

# Auxiliary calculations

Here the auxiliary calculations of the manuscript ‘Direct Inversion of Circulation and Mixing from Tracer Measurements: I. Theory’ by T. von Clarmann et al. are presented in full detail; this document is intended to guide the interested reader through the equations. The auxiliary calculations are not included in the main publications because most steps are trivial while lengthy. Notation follows that of the main manuscript. This auxiliary document is intended to save the reviewers and interested readers some time and headache.

## 1 Divergence

The divergence in polar coordinates (polar angle  $\Phi$ , longitude  $\lambda$ ) is:

$$\nabla \cdot \vec{a} = \frac{1}{r \sin \Phi} \frac{\partial(\sin \Phi a_\Phi)}{\partial \Phi} + \frac{1}{r^2} \frac{\partial(r^2 a_r)}{\partial r} + \frac{1}{r \sin \Phi} \frac{\partial a_\lambda}{\partial \lambda} \quad (1)$$

From this we get the divergence in geographical coordinates (latitude  $\phi = \frac{\pi}{2} - \Phi$ ) by

$$\sin \Phi = \cos \phi, \quad (2)$$

$$\frac{\partial}{\partial \Phi} = -\frac{\partial}{\partial \phi} \quad (3)$$

and

$$a_\Phi\left(\frac{\pi}{2} - \phi\right) = -a_\phi(\phi) \quad (4)$$

as

$$\begin{aligned} \nabla \cdot \vec{a} &= \frac{1}{r \cos \phi} \frac{\partial(\cos \phi a_\phi)}{\partial \phi} + \frac{1}{r^2} \frac{\partial(r^2 a_r)}{\partial r} + \frac{1}{r \cos \phi} \frac{\partial a_\lambda}{\partial \lambda} = \\ &= \frac{1}{r} \frac{\partial a_\phi}{\partial \phi} - \frac{a_\phi}{r} \tan(\phi) + \frac{\partial a_r}{\partial r} + \frac{2a_r}{r} + \frac{1}{r \cos(\phi)} \frac{\partial a_\lambda}{\partial \lambda}. \end{aligned} \quad (5)$$

## 2 MacCormack Integration

The MacCormack scheme uses the predictor

$$c_{i+1}^*(x_0, y_0) = c_i(x_0, y_0) - \frac{\Delta t}{\Delta x} \left( e_i(x + \Delta x, y) - e_i(x, y) \right) - \frac{\Delta t}{\Delta y} \left( f_i(x, y + \Delta y) - f_i(x, y) \right) \quad (6)$$

and the corrector

$$\begin{aligned} c_{i+1}(x_0, y_0) &= \\ &= \frac{1}{2} \left[ c_i(x, y) + c_{i+1}^*(x, y) - \frac{\Delta t}{\Delta x} \left( e_{i+1}^*(x, y) - e_{i+1}^*(x - \Delta x, y) \right) - \frac{\Delta t}{\Delta y} \left( f_{i+1}^*(x, y) - f_{i+1}^*(x, y - \Delta y) \right) \right] \end{aligned} \quad (7)$$

### 3 Integration of tendencies of air density

We specify

$$c = \cos(\phi)r^2\rho, \quad (8)$$

$$e = \cos(\phi)r\rho v, \quad (9)$$

and

$$f = \cos(\phi)r^2\rho w. \quad (10)$$

The continuity equation is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0. \quad (11)$$

Transformation to geographical coordinates (longitude  $\lambda$  and latitude  $\phi$ ) gives, without application of the shallowness approximation <sup>1</sup>

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial \rho v}{\partial \phi} - \frac{\rho v}{r} \tan(\phi) + \frac{\partial \rho w}{\partial r} + \frac{2\rho w}{r} + \frac{1}{r \cos(\phi)} \frac{\partial \rho u}{\partial \lambda} = 0. \quad (12)$$

From here on colours are used for better traceability. Reduction to two dimensions ( $u = 0$ ) gives

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial \rho v}{\partial \phi} - \frac{\rho v}{r} \tan(\phi) + \frac{\partial \rho w}{\partial r} + \frac{2\rho w}{r} = 0. \quad (13)$$

