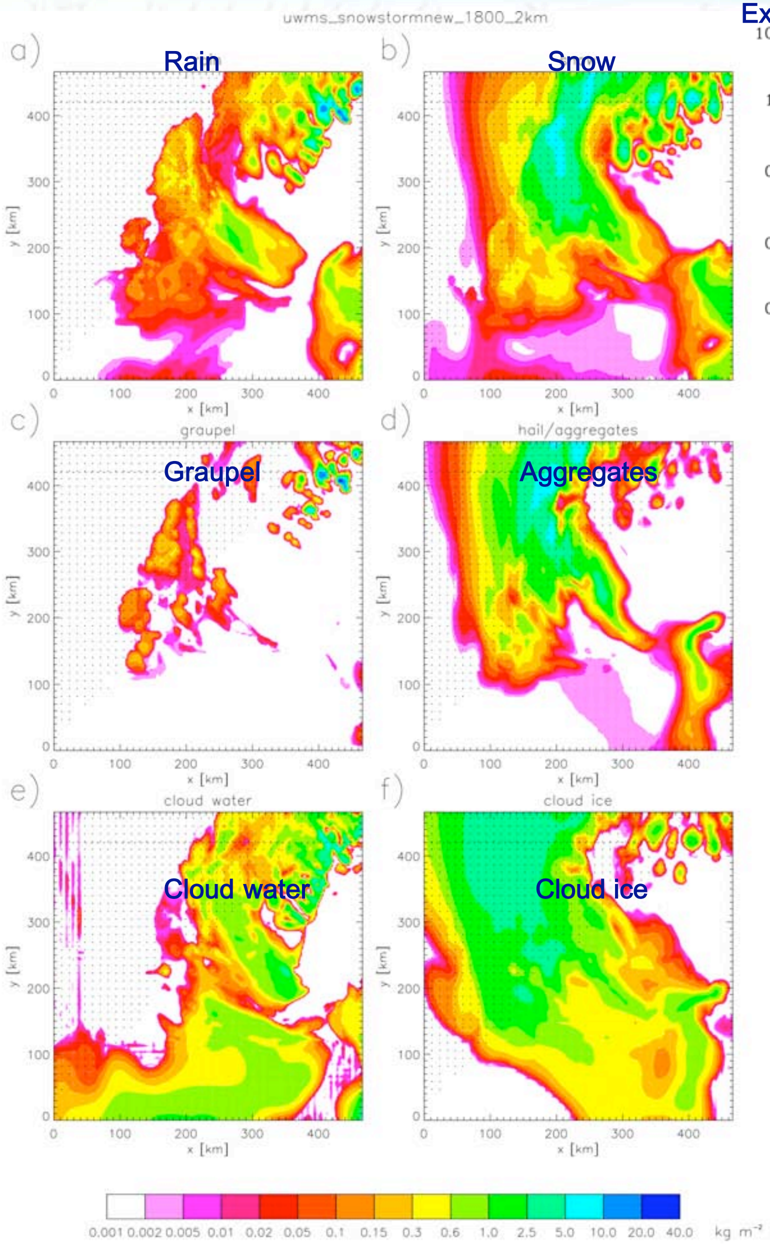
$$\frac{dI(\hat{\Omega})}{d\tau} = I(\hat{\Omega}) - (1-\overline{\omega})B - \frac{\overline{\omega}}{4\pi}\int_{4\pi} \underline{p(\hat{\Omega}', \hat{\Omega})} I(\hat{\Omega}') d\omega'$$

