Météo-France T-matrix code documentation

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Contents

1 Introduction

The T-matrix method is a computational technique of light scattering by nonspherical particles originally formulated by [Waterman](#page-16-0) (1965) . The T-Matrix (**T** for **Transition-matrix**) allows to calculate the scattered field for a given incident field. More explanations are given for example in the PhD manuscrit section 1.2.1 of [Le Bastard](#page-15-0) [\(2019\)](#page-15-0)). The dual-polarization radar variables can then be calculated from the scattering coefficients, for a given radar wavelength.

The code used at Météo France is derived from [Mishchenko and Travis](#page-15-1) [\(1994\)](#page-15-1) code and has originally been downloaded from:

http://www.giss.nasa.gov/staff/mmishchenko/t_matrix.html

The version used is : Extended-precision T-matrix code for nonspherical particles in a fixed orientation: amplq.lp.f, lpq.f, and amplq.par.f In order to run the code, it is necessary to install LAPACK packages:

<http://www.netlib.org/lapack/>

The Météo-France T-matrix version includes 2 programs:

- Tmatrix.f (fortran 77): computation of the scattering coefficients for a single hydrometeor with a given shape/diameter/dielectric constant
- TmatInt.f90 (fortran 90): integration of the scattering coefficients over the particle size distribution

This code was first created at Météo-France by [Al-Sakka](#page-14-2) et al. [\(2013\)](#page-14-2) and has been continually upgraded, and used for the studies of [Augros](#page-14-3) et al. [\(2016\)](#page-14-3), [Taufour](#page-16-1) et al. [\(2018\)](#page-16-1), [Borderies](#page-14-4) [et al.](#page-14-4) [\(2018\)](#page-14-4), [Le Bastard](#page-15-2) et al. [\(2019\)](#page-15-2) and [Thomas](#page-16-2) et al. [\(2020\)](#page-16-2).

2 Program Tmatrix.f

This program computes back- and forward scattering coefficients (from which one can calculate the polarimetric variables) for a given radar wavelength. The coefficients are computed for different particle sizes. They are function of elevation angle, radar wavelength, temperature, liquid water fraction and hydrometeor type. The program parameters are defined in a parameter file, which is read in the beginning of the program. Calculation of scattering coefficients is made by the procedure TMD.

Out of this procedure, the scattering coefficients (S11, S22, S11f, S22f) and DPOL variables are written in two different files, for a range a temperature values, elevation angles, diameters and liquid water fraction (for graupel).

2.1 Steps of the program

- 1. Reading of the hydrometeor constants file: contains a_j and b_j coefficients for the mass diameter relation: $m(D) = a_i * D^{b_j}$
- 2. Reading of the parameter file "TmatParam_BandType" (see example in [Figure 1\)](#page-2-2):

contains the hydrometeor type, the options for oscillation (oscill and sigbeta), for the dieletric constant (DIEL), for the aspect ratio (CEPS) and the min/step/max ranges of the varying parameters: radar wavelength (LAM), radar elevation (ELEV), temperature in degree C (Tc), exponent (expD) of the spherical equivalent diameter (D) , and mass water fraction (F_w) .

3. Loops over LAM, Tc, ELEV, F_w and D (spherical equivalent diameter)

Calculation of:

- aspect ratio $r = \frac{1}{\sqrt{15}}$ EP S
- maximum diameter D_m
- partially melted equivalent diameter $(D_{eq}:$ needed as input of the TMD subroutine) and fully melted equivalent diameter (D_{eqr})
- dielectric constant EPSX
- 4. Call of procedure TMD, which retrieves the scattering coefficients S11, S22, S11f, S22f as a function of LAM, ELEV, Tc, D_{eq} , oscill, sigbeta, EPSX, EPS
- 5. Calculation of DPOL variables from the T-matrix scattering coefficients using the equations detailed in Appendix of [Augros](#page-14-3) et al. [\(2016\)](#page-14-3).

Ouvrir ⊡			TmatParam_Srr ~/Programmes/T
		l type:rr	
		2 oscill:0	
		3 sigbeta:1	
		4 DIEL: 1	
		5 CEPS: 1	
		6 LAMmin: 106.2	
		7 LAMmax: 106.2	
		8 LAMstep:0.1	
		9 ELEVmin:0.0	
		10 ELEVmax:20.0	
		11 ELEVstep:4.0	
		12 Tcmin:-20.0	
		13 Tcmax:40.0	
		14 Tcstep:1.0	
		15 expDmin:0.0	
		16 expDmax:3.0	
		17 expDstep:0.1	
		18 Fwmin:0.0	
		19 Fwstep:0.1	
		20 Fwmax: 0.0	

Figure 1: Example of a parameter file for rain at S-band

- 6. Calculation of DPOL variables (ZhhR, ZvvR et KdpR) using the theory of Rayleigh for spheroids. The corresponding equations are detailed in section 3.4.3 of [Caumont](#page-15-3) [\(2007\)](#page-15-3).
- 7. Writing of the scattering coefficients and DPOL variables in two distinct files: TmatCoefDiff_Srr and TmatVarPol_Srr (example for rain at S band)

2.2 Options and equations for aspect ratio, diameters, dieletric constant and oscillation

2.2.1 Aspect ratio r

The option for aspect ratio r is determined by parameter CEPS.

The variable needed as input of the T-matrix TMD routine is:

$$
EPS = \frac{1}{r}
$$

1. Rain

 $CEPS = 1$

The aspect ratio of raindrops r_r follows the formulation of [Brandes](#page-15-4) *et al.* [\(2002\)](#page-15-4), as in [Ryzhkov](#page-16-3) et al. [\(2011\)](#page-16-3).

$$
r_r = 0.9951 + 0.02510D - 0.03644D^2 + 0.005303D^3 - 0.0002492D^4 \tag{1}
$$

with D the spherical equivalent diameter in mm

2. Primary ice

In a first approximation, pristine ice crystals are modelled as spheres because of their random orientation, as done in [Caumont](#page-15-5) et al. [\(2006\)](#page-15-5).

