1) Total (or material) derivative

Make sure you understand the important distinction between the total and partial derivative on page 6 of Stull Chapter 1. We need them both, because we use the total derivitive to write *conservation laws* (for mass, momentum, energy and entropy) in a reference frame moving with the flow, but models and observations are generally constructed/measured in a fixed (eulerian) reference frame with x, y, z constant. Here are two different approaches to deriving the p. 6 expression. For the first derivation it helps to to recall some basic facts about Taylor's series (actually Gregory's series) and Taylor's theorem

In particular in the neighborhood of the point $t = t_0$, $x = a$, $y = b$

$$\begin{aligned} f(x,y) &\approx f(a,b,t_0) + (t-t_0)\frac{\partial f}{\partial t}(a,b,t_0) + (x-a)\frac{\partial f}{\partial x}(a,b,t_0) + (y-b)\,\frac{\partial f}{\partial y}(a,b,t_0) \\ &+ \text{higher order terms} \end{aligned}$$

or keeping only terms of first order and rearranging

$$f(x,y,t) - f(a,b,t_0) = \Delta f \approx \Delta t\frac{\partial f}{\partial t}(a,b,t_0) + \Delta x\frac{\partial f}{\partial x}(a,b,t_0) + \Delta y\,\frac{\partial f}{\partial y}(a,b,t_0)$$

and dividing through by Δt:

$$\begin{aligned} \frac{\Delta f}{\Delta t} &\approx \frac{\Delta t}{\Delta t}\frac{\partial f}{\partial t}(a,b,t_0) + \frac{\Delta x}{\Delta t}\frac{\partial f}{\partial x}(a,b,t_0) + \frac{\Delta y}{\Delta t}\frac{\partial f}{\partial y}(a,b,t_0) \\ &= \frac{\partial f}{\partial t} + u \cdot \nabla f \end{aligned}$$

But how do we know that $\frac{\Delta f}{\Delta t}$ is the *material* derivative – i.e. the derivative in a reference frame moving with the flow? Take a look at two fluid mechanics lectures by Moira Jardine of the University of St. Andrews, Fluid lecture 1 and Fluid lecture 2.

Her definition of $\frac{dQ}{dt}$ is:

$$\frac{dQ}{dt} = \frac{Q(r+\delta r, t+\delta t) - Q(r,t)}{\delta t} \tag{1}$$

with the implicit idea that $Q(r+\delta r, t+\delta t)$ is the same piece of fluid as $Q(r,t)\delta t$, observed at time $t + \delta t$ – that is, the displacement δr is whatever is needed to track the fluid parcel.

If this seems a little ad hoc, it is possible to make this more explicit by specifically labeling the fluid volumes by their initial positions, and being clear about the fact that we are following the volumes as time progresses. Here I'm relying on a derivation given in Salmon, 1998, Lectures on Geophysical Fluid Dynamics.

In Salmon's notation, for the *Eulerian description*, the independent variables are the space coordinates $\mathbf{x} = (x, y, z)$ and the time t. In the *Lagrangian description*, the independent coordinates are a set of particle labels which uniquely identify a small region of the fluid. For example the label could be the three coordinates $\mathbf{a} = (a, b, c)$, where (a, b, c) have the numerical values of (x, y, z) at time $t = 0$. It is also helpful to give a separate symbol to the time in the Lagrangian frame, τ, to remind us that as τ varies the label (a, b, c) is kept fixed, while as t, varies the position (x, y, z) is kept fixed. In this notation the material or total derivative is by definition the time derivitive keeping the labels constant:

$$\frac{\partial Q}{\partial \tau} = \frac{dQ}{dt} \tag{2}$$

where Q is a property of the fluid, like vapor mixing ratio or energy. Eq. (2) gives the rate of change of Q for a tagged region of of fluid, with evolving spatial coordinates given by $x(a, b, c, \tau)$, $y(a, b, c, \tau)$, $z(a, b, c, \tau)$.

Then using the chain rule we have:

$$\frac{\partial Q}{\partial \tau} = \frac{dQ}{dt} = \frac{\partial Q}{\partial t}\frac{\partial t}{\partial \tau} + \frac{\partial Q}{\partial x}\frac{\partial x}{\partial \tau} + \frac{\partial Q}{\partial y}\frac{\partial y}{\partial \tau} + \frac{\partial Q}{\partial z}\frac{\partial z}{\partial \tau} \tag{3}$$

But the velocity of the infinitesimal volume is by definition:

$$\mathbf{v} \equiv \left(\frac{\partial x}{\partial \tau}, \frac{\partial y}{\partial \tau}, \frac{\partial z}{\partial \tau}\right) = (u, v, w) \tag{4}$$

So we can rewrite (3) as:

$$\frac{\partial Q}{\partial \tau} = \frac{dQ}{dt} = \frac{\partial Q}{\partial t} + u\frac{\partial Q}{\partial x} + v\frac{\partial Q}{\partial y} + w\frac{\partial Q}{\partial y} = \frac{\partial Q}{\partial t} + \mathbf{v} \cdot \nabla Q \tag{5}$$

Thus $\mathbf{v} \equiv \left(\frac{\partial x}{\partial \tau}, \frac{\partial y}{\partial \tau}, \frac{\partial z}{\partial \tau}\right)$ makes explicit the idea that $\frac{\delta r}{\delta t}$ is the velocity "following the flow".