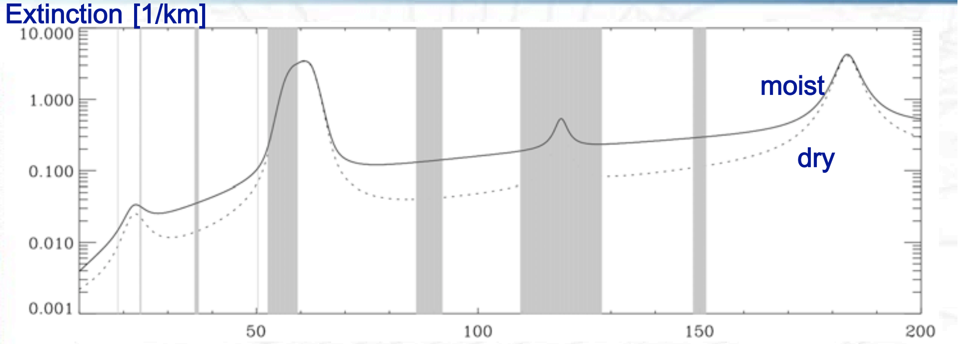
scattering albedo

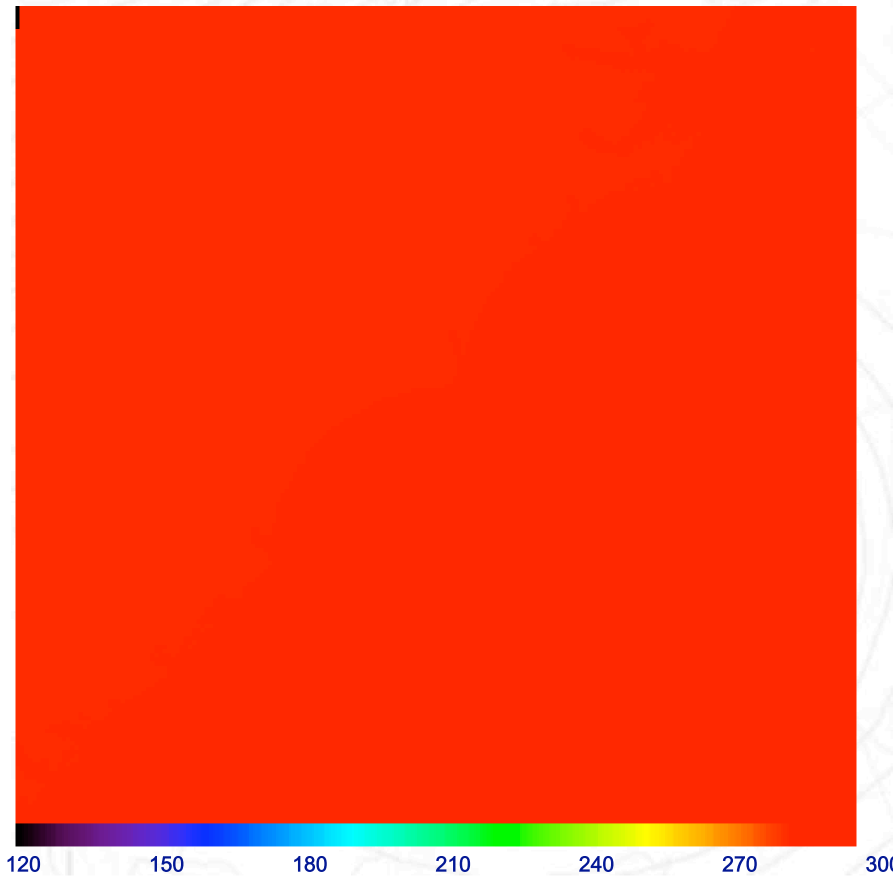
phase function

- Scattering albedo and phase function (asymmetry parameter for Henyey-Greenstein phase function) are pre-computed using Mie theory, and stored in look up tables.
- Look-up tables are indexed by hydrometeor amounts (for rain, snow, cloud water, cloud ice)
- See Appendix for details, also Bauer *et al*, QJRMS, 2006, Vol.132, pp.1259-1281.