 $CEPS = 5$

3. Snow

 $CEPS = 6$

• Dry snow

The aspect ratio of dry aggregated snow varies between 0.6 and 0.8 [Straka](#page-16-4) [\(2000\)](#page-16-4). In this code, it is assumed to be 0.75 as in Jung *[et al.](#page-15-6)* [\(2008\)](#page-15-6). But to avoid higher Z_{dr} for low diameters due to higher snow density, a linear decrease in the axis ratio from 1 to 0.75 for diameters from 0 to 8 mm and a constant axis ratio of 0.75 for diameters higher than 8 mm is simulated (see section 3.3.2 of [Augros](#page-14-3) *et al.* [\(2016\)](#page-14-3)):

$$
r_s = \begin{cases} 1 - \frac{1 - 0.75}{8 - 0} D & \text{si } D \le 8 \text{ mm} \\ 0.75 & \text{si } D > 8 \text{ mm} \end{cases}
$$
(3)

• Wet snow

In [Augros](#page-14-3) et al. [\(2016\)](#page-14-3), snow is considered dry only because in the ICE3 microphysics scheme, graupel is the only ice species that can have a wet growth mode. When the air temperature is warmer than $0 °C$, small primary ice crystals are immediately converted into cloud water, snowflakes are transferred into the graupel category and finally graupel particles melt by shedding all the liquid water into raindrops (see Appendix of [Lascaux](#page-15-7) *et al.* [\(2006\)](#page-15-7)).

However, in the T-matrix code, the parametrization of wet snow is possible, if a dedicated parameter file for wet snow (TmatParam_Sws) is created with a range of F_w values between 0 and 1.

In that case, the axis ratio of wet snow is parametrized as a combination of the axis ratios of dry snow and rain, following equation (14) of [Ryzhkov](#page-16-3) *et al.* (2011) :

$$
r_{ws} = r_s + F_w(r_r - r_s) \tag{4}
$$

In this equation, the axis ratio of rain r_r is estimated with [Equation 1](#page-2-3) but the spherical equivalent diameter D is replaced by the fully melted equivalent diameter D_{ear} (see estimation in [2.2.3\)](#page-4-1).

4. Graupel

 $CEPS = 9$

• Dry Graupel

The aspect ratio of dry graupel r_q is the one proposed by [Ryzhkov](#page-16-3) *et al.* [\(2011\)](#page-16-3):

$$
r_g = \begin{cases} 1 - 0.02D & \text{if } D \le 10 \text{ mm} \\ 0.8 & \text{if } D > 10 \text{ mm} \end{cases}
$$
 (5)

$$
r_i = 1 \tag{2}
$$

 $r_g = 0.8$ mm for $D > 10$ mm in the study of [Le Bastard](#page-15-0) [\(2019\)](#page-15-0) but $r_g = 0.85$ mm for $D > 10$ mm in the study of [Augros](#page-14-3) *et al.* [\(2016\)](#page-14-3) to account for oscillation that is neglected as explained in section 3.3.3 of [Augros](#page-14-3) et al. [\(2016\)](#page-14-3).

• Wet graupel

The aspect ratio of wet graupel r_{wg} follows the formulation of [Ryzhkov](#page-16-3) *et al.* [\(2011\)](#page-16-3), deduced from the experimental results of [Rasmussen](#page-16-5) et al. [\(1984\)](#page-16-5):

$$
\begin{bmatrix}\nr_{wg} = \n\begin{cases}\nr_g - 5.0(r_g - 0.8)F_w & \text{if } F_w \leq 0.2 \\
0.88 - 0.40F_w & \text{if } 0.2 < F_w \leq 0.8 \\
2.8 - 4.0r_w + 5.0(r_w - 0.56)F_w & \text{if } F_w > 0.8\n\end{cases}\n\end{bmatrix}\n\tag{6}
$$

where r_w is the aspect ratio of a raindrop of diameter D_{eqr} , which is produced as a result of the graupel melting.

2.2.2 Maximum diameter D_m

The maximum diameter D_m of the spheroid is expressed as a function of the spherical equivalent diameter D using:

$$
D_m = D EPS^{\frac{1}{3}}
$$

$$
D_m = D r^{-\frac{1}{3}}
$$
(7)

2.2.3 Description of the melting process and estimation of D_{eq} and D_{eqr}

In MesoNH, graupel is the only specie that can have a wet growth mode or that can be melting (see [Lascaux](#page-15-7) *et al.* [\(2006\)](#page-15-7)). However, in the T-matrix code, the parametrization of wet snow is possible as proposed by [Le Bastard](#page-15-0) [\(2019\)](#page-15-0), if a dedicated parameter file for wet snow is created with a range of F_w values between 0 and 1 (see their chapter 4.1).

 D_{eq} and D_{eq} are the partially and fully melted equivalent diameters. D_{eq} is needed as input of the TMD subroutine to compute the scattering coefficients. D_{ear} is needed for the melting species to estimate their axis ratio. D_{eqr} is also used in the integration of the scattering coefficients over the full Particule Size Distribution (PSD) that is done in TmatInt.f90 (see [section 3\)](#page-12-0). It is thus estimated for all species even those that are not potentially melted species (rain and primary ice).

1. Rain

$$
D_{eq} = D_{eqr} = D \tag{8}
$$

2. Primary ice

For primary ice, the liquid water fraction F_w is set to 0:

$$
D_{eq} = D \tag{9}
$$

The fully melted equivalent diameter D_{eqr} is calculated as a function of the density of liquid water ρ_w (1000 kg m⁻³) and primary ice ρ_i (kg m⁻³)

$$
D_{eqr} = \left(\frac{\rho_i}{\rho_w}\right)^{\frac{1}{3}} D \tag{10}
$$

with

$$
\rho_i = \frac{a_i D_m^{b_i}}{\frac{\pi}{6} D^3} \tag{11}
$$

 $a_i = 0.82$ and $b_i = 2.5$ are the ICE3 mass-diameter coefficients for primary ice. [Equation 10](#page-5-0) is also used by [Wolfensberger and Berne](#page-16-6) [\(2018\)](#page-16-6).