Multiplication by  $r^2 \cos(\phi)$  gives

$$r^2 \cos(\phi) \frac{\partial \rho}{\partial t} + r^2 \cos(\phi) \frac{1}{r} \frac{\partial \rho v}{\partial \phi} - r^2 \cos(\phi) \frac{\rho v}{r} \tan(\phi) + r^2 \cos(\phi) \frac{\partial \rho w}{\partial r} + 2r \rho w \cos(\phi) = 0. \quad (14)$$

$r^2$  and  $\cos \phi$  are time-independent, so we have

$$\frac{\partial r^2 \cos(\phi) \rho}{\partial t} + r \cos(\phi) \frac{\partial \rho v}{\partial \phi} - r \sin(\phi) \rho v + r^2 \cos(\phi) \frac{\partial \rho w}{\partial r} + 2r \rho w \cos(\phi) = 0. \quad (15)$$

With

$$\frac{\partial r \cos(\phi) \rho v}{\partial \phi} = r \cos(\phi) \frac{\partial \rho v}{\partial \phi} + \rho v r \frac{\partial \cos(\phi)}{\partial \phi} = r \cos(\phi) \frac{\partial \rho v}{\partial \phi} - \rho v r \sin(\phi) \quad (16)$$

and

$$\frac{\partial r^2 \cos(\phi) \rho w}{\partial r} = r^2 \cos(\phi) \frac{\partial \rho w}{\partial r} + 2\rho w r \cos(\phi) \quad (17)$$

and with application of the  $c$ ,  $e$ , and  $f$  terms defined above (Eqs. (8–10)) we get

$$\begin{aligned} \frac{\partial r^2 \cos(\phi) \rho}{\partial t} + \frac{\partial r \cos(\phi) \rho v}{\partial \phi} + \frac{\partial r^2 \cos(\phi) \rho w}{\partial r} = \\ \frac{\partial c}{\partial t} + \frac{\partial e}{\partial \phi} + \frac{\partial f}{\partial r} = 0, \end{aligned} \quad (18)$$

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<sup>1</sup>this is not because we intend to challenge the shallowness approximation but because without this approximation the continuity equation can better be transformed in a MacCormack-integrable form)

which is of a form that the MacCormack scheme (Eqs. 6–7) can be applied. We have  $r = r_e + z$  and  $\Delta r = \Delta z$ . The prediction at  $(\phi, z)$  is

$$\begin{aligned} r^2 \cos(\phi) \rho_{i+1}(\phi, z)^* &= r^2 \cos(\phi) \rho_i(\phi, z) - \\ &\frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi + \Delta \phi) \rho_i(\phi + \Delta \phi, z) v(\phi + \Delta \phi, z) - r \cos(\phi) \rho_i(\phi, z) v(\phi, z) \right) - \\ &\frac{\Delta t_p}{\Delta z} \left( (r + \Delta z)^2 \cos(\phi) \rho_i(\phi, z + \Delta z) w(\phi, z + \Delta z) - r^2 \cos(\phi) \rho_i(\phi, z) w(\phi, z) \right) \end{aligned} \quad (19)$$

The prediction at  $(\phi - \Delta \phi, z)$  is

$$\begin{aligned} r^2 \cos(\phi - \Delta \phi) \rho_{i+1}(\phi - \Delta \phi, z)^* &= r^2 \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z) - \\ &\frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi) \rho_i(\phi, z) v(\phi, z) - r \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z) v(\phi - \Delta \phi, z) \right) - \\ &\frac{\Delta t_p}{\Delta z} \left( (r + \Delta z)^2 \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z + \Delta z) w(\phi - \Delta \phi, z + \Delta z) - \right. \\ &\quad \left. r^2 \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z) w(\phi - \Delta \phi, z) \right) \end{aligned} \quad (20)$$