Then Taylor's frozen turbulence hypothesis is equivalent to the statement that:

$$\frac{\partial Q}{\partial \tau} = \frac{dQ}{dt} = 0 \tag{6}$$

i.e., there are no sources or sinks of Q changing the properties of the fluid in the infinitesimal box. In particular, the turbulence is *frozen*, and is not able to mix adjacent boxes on the time and space scales of interest in the problem. This doesn't mean that there are no fluctuations, it just means that the *statistics* of the fluctuations are stationary. (Note that the idea of frozen turbulence is due to G. I. Taylor (b. 1886, d. 1975) not Brook Taylor (b. 1685, d. 1731).

2) Virtual temperature

A nice example of the use of Taylor's series is Stull (1.5.1a) on p. 7:

$$\theta_v = \theta(1 + 0.61 r_{sat} - r_l)$$

where θ called the *potential temperature* is acutally a measure of the entropy of dry air (to be derived later), r_{sat} is the saturation mixing ratio for water vapor (kg water/kg dry air) and r_l is the mixing ratio for cloud droplets (kg water/kg dry air).

We'll go into all of this in more detail, but it's worth looking at how the factor 0.61 comes about, extending the derivation on Wallace and Hobbs (Chapter 3.1.1, p. 4) Virtual temperature provides a succinct way to describe the density of a mixture of dry air, water vapor, and hydrometeors like cloud droplets, raindrops, snow and ice. Specifically, write this density as:

$$\rho = \rho_d + \frac{e}{R_v T} + \rho_l + \rho_r + \rho_i \tag{7}$$

where ρ_d is the density of dry air, e is the vapour pressure, R_v is the gas constant for water vapor ($461\ \ \mathrm{J\,kg^{-1}\,K^{-1}}$), T is the temperature and $\rho_l,\ \rho_r,\ \rho_i$ are the densities of cloud droplets, rain drops and ice crystals. (When we begin comparing densities to find the *buoyancy* we'll need the additional assumption that the droplets, drops and crystals are all falling at constant velocity, so we can calculate the downward force they exert on the surrounding air). From the definition of the mixing ratio we know that:

$$r_v = \frac{\rho_v}{\rho_d} = \frac{\frac{e}{R_v T}}{\frac{p_d}{R_d T}} = \frac{R_d}{R_v}\frac{e}{p-e} = \epsilon\frac{e}{p-e} \approx 0.622\frac{e}{p-e} \tag{8}$$

Inverting (8) gives:

$$\frac{e}{p} = \frac{r_v}{r_v + \epsilon} \tag{9}$$

Putting in the equation of state for dry air and group terms, (7) becomes:

$$\rho = \frac{p}{R_d T}\left(1 - \frac{e}{p}(1-\epsilon)\right) + \rho_l + \rho_r + \rho_i \tag{10}$$

and using (9):

$$\rho = \frac{p}{R_d T}\left(1 - \frac{r_v}{r_v+\epsilon}(1-\epsilon)\right) + \rho_l + \rho_r + \rho_i \tag{11}$$

Now divide both sides of (11) by $\rho_d = (p-e)/(R_d T)$

$$\frac{\rho}{\rho_d} = \left(\frac{p}{R_d T_v}\frac{R_d T}{p-e}\right) = \frac{p}{R_d T}\frac{R_d T}{p-e}\left[1 - \frac{r_v}{r_v+\epsilon}(1-\epsilon)\right] + r_l + r_r + r_i \tag{12}$$

where we've defined the virtual temperature, T_v as the temperature that produces the correct density ρ for the mixture given the (incorrect) dry air gas constant R_d.

Cleaning this up by moving multiplying by $(p-e)/p$:

$$\frac{T}{T_v} = \left[1 - \frac{r_v}{r_v+\epsilon}(1-\epsilon)\right] + \frac{p-e}{p}\left[r_l + r_r + r_i\right] \tag{13}$$

But we know that in the atmosphere, $e/p,\ r_l,\ r_r,\ r_i$ are all small (below 0.02) so neglect their products, which leaves:

$$\frac{T}{T_v} = \left[1 - \frac{r_v}{r_v+\epsilon}(1-\epsilon)\right] + r_l + r_r + r_i \tag{14}$$

Now rearrange (14), dropping all second order terms:

$$\frac{T}{T_v} = \frac{r_v + \epsilon - r_v + r_v\epsilon + \epsilon(r_l + r_r + r_i)}{r_v + \epsilon} \tag{15}$$

or flipping:

$$T_v = T\left(\frac{r_v + \epsilon}{\epsilon}\right)\left(\frac{1}{1 + (r_l + r_r + r_i)}\right) \tag{16}$$

To get the mixing ratios out of the denominator, use a Taylor series expansion:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + \frac{f'''(x_0)}{2 \cdot 3}(x - x_0)^3 + \ldots \tag{17}$$

You should show that expanding about $x_0 = 0$ yields:

$$\frac{1}{1+r} = 1 - r + r^2 - r^3 + \ldots \tag{18}$$

So that

$$T_v \approx T\left(\frac{r_v + \epsilon}{\epsilon}\right)(1 - (r_l + r_r + r_i)) \tag{19}$$

and rearranging and again dropping second order terms:

$$T_v \approx \frac{T(\epsilon + (1-\epsilon)r_v - \epsilon(r_l + r_r + r_i))}{\epsilon} \tag{20}$$

and finally:

$$T_v \approx T\left(1 + \frac{(1-\epsilon)}{\epsilon}r_v - (r_l + r_r + r_i)\right) = T\left(1 + 0.608\, r_v - (r_l + r_r + r_i)\right) \tag{21}$$

In words (21) says that air becomes more buoyant (effectively "warmer") as r_v increases (because light H_2O replaces heavy N_2), and droplets, drops and ice concentrations decrease (because falling hydrometeors exert downward drag on the atmosphere).