3. Snow

In [Augros](#page-14-3) *et al.* [\(2016\)](#page-14-3), the liquid water fraction F_w is set to 0: $D_{eq} = D$

But in the T-matrix code, the parametrization of a wet snow specie is possible, following [Le Bastard](#page-15-0) [\(2019\)](#page-15-0). In that case, the partially melted equivalent diameter D_{eq} is calculated as:

$$
D_{eq} = \left(\frac{\rho_s}{\rho_{ws}}\right)^{\frac{1}{3}} D \tag{12}
$$

where the density of wet snow ρ_{ws} (kg m⁻³) is estimated as a function of the mass water fraction F_w following equation (4) of Jung [et al.](#page-15-6) [\(2008\)](#page-15-6):

$$
\rho_{ws} = \rho_s (1 - F_w^2) + \rho_w F_w^2 \tag{13}
$$

 ρ_s is calculated like for primary ice with [Equation 11](#page-5-1) with $a_s = 0.02$ and $b_s = 1.9$.

 D_{eqr} is calculated like for primary ice with [Equation 10](#page-5-0) by replacing ρ_i by ρ_s .

4. Graupel

[Ryzhkov](#page-16-3) et al. [\(2011\)](#page-16-3) and [Rasmussen and Heymsfield](#page-16-7) [\(1987\)](#page-16-7) suggest that if the initial density of the dry hail or graupel is less than the one of a solid ice, water first soaks particle interior and fills all air cavities. Once melted water saturates the particle interior $(F_w = F_{w_{sat}})$, it starts building a water shell.

The different steps of the melting process are described hereafter following [Le Bastard](#page-15-0) [\(2019\)](#page-15-0) and illustrated in [Figure 2](#page-6-0) (see also Figure 1 of [Rasmussen and Heymsfield](#page-16-7) [\(1987\)](#page-16-7)).

• Step 0: $F_w = 0$

The initial volume of air cavities $V_c^{(i)}$ within the dry graupel $(F_w = 0)$ can be expressed using:

$$
V_c^{(i)} = V_g - V_i
$$

with V_i the volume occupied by pure ice

$$
V_i = \frac{m_i}{\rho_i} = \frac{m_g}{\rho_i} = \frac{\pi}{6} D^3 \frac{\rho_g}{\rho_i}
$$
\n(14)

with ρ_i the density of pure ice (916 kg m³)

Figure 2: Illustration of the graupel melting process as a function of mass water fraction F_w . Air (A), ice (I) and liquid water (W) are shown respectively in grey, white, and blue. The various combinations [matrix, inclusions] used to calculate the dielectric constant according to the Maxwell-Garnett approximation (see [2.2.5\)](#page-8-1) are also shown. Taken from Figure 4.1 of [Le Bastard](#page-15-0) [\(2019\)](#page-15-0).

 $\left(m_g = m_c + m_i = m_i\right)$ because the mass of air cavities $m_c{=}0)$ $V_c^{(i)}$ can thus be expressed as:

$$
V_c^{(i)} = \frac{\pi}{6} D^3 (1 - \frac{\rho_g}{\rho_i})
$$
\n(15)

• Step 1: $0 < F_w \leq F_{w_{sat}}$

When the graupel starts melting, the melted water first soaks the air cavities reducing the particle volume V_{wg} :

$$
V_{wg} = \frac{\pi}{6} D_{eq}^{3}
$$

$$
= \frac{\pi}{6} D^{3} - \frac{F_{w} m_{g}}{\rho_{g}}
$$

$$
V_{wg} = \frac{\pi}{6} D^{3} (1 - F_{w})
$$
 (16)

The equivalent diameter of the wet graupel D_{eq} is then:

$$
D_{eq} = (1 - F_w)^{\frac{1}{3}} D \tag{17}
$$

The volume of liquid water V_w formed due to the ice melting can be expressed as a function of the mass water fraction F_w , the particle mass $m_{wg} = m_g$ and the density of liquid water ρ_w :

$$
V_w = \frac{F_w m_g}{\rho_w}
$$

$$
V_w = \frac{\pi}{6} D^3 F_w \frac{\rho_g}{\rho_w}
$$
 (18)

As the graupel melts, the density of the cavities within the graupel is constant but their total volume (including both air and water) is reduced as is the graupel volume. The volume of the cavities can be expressed as:

$$
V_c = \frac{\pi}{6} D_{eq}^3 (1 - \frac{\rho_g}{\rho_i})
$$
\n(19)

The cavities are fully soaked when $V_c = V_w$. $F_{w_{sat}}$ can thus be estimated using:

$$
\frac{\pi}{6}D_{eq}^3(1-\frac{\rho_g}{\rho_i}) = \frac{\pi}{6}D^3F_{w_{sat}}\frac{\rho_g}{\rho_w}
$$

$$
(1-F_{w_{sat}})D^3(1-\frac{\rho_g}{\rho_i}) = D^3F_{w_{sat}}\frac{\rho_g}{\rho_w}
$$

$$
1-\frac{\rho_g}{\rho_i} = F_{w_{sat}}(\frac{\rho_g}{\rho_w}+1-\frac{\rho_g}{\rho_i})
$$

$$
F_{w_{sat}} = \frac{1-\frac{\rho_g}{\rho_i}}{1-\frac{\rho_g}{\rho_i}+\frac{\rho_g}{\rho_w}}
$$

$$
F_{w_{sat}} = \frac{\frac{1}{\rho_i}-\frac{1}{\rho_g}}{\frac{1}{\rho_i}-\frac{1}{\rho_g}-\frac{1}{\rho_w}}
$$
(20)

• Step 2: $F_w > F_{w_{sat}}$

Once fully soaked, the particle starts building a water shell.