The prediction at  $(\phi, z - \Delta z)$  is

$$\begin{aligned} (r - \Delta z)^2 \cos(\phi) \rho_{i+1}(\phi, z - \Delta z)^* &= (r - \Delta z)^2 \cos(\phi) \rho_i(\phi, z - \Delta z) - \\ &\frac{\Delta t_p}{\Delta \phi} \left( (r - \Delta z) \cos(\phi + \Delta \phi) \rho_i(\phi + \Delta \phi, z - \Delta z) v(\phi + \Delta \phi, z - \Delta z) - \right. \\ &\quad \left. (r - \Delta z) \cos(\phi) \rho_i(\phi, z - \Delta z) v(\phi, z - \Delta z) \right) - \\ &\frac{\Delta t_p}{\Delta z} \left( r^2 \cos(\phi) \rho_i(\phi, z) w(\phi, z) - (r - \Delta z)^2 \cos(\phi) \rho_i(\phi, z - \Delta z) w(\phi, z - \Delta z) \right) \end{aligned} \quad (21)$$

The correction gives for air density according to Eq. (7)

$$\begin{aligned} \rho_{i+1}(\phi, z) &= \\ &\frac{1}{2r^2 \cos(\phi)} \left[ r^2 \cos(\phi) \rho_i(\phi, z) + r^2 \cos(\phi) \rho_{i+1}(\phi, z)^* \right. \\ &\quad \left. - \frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi) v(\phi, z) \rho_{i+1}(\phi, z)^* - r \cos(\phi - \Delta \phi) v(\phi - \Delta \phi, z) \rho_{i+1}(\phi - \Delta \phi, z)^* \right) \right. \\ &\quad \left. - \frac{\Delta t_p}{\Delta z} \left( r^2 \cos(\phi) w(\phi, z) \rho_{i+1}(\phi, z)^* - (r - \Delta z)^2 \cos(\phi) w(\phi, z - \Delta z) \rho_{i+1}(\phi, z - \Delta z)^* \right) \right] = \\ &= \frac{1}{2r^2 \cos(\phi)} \left[ r^2 \cos(\phi) \rho_i(\phi, z) + r^2 \cos(\phi) \rho_i(\phi, z) \right. \\ &\quad \left. - \frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi + \Delta \phi) \rho_i(\phi + \Delta \phi, z) v(\phi + \Delta \phi, z) - r \cos(\phi) \rho_i(\phi, z) v(\phi, z) \right) \right. \\ &\quad \left. - \frac{\Delta t_p}{\Delta z} \left( (r + \Delta z)^2 \cos(\phi) \rho_i(\phi, z + \Delta z) w(\phi, z + \Delta z) - r^2 \cos(\phi) \rho_i(\phi, z) w(\phi, z) \right) \right. \\ &\quad \left. - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( r^2 \cos(\phi) \rho_i(\phi, z) \right) \right] \right] \end{aligned} \quad (22)$$