Combined cloud-radiative transfer modelling







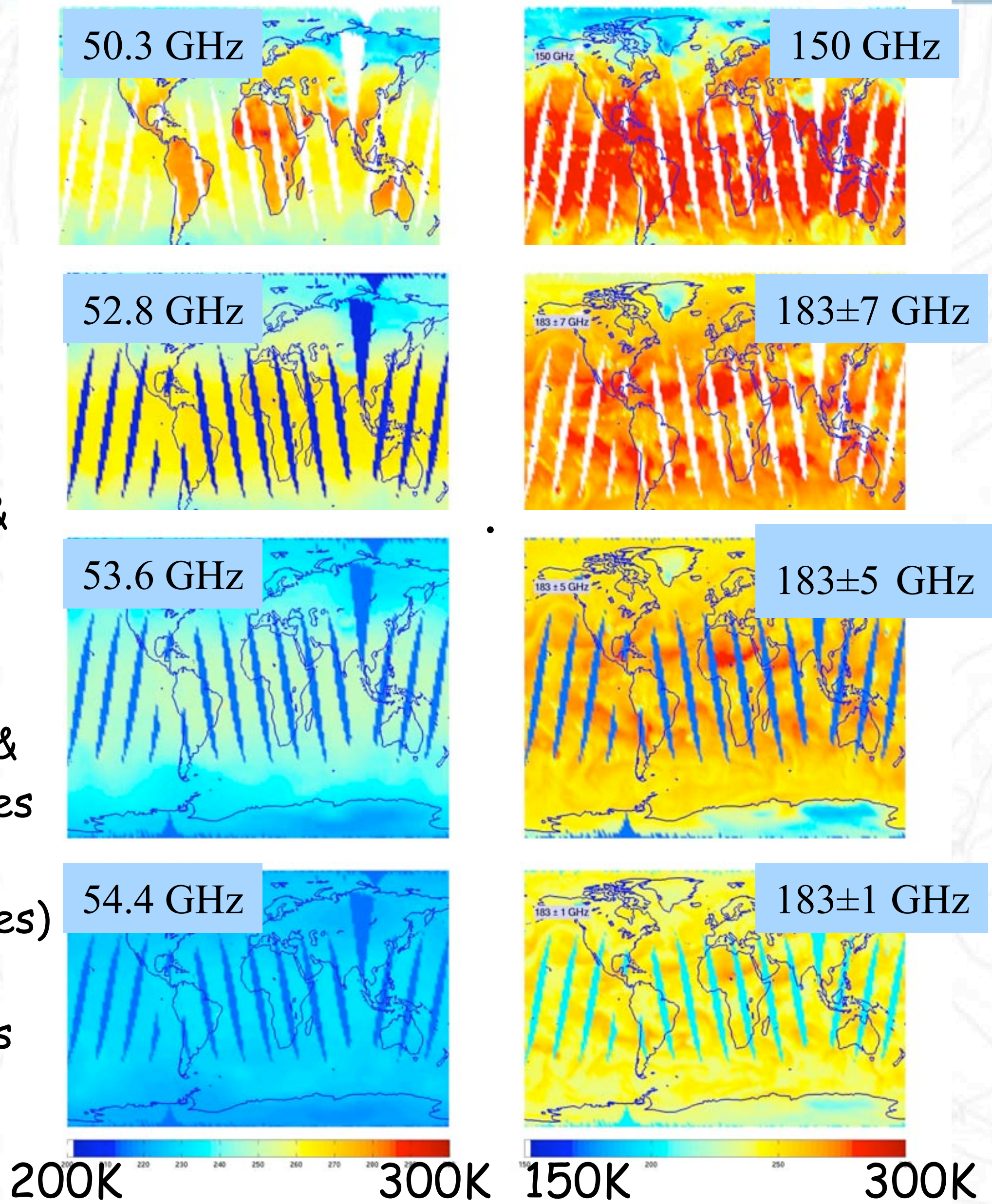
Summary

MW data
v. important
for NWP !