At this stage, the graupel is composed of pure ice and water only. Its mass m_{wg} can be expressed as a function of the mass of ice m_i + the mass of water $m_{w_{tot}}$, including the water within the core and in the shell:

$$
m_{wg} = m_g = m_i + m_{w_{tot}} \tag{21}
$$

Thus, its volume V_{wg} is:

$$
V_{wg} = \frac{m_i}{\rho_i} + \frac{m_{w_{tot}}}{\rho_w}
$$

= $m_g \left(\frac{1 - F_w}{\rho_i} + \frac{F_w}{\rho_w} \right)$
= $\frac{\pi}{6} D^3 \rho_g \left(\frac{1 - F_w}{\rho_i} + \frac{F_w}{\rho_w} \right)$

We can deduce the equivalent diameter D_{eq} :

$$
D_{eq} = \left[\rho_g \left(\frac{1 - F_w}{\rho_i} + \frac{F_w}{\rho_w}\right)\right]^{\frac{1}{3}} D\right]
$$
 (22)

For graupel, the fully melted equivalent diameter D_{eqr} is calculated like for primary ice and snow with [Equation 10](#page-5-0) by replacing ρ_i by ρ_g .

2.2.4 Wet hydrometeor content and mass water fraction

As in Jung *[et al.](#page-15-6)* [\(2008\)](#page-15-6), graupel is assumed to be wet when graupel and rainwater coexist. Two options have been parametrized in the python forward operator program (the program that reads the output of the T-matrix code) to estimate the wet graupel content M_{wg} (kg m⁻³):

1. The rainwater content M_r (kg m⁻³) is added to the graupel content M_g , as done in [Le Bastard](#page-15-0) [\(2019\)](#page-15-0) and in [Wolfensberger and Berne](#page-16-6) [\(2018\)](#page-16-6):

$$
M_{wg} = M_g + M_r \tag{23}
$$

 M_q and M_r are set to 0

2. Only the dry graupel content M_{wg} is transferred to the wet graupel content, as done in [Augros](#page-14-3) et al. [\(2016\)](#page-14-3) and Jung [et al.](#page-15-6) [\(2008\)](#page-15-6):

$$
M_{wg} = M_g \tag{24}
$$

 M_q is set to 0 and rainwater coexists with wet graupel

In both cases, the mass water fraction within wet graupel F_w is estimated as:

$$
F_w = \frac{M_r}{M_g + M_r} \tag{25}
$$

2.2.5 Dielectric constant EPSX

1. Rain

 $DIEL=1$

The Debye model is used for rain as in [Caumont](#page-15-5) *et al.* [\(2006\)](#page-15-5):

$$
\epsilon_w = \epsilon_\infty + \frac{\epsilon_0 - \epsilon_\infty}{1 - i f/f_D},\tag{26}
$$

where ϵ_0 and ϵ_∞ are respectively the dielectric static and high frequency coefficients and f is the radar frequency (Hz), and f_D is the relaxation frequency (Hz). [Liebe](#page-15-8) *et al.* [\(1991\)](#page-15-8) gave the following values for these parameters :

$$
\epsilon_0 = 77,66 - 103,3\Theta \tag{27}
$$

$$
\epsilon_{\infty} = 0,066\epsilon_0 \tag{28}
$$

$$
f_D = (20, 27 + 146, 5\Theta + 314\Theta^2)10^9\tag{29}
$$

where the inverse relative temperature Θ is related to T (K) with the following formula:

$$
\Theta = 1 - \frac{300}{T} \tag{30}
$$

2. Snow, graupel and ice crystals

The effective permittivity ϵ_{eff} of non homogeneous hydrometeors can be estimated based on the Maxwell-Garnett approximation [\(Maxwell Garnett,](#page-15-9) [1904\)](#page-15-9), considering a matrix

medium with permittivity ϵ^{mat} and inclusions with permittivity ϵ^{inc} (e.g [Wolfensberger](#page-16-6) [and Berne](#page-16-6) [\(2018\)](#page-16-6)):

$$
\epsilon_{eff}(\epsilon^{mat}, \epsilon^{inc}, f_{vol}^{inc}) = \epsilon^{mat} \left(\frac{1 + 2f_{vol}^{inc} \epsilon^{inc} - \epsilon^{mat}}{1 - f_{vol}^{inc} \epsilon^{inc} + 2\epsilon^{mat}} \right) \tag{31}
$$

with f_{vol}^{inc} the volume fraction of the inclusions.

• Dry snow (DIEL=3), dry graupel (DIEL=7) and primary ice (DIEL=11) Dry solid hydrometeors consist of inclusions of ice in a matrix of air. In this case $\epsilon^{mat} \approx 1$, and $f_{vol}^{inc} = \frac{V_i}{V_i}$ $\frac{V_i}{V_d} = \frac{\rho_d}{\rho_i}$ $\frac{\rho u}{\rho_i}.$

The permittivity of the dry hydrometeor ϵ_d can be estimated following equation (4) in [Ryzhkov](#page-16-3) et al. (2011) :

$$
\epsilon_d = \frac{1 + 2\frac{\rho_d}{\rho_i} \frac{\epsilon_i - 1}{\epsilon_i + 2}}{1 - \frac{\rho_d}{\rho_i} \frac{\epsilon_i - 1}{\epsilon_i + 2}}
$$
(32)

where ρ_d is the density of the dry hydrometeor (snow, graupel or ice crystals), ϵ_i the dielectric constant of pure ice (estimated from [Hufford](#page-15-10) [\(1991\)](#page-15-10)), and ρ_i the density of pure ice $(0.916 \text{ g cm}^{-3}).$

• Wet graupel

$DIEL = 7$

The melting process of the graupel implemented is summarized in [Figure 2.](#page-6-0) In its initial state, the particle is dry and of fairly low density (between 100 and 200 kg m^{-3} depending on its size). When melting, the water first fills the outer cavities of the particle, forming a layer which is treated as an ice matrix with water inclusions. This outer layer plays the role of matrix for the whole particle while the core (still an air matrix with ice inclusions) plays the role of an inclusion. When the graupel is fully soaked with water $(F_w = F_{w_{sat}})$ it is considered as an ice matrix with water inclusions. Then, additional water accumulates at the surface of the particle. The latter is then represented as a matrix of liquid water with a water-saturated graupel inclusion.