$$\begin{aligned}
& -\frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi + \Delta \phi) \rho_i(\phi + \Delta \phi, z) v(\phi + \Delta \phi, z) - r \cos(\phi) \rho_i(\phi, z) v(\phi, z) \right) \\
& -\frac{\Delta t_p}{\Delta z} \left( (r + \Delta z)^2 \cos(\phi) \rho_i(\phi, z + \Delta z) w(\phi, z + \Delta z) - r^2 \cos(\phi) \rho_i(\phi, z) w(\phi, z) \right) \\
& -\frac{v(\phi - \Delta \phi, z)}{r} \left( r^2 \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z) \right. \\
& -\frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi) \rho_i(\phi, z) v(\phi, z) - r \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z) v(\phi - \Delta \phi, z) \right) \\
& -\frac{\Delta t_p}{\Delta z} \left( (r + \Delta z)^2 \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z + \Delta z) w(\phi - \Delta \phi, z + \Delta z) \right. \\
& \quad \left. - r^2 \cos(\phi - \Delta \phi) \rho_i(\phi - \Delta \phi, z) w(\phi - \Delta \phi, z) \right) \left. \right] \\
& -\frac{\Delta t}{\Delta z} \left[ w(\phi, z) \left( r^2 \cos(\phi) \rho_i(\phi, z) \right) \right. \\
& -\frac{\Delta t_p}{\Delta \phi} \left( r \cos(\phi + \Delta \phi) \rho_i(\phi + \Delta \phi, z) v(\phi + \Delta \phi, z) - r \cos(\phi) \rho_i(\phi, z) v(\phi, z) \right) \\
& -\frac{\Delta t_p}{\Delta z} \left( (r + \Delta z)^2 \cos(\phi) \rho_i(\phi, z + \Delta z) w(\phi, z + \Delta z) - r^2 \cos(\phi) \rho_i(\phi, z) w(\phi, z) \right) \\
& -w(\phi, z - \Delta z) \left( (r - \Delta z)^2 \cos(\phi) \rho_i(\phi, z - \Delta z) \right. \\
& -\frac{\Delta t_p}{\Delta \phi} \left( (r - \Delta z) \cos(\phi + \Delta \phi) \rho_i(\phi + \Delta \phi, z - \Delta z) v(\phi + \Delta \phi, z - \Delta z) \right. \\
& \quad \left. - (r - \Delta z) \cos(\phi) \rho_i(\phi, z - \Delta z) v(\phi, z - \Delta z) \right) \\
& \left. -\frac{\Delta t_p}{\Delta z} \left( r^2 \cos(\phi) \rho_i(\phi, z) w(\phi, z) - (r - \Delta z)^2 \cos(\phi) \rho_i(\phi, z - \Delta z) w(\phi, z - \Delta z) \right) \right] \left. \right]
\end{aligned}$$

#### 4 Derivatives of predicted air densities w.r.t. initial air densities

We differentiate Eq. 22 with respect to air densities at the same location.

$$\begin{aligned}
\frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z)} &= \frac{1}{2r^2 \cos(\phi)} \left[ 2r^2 \cos(\phi) \right. \\
& -\frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( \frac{(\Delta t_p) r \cos(\phi) v(\phi, z)}{\Delta \phi} + \frac{(\Delta t_p) r^2 \cos(\phi) w(\phi, z)}{\Delta z} \right) \right. \\
& \quad \left. + \frac{v(\phi - \Delta \phi, z) (\Delta t_p) \cos(\phi) v(\phi, z)}{\Delta \phi} \right] \\
& -\frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{(\Delta t_p) r \cos(\phi) v(\phi, z)}{\Delta \phi} + \frac{(\Delta t_p) r^2 \cos(\phi) w(\phi, z)}{\Delta z} \right) \right. \\
& \quad \left. + \frac{w(\phi, z - \Delta z) (\Delta t_p) r^2 \cos(\phi) w(\phi, z)}{\Delta z} \right] \left. \right] =
\end{aligned} \tag{23}$$

$$\begin{aligned} & \frac{1}{2} \left[ 2 - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi - \Delta \phi, z) v(\phi, z)}{r^2} \right] \right. \\ & \left. - \frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) w(\phi, z) \right] \right] \end{aligned}$$

We further differentiate predicted air densities (Eq. 22) with respect to air densities at the adjacent southern latitude but the same altitude.

$$\begin{aligned} & \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi - \Delta \phi, z)} = \tag{24} \\ & \frac{1}{2r^2 \cos(\phi)} \cdot \left[ - \frac{\Delta t_p}{\Delta \phi} \left[ - \frac{v(\phi - \Delta \phi, z)}{r} \cdot \right. \right. \\ & \left. \left. \left( r^2 \cos(\phi - \Delta \phi) + \frac{\Delta t_p}{\Delta \phi} r \cos(\phi - \Delta \phi) v(\phi - \Delta \phi, z) + \frac{\Delta t_p}{\Delta z} r^2 \cos(\phi - \Delta \phi) w(\phi - \Delta \phi, z) \right) \right] \right] = \\ & \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi - \Delta \phi, z) \right) \right] \end{aligned}$$

Then we differentiate predicted air densities (Eq. 22) with respect to air densities at the adjacent northern latitude but the same altitude.

$$\begin{aligned} & \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta \phi, z)} = \frac{1}{2r^2 \cos(\phi)} \cdot \