50 GHz
W. Fns span
troposphere/
stratosphere &
give info on T

MW
Spectroscopy &
RT in clear skies
is relatively
simple (few lines)

Fast RT models
used in DA



183 GHz channels
are centred on
H_2O line,
channels selected
to give vertical
coverage.

MW scattering
RT more complex
but Fast RT
models now
available

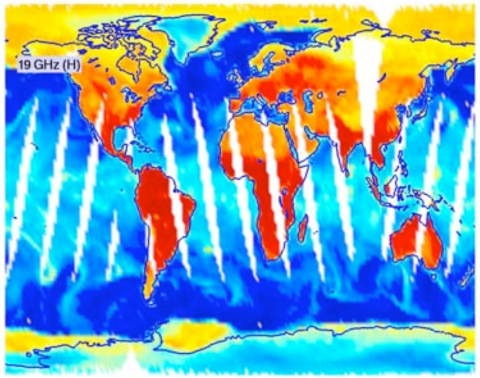
Summary

Ocean surface is polarising, This gives ocean WS information

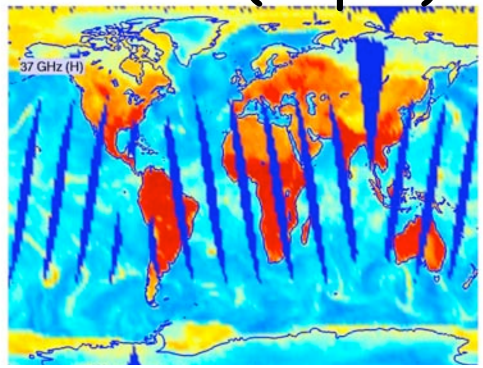
22 GHz (& 19/37/85) gives information on WV and cloud although vertical resolution is limited (wrt IR)

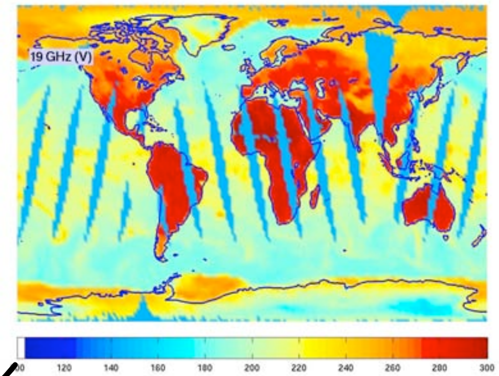
Land surface emissivity is more difficult to model, this restricts use of data over land

19 GHz (H pol)



37 GHz (H pol)

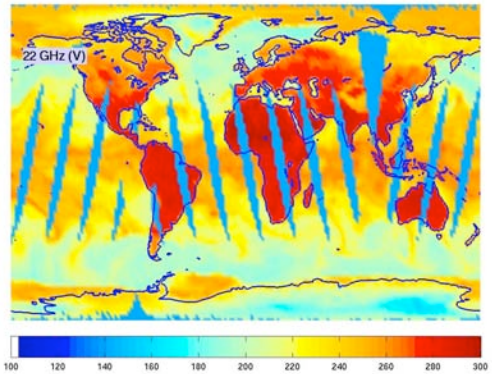




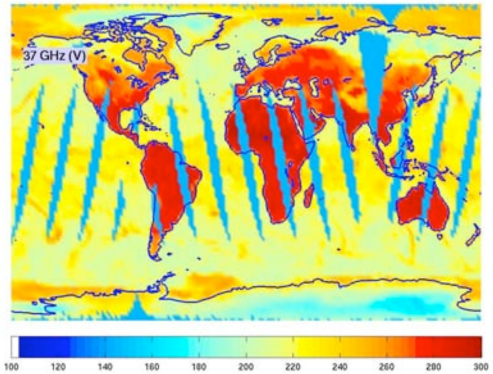
100K

300K

19 GHz (V pol)



22 GHz (V pol)



37 GHz (V pol)