In summary, when the water fraction increases, the particle can be successively considered as a matrix of water-saturated graupel (matrix of ice with water inclusions) with dry graupel inclusions (matrix of air with ice inclusions) and as a matrix of water with water-saturated graupel (matrix of ice with water inclusions). Then, we can express the effective permittivity as follows:

$$
\epsilon_{wg} = \begin{cases}\n\epsilon_{eff}(\epsilon_{eff}(\epsilon_i, \epsilon_w, f_{vol}^{iw}), \epsilon_{eff}(\epsilon_a, \epsilon_i, f_{vol}^{ai}), f_{vol}^{iw}^{-ai}) & \text{, if } F_w \leq F_{w_{sat}} \\
\epsilon_{eff}(\epsilon_w, \epsilon_{eff}(\epsilon_i, \epsilon_w, f_{vol}^{iw}), f_{vol}^{w}^{-iw}) & \text{, if } F_w > F_{w_{sat}}\n\end{cases},
$$
\n(33)

where f_{vol}^{iw} , f_{vol}^{ia} , f_{vol}^{iw} ^{ai} and f_{vol}^{w} are the volume fractions of the corresponding inclusions.

 f_{vol}^{iw} is the volume fraction of the cavities. It is constant all along the early stage of the melting process $(F_w \leq F_{w_sat})$. Consequently, f_{vol}^{iw} is equal to the ratio between the initial volume of the cavities (see [Equation 15\)](#page-6-1) and the initial volume of the particle:

$$
f_{vol}^{iw} = \frac{V_c^{(i)}}{V_g} = 1 - \frac{\rho_g}{\rho_i}
$$
\n(34)

 f_{vol}^{ai} is the volume fraction of ice in the initial particle:

$$
f_{vol}^{ai} = \frac{V_i}{V_g} = \frac{\rho_g}{\rho_i} \tag{35}
$$

The cavities are supposed to be evenly distributed within the graupel. Thus, the volume fraction of the core (made of ice and air) within the particle f_{vol}^{iw} ^{-ai} can be expressed as the ratio between the volume of the unfilled cavities in the core $V_c - V_w$ and the total volume of the cavities V_c :

$$
f_{vol}^{iw} = \frac{V_c - V_w}{V_c} \tag{36}
$$

Combining equations [17,](#page-6-2) [18](#page-6-3) and [19,](#page-7-0) we can retrieve:

$$
f_{vol}^{iw} = 1 - \frac{D^3}{D_{eq}^3} \frac{F_w \rho_g}{\rho_w \left(1 - \frac{\rho_g}{\rho_i}\right)}
$$

$$
f_{vol}^{iw} = 1 - \frac{F_w}{1 - F_w} \frac{\rho_i \rho_g}{\rho_i \rho_w - \rho_g \rho_w} \tag{37}
$$

 $f_{vol}^{w_iw}$ is the volume fraction of the inner core of the particle (ice + water filled cavities) once $F_w > F_{w_sat}$.

The volume of the core V_{core} can be estimated by considering the mass of ice within the core, which is equal to the total mass of ice of the particle:

$$
m_i = (1 - F_w)m_g
$$

 m_i can be also expressed as a function of the volume of the core V_{core} if we consider that the water is removed from the cavities:

$$
m_i = \rho_g V_{core}
$$

$$
V_{core} = (1 - F_w) \frac{m_g}{\rho_g}
$$

$$
= (1 - F_w) V_g
$$

$$
V_{core} = (1 - F_w)\frac{\pi}{6}D^3
$$
 (38)

$$
f_{vol}^{w} = \frac{V_{core}}{V_{wg}}
$$

$$
= \frac{(1 - F_w) \frac{\pi}{6} D^3}{\frac{\pi}{6} D_{eq}^3}
$$

$$
f_{vol}^{w_iw} = \frac{(1 - F_w)}{\rho_g \left(\frac{1 - F_w}{\rho_i} + \frac{F_w}{\rho_w}\right)}\tag{39}
$$

In summary, the volume fractions involved in the calculation of the effective permittivity of the melting graupel are:

$$
\begin{cases}\nf_{vol}^{iw} = 1 - \frac{\rho_g}{\rho_i} \\
f_{vol}^{ai} = \frac{\rho_g}{\rho_i} \\
f_{vol}^{iw_{ai}} = 1 - \frac{F_w}{1 - F_w} \frac{\rho_i \rho_g}{\rho_i \rho_w - \rho_g \rho_w} \\
f_{vol}^{w_{i}} = \frac{(1 - F_w)}{\rho_g \left(\frac{1 - F_w}{\rho_i} + \frac{F_w}{\rho_w}\right)}\n\end{cases} \tag{40}
$$

2.2.6 Compiling

• Before compiling:

for calculations for one hydrometeor type only, modify the loop over types:

DO idtype=1,1 for rain only, for example.

for calculations for one radar frequency band only, modify the loop over bandes:

DO idbande=3,3 for S-band only, for example.

• Compile with make: builds the executable Tmat

2.2.7 Running the program

- make sure an empty directory OUTPUT is present in DPOLSIMUL (otherwise create this directory: mkdir OUTPUT)
- make sure that the file ampl.par.f is present (in the same directory)
- make sure that the parameter files corresponding to the frequency band defined (band="S" for example) are present in the same directoty. For this example, files: TmatParam_Swg, TmatParam_Sgg, TmatParam_Srr, TmatParam_Sss, TmatParam_Sii
- Launch the command ./Tmat : creation of the following files for each hydrometeor type (example for rain here) :
	- TmatVarPol_Srr : contains
		- ∗ 3 first lines describing the content of the file : LAMmin LAMstep LAMmax ELEVmin ELEVstep ELEVmax Tcmin Tcstep Tcmax expDmin expDstep expDmax Fwmin Fwstep Fwmax
		- ∗ the dualpol variables for a range of wavelengths, temperatures, elevation angles, liquid water fractions (Fw) in case of type w (melting graupel), and diameters: LAM, Tc, ELEV, Fw, D, Deq, ZhhlgR, ZvvlgR, Zhhlg, Zvvlg, Zdrlg, Rhv, KDP, KdpR, Adp, Ah, Av, Deltaz
	- TmatCoefDiff_Srr : contains
- ∗ 3 first lines describing the content of the file : LAMmin LAMstep LAMmax ELEVmin ELEVstep ELEVmax Tcmin Tcstep Tcmax expDmin expDstep expDmax Fwmin Fwstep Fwmax
- ∗ the real and imaginary parts of the scattering coefficients (f for forward scattering), and Zhh, Zvv et Kdp calculated with Rayleigh for spheroid scattering method:

LAM, Tc, ELEV, Fw, D, Dm, Deq, Deqm, Deqr, Deqrm, REAL(S11), AIMAG(S11), REAL(S22), AIMAG(S22), REAL(S11f), AIMAG(S11f), REAL(S22f), AIMAG(S22f), ZhhR, ZvvR, KdpR

 $-$ TmatResu Srr : this file contains just some information that the user can select to print if needed (like the dielectric constant)

3 Program TmatInt.f90

Reading of scattering coefficients files (like TmatCoefDiff Srr) produced by the previous program and integration over diameters (from the particle size distribution PSD) in order to build new tables with integrated coefficients.

3.1 Steps of the program

- 1. Loops over the band and the hydrometeor type
- 2. Reading of the hydrometeor constants file for PSD calculations $+$ the rain constant file (for the equivalent melted hydrometeor)
- 3. Reading of the min/step/max for LAM, ELEV, Tc, expD and Fw in the 2nd line of the scattering coefficients file
- 4. Reading of the coefficients RES11, IMS11, RES22, IMS22, RES11f, IMS11f, RES22f, IMS22f for each values of LAM, ELEV, Tc, expD and Fw
- 5. Loops over wavelengths LAM, temperature Tc, elevation ELEV, 3d parameter of the table P3 (liquid water fraction Fw if 1-moment, concentration CC if 2-moments), and hydrometeor content M
	- (0) Step 0: calculation of the "liquid" and "solid" parts of the contents (M_{rr}) and M_{ss}) with a Riemman sum (integration over diameters)

The purpose of this step is to calculate a first estimation of the "liquid" and "solid" parts of the distribution $(N_{rr}$ and $N_{ss})$ and of the "liquid" and "solid" parts of the hydrometeor content when doing the Riemann sum $(M_{rr}$ and $M_{ss})$.

- loop over diameters (D in mm)
	- calculation of the position (kTmat) of the parameters (LAM, Tc, ELEV, P3, M, D) in the table
	- reading of all diameters and coefficients in the table
	- number concentration of the "solid part" $N_{ss} = PSD_{ss} [(1 F_w)M, D_m],$ and "liquid part" of the distribution $N_{rr} = PSD_{rr}(F_wM, D_{eqr_m})$

– Liquid M_{rr} and solid M_{ss} parts of the content (in case of a wet specie):

$$
M_{rr} = \sum_{D_{min}}^{D_{max}} a_{rr} D_{eqr_m}^{b_{rr}} N_{rr} (D_{eqr_m}) \times 0.5 (D_{eqr_{m_{sup}}} - D_{eqr_{m_{inf}}}) \tag{41}
$$

$$
M_{ss} = \sum_{D_{min}}^{D_{max}} a_{ss} D_m^{b_{ss}} N_{ss}(D_m) \times 0.5(D_{m_{sup}} - D_{m_{inf}})
$$
(42)

(1) Step 1: correction of N_{rr} and N_{ss}

To ensure the correspondence between the initial content M and the recalculated content M_{int} after integration with the Riemann sum, a corrective factor $\frac{M}{M_{int}}$ is applied to the particle numbers N_{rr} and N_{ss} before computation of the radar variables through integration over the PSD.

- loop over diameters (D in mm)
	- calculation of the position (kTmat) of the parameters (LAM, Tc, ELEV, P3, M, D) in the table
	- reading of all diameters and coefficients in the table
	- estimation of the fall velocity of the wet specie v_w by combining the rain and solid hydrometeor fall velocities $(v_{rr}$ and $v_{ss})$: eq 4.15 p 93 in [Le Bastard](#page-15-0) [\(2019\)](#page-15-0), following [Wolfensberger and Berne](#page-16-6) [\(2018\)](#page-16-6) and Mitra (1990)
	- Application of the corrective factor to the number concentrations:

*
$$
N_{ss}
$$
 is multiplied by $\frac{(1 - F_w)M}{M_{ss}}$
\n* N_{rr} is multiplied by $\frac{F_w M}{M}$

number concentration $N(D_{eq})$:

 M_{rr} – Combination of the liquid and solid parts of the distribution following Szyrmer and Zawadzki (1999) and used by [Wolfensberger and Berne](#page-16-6) [\(2018\)](#page-16-6) and [Le Bas](#page-15-0)[tard](#page-15-0) [\(2019\)](#page-15-0) (see their equation 4.20 p 107) to compute the total particle

$$
N(D_{eq}) = (1 - F_w) \frac{v_{ss}}{v_w} N_{ss}(D_{eq}) + F_w \frac{v_r}{v_w} N_{rr}(D_{eq})
$$
 (43)

Another formulation for the estimation of the number concentration for wet hydrometeors (called the "weighted PSD approach") is also proposed by [Wolfensberger and Berne](#page-16-6) [\(2018\)](#page-16-6) with their equation (41). This formulation has not yet been implemented in the T-matrix code.

– Recalculation of the total content M_{int} after integration using the total particle number concentration $N(D_{eq})$

$$
M_{int} = \sum_{D_{min}}^{D_{max}} a_{rr} D_{eqr_m}^{b_{rr}} N(D_{eq}) \times 0.5 \left(D_{eq_{m_{sup}}} - D_{eq_{m_{inf}}} \right) \tag{44}
$$

(2) Step 2: correction of the total particle number concentration N

- loop over diameters
	- re-computation of N_{rr} and N_{ss} and application of the corrective factors as in Step 1
	- re-computation of $N(D_{eq})$ as in Step 1
- application of the corrective factor $\frac{M}{M}$ $\frac{m}{M_{int}}$ to $N(D_{eq})$
- computation of the integrated rainfall rate RR_{int}
- integration of the scattering coefficients over the PSD:
- integration of Zhh, Zvv et Kdp calculated with Rayleigh for spheroid scattering
- writing of the integrated coefficients in the output file: TmatCoefInt ICE3 S106.2 rr (example for ICE3, S band and rain)
- computation of the radar variables (but for a single hydrometeor type) Z_{hh} , Z_{dr} , K_{dp} , ρ_{hv} , A_{dp} (differential attenuation), A_h and A_v (specific attenuation on the H and V polarizations), δ_{hv} (back-scattering differential phase)
- writing of the radar variables in the output file (for example TmatVarInt ICE3 S106.2 rr)

3.2 Compiling

- before compiling, choose the frequency band in the beginning of the file (they should be the same as those selected in the previous program)
- compiling with the command make $-$ f makeTmatInt \Rightarrow build the executable TmatInt

3.3 Running the program

- INPUT: you need to have files like TmatCoefDiff Sgg, for each hydrometeor type
- RUN: ./TmatInt
- OUTPUT: files TmatCoefInt Srr and TmatVarInt Srr with integrated scattering coefficients and dualpol variables
	- TmatCoefInt_Srr: Tc, ELEV, P3, M, S11carre, S22carre, REAL(S22S11), AIMAG(S22S11), ReS22fmS11f, ImS22ft, ImS11ft, RRint
	- TmatVarInt_Srr: Tc, ELEV, P3, M, Zhhlg, Zvvlg, Zdrlg, Rhv, KDP

References

- Al-Sakka H, Boumahmoud AA, Fradon B, Frasier SJ, Tabary P. 2013. A new fuzzy logic hydrometeor classification scheme applied to the French X, C and S-band polarimetric radars. Journal of Applied Meteorology and Climatology 52(2013): 2328–2344, URL [http:](http://journals.ametsoc.org/doi/abs/10.1175/JAMC-D-12-0236.1) [//journals.ametsoc.org/doi/abs/10.1175/JAMC-D-12-0236.1](http://journals.ametsoc.org/doi/abs/10.1175/JAMC-D-12-0236.1).
- Augros C, Caumont O, Ducrocq V, Gaussiat N, Tabary P. 2016. Comparisons between S, C, and X band polarimetric radar observations and convective-scale simulations of HyMeX first special observing period. Quarterly Journal of the Royal Meteorological Society 142, Issue S1: $347-362$, doi:10.1002/qj.2572, URL <http://dx.doi.org/10.1002/qj.2572>.
- Borderies M, Caumont O, Augros C, Bresson E, Delanoë J, Ducrocq V, Fourrié N, Bastard TL, Nuret M. 2018. Simulation of w-band radar reflectivity for model validation and data assimilation. Quarterly Journal of the Royal Meteorological Society 144(711): 391–403, doi:10. 1002/qj.3210, URL <https://rmets.onlinelibrary.wiley.com/doi/abs/10.1002/qj.3210>.
- Brandes EA, Zhang G, Vivekanandan J. 2002. Experiments in rainfall estimation with a polarimetric radar in a subtropical environment. Journal of Applied Meteorology 41(6): 674–685, URL [http://journals.ametsoc.org/doi/abs/10.1175/1520-0450\(2002\)](http://journals.ametsoc.org/doi/abs/10.1175/1520-0450(2002)041%3C0674:EIREWA%3E2.0.CO;2) [041%3C0674:EIREWA%3E2.0.CO;2](http://journals.ametsoc.org/doi/abs/10.1175/1520-0450(2002)041%3C0674:EIREWA%3E2.0.CO;2).
- Caumont. 2007. Simulation et assimilation de données radar pour la prévision de la convection profonde à fine échelle. PhD thesis, UNIVERSITÉ TOULOUSE III — PAUL SABATIER, URL <http://www.theses.fr/2007TOU30217>.
- Caumont O, Ducrocq V, Delrieu G, Gosset M, Pinty JP, Parent du Châtelet J, Andrieu H, Lemaître Y, Scialom G. 2006. A radar simulator for high-resolution nonhydrostatic models. Journal of Atmospheric and Oceanic Technology 23(8): 1049–1067, URL [http://journals.](http://journals.ametsoc.org/doi/abs/10.1175/JTECH1905.1) [ametsoc.org/doi/abs/10.1175/JTECH1905.1](http://journals.ametsoc.org/doi/abs/10.1175/JTECH1905.1).
- Hufford G. 1991. A model for the complex permittivity of ice at frequencies below 1 thz. International Journal of Infrared and Millimeter Waves $12(7)$: 677–682, URL [http://link.](http://link.springer.com/article/10.1007/BF01008898) [springer.com/article/10.1007/BF01008898](http://link.springer.com/article/10.1007/BF01008898).
- Jung Y, Zhang G, Xue M. 2008. Assimilation of simulated polarimetric radar data for a convective storm using the ensemble kalman filter. part i: Observation operators for reflectivity and polarimetric variables. Monthly Weather Review 136(6): 2228-2245, URL <http://journals.ametsoc.org/doi/pdf/10.1175/2007MWR2083.1>.
- Lascaux F, Richard E, Pinty JP. 2006. Numerical simulations of three different map iops and the associated microphysical processes. Quarterly Journal of the Royal Meteorological Society 132(619): 1907–1926, doi:10.1256/qj.05.197, URL [https://rmets.onlinelibrary.wiley.](https://rmets.onlinelibrary.wiley.com/doi/abs/10.1256/qj.05.197) [com/doi/abs/10.1256/qj.05.197](https://rmets.onlinelibrary.wiley.com/doi/abs/10.1256/qj.05.197).
- Le Bastard T. 2019. Utilisation des données radar volumiques et d'un modèle de pnt à haute résolution pour une meilleure estimation quantitative des précipitations en plaine et sur les massifs montagneux. PhD thesis, École doctorale Sciences de l'univers, de l'environnement et de l'espace (Toulouse), URL <https://www.theses.fr/2019INPT0140>.
- Le Bastard T, Caumont O, Gaussiat N, Karbou F. 2019. Combined use of volume radar observations and high-resolution numerical weather predictions to estimate precipitation at the ground: methodology and proof of concept. Atmospheric Measurement Techniques 12(10): 5669–5684, doi:10.5194/amt-12-5669-2019, URL [https://www.atmos-meas-tech.](https://www.atmos-meas-tech.net/12/5669/2019/) [net/12/5669/2019/](https://www.atmos-meas-tech.net/12/5669/2019/).
- Liebe HJ, Hufford GA, Manabe T. 1991. A model for the complex permittivity of water at frequencies below 1 thz. International Journal of Infrared and Millimeter Waves 12(7): 659– 675, URL <http://link.springer.com/article/10.1007/BF01008897>.
- Maxwell Garnett J. 1904. Colours in metal glasses and in metallic films. Proceedings of the Royal Society of London 73(488-496): 443-445, URL [http://rspl.royalsocietypublishing.org/](http://rspl.royalsocietypublishing.org/content/73/488-496/443.full.pdf) [content/73/488-496/443.full.pdf](http://rspl.royalsocietypublishing.org/content/73/488-496/443.full.pdf).
- Mishchenko MI, Travis LD. 1994. T-matrix computations of light scattering by large spheroidal particles. Optics communications 109(1): 16–21, URL [http://www.sciencedirect.com/](http://www.sciencedirect.com/science/article/pii/0030401894907315) [science/article/pii/0030401894907315](http://www.sciencedirect.com/science/article/pii/0030401894907315).
- Rasmussen RM, Heymsfield AJ. 1987. Melting and shedding of graupel and hail. part i: Model physics. Journal of the Atmospheric Sciences 44(19): 2754–2763, doi: 10.1175/1520-0469(1987)044<2754:MASOGA>2.0.CO;2, URL [https://doi.org/10.1175/](https://doi.org/10.1175/1520-0469(1987)044<2754:MASOGA>2.0.CO;2) [1520-0469\(1987\)044<2754:MASOGA>2.0.CO;2](https://doi.org/10.1175/1520-0469(1987)044<2754:MASOGA>2.0.CO;2).
- Rasmussen RM, Levizzani V, Pruppacher HR. 1984. A wind tunnel and theoretical study on the melting behavior of atmospheric ice particles: Iii. experiment and theory for spherical ice particles of radius > 500 µm. *Journal of the Atmospheric Sciences* 41(3): 381–388, doi: 10.1175/1520-0469(1984)041<0381:AWTATS>2.0.CO;2, URL [https://doi.org/10.1175/](https://doi.org/10.1175/1520-0469(1984)041<0381:AWTATS>2.0.CO;2) [1520-0469\(1984\)041<0381:AWTATS>2.0.CO;2](https://doi.org/10.1175/1520-0469(1984)041<0381:AWTATS>2.0.CO;2).
- Ryzhkov A, Pinsky M, Pokrovsky A, Khain A. 2011. Polarimetric radar observation operator for a cloud model with spectral microphysics. Journal of Applied Meteorology and Climatology 50(4): 873–894, doi:10.1175/2010JAMC2363.1, URL [http://dx.doi.org/10.1175/](http://dx.doi.org/10.1175/2010JAMC2363.1) [2010JAMC2363.1](http://dx.doi.org/10.1175/2010JAMC2363.1).
- Straka. 2000. Bulk hydrometeor classification and quantification using polarimetric radar data: Synthesis of relations. JOURNAL OF APPLIED METEOROLOGY .
- Taufour M, Vié B, Augros C, Boudevillain B, Delanoë J, Delautier G, Ducrocq V, Lac C, Pinty JP, Schwarzenböck A. 2018. Evaluation of the two-moment scheme lima based on microphysical observations from the hymex campaign. Quarterly Journal of the Royal Meteorological Society 144(714): 1398-1414, doi:10.1002/qj.3283, URL [https://rmets.onlinelibrary.](https://rmets.onlinelibrary.wiley.com/doi/abs/10.1002/qj.3283) [wiley.com/doi/abs/10.1002/qj.3283](https://rmets.onlinelibrary.wiley.com/doi/abs/10.1002/qj.3283).
- Thomas G, Mahfouf JF, Montmerle T. 2020. Toward a variational assimilation of polarimetric radar observations in a convective-scale numerical weather prediction (nwp) model. Atmospheric Measurement Techniques 13(5): 2279–2298, doi:10.5194/amt-13-2279-2020, URL <https://www.atmos-meas-tech.net/13/2279/2020/>.
- Waterman PC. 1965. Matrix formulation of electromagnetic scattering. Proceedings of the IEEE 53(8): 805–812.
- Wolfensberger D, Berne A. 2018. From model to radar variables: a new forward polarimetric radar operator for cosmo. Atmospheric Measurement Techniques 11(7): 3883-3916, doi:10. 5194/amt-11-3883-2018, URL <https://www.atmos-meas-tech.net/11/3883/2018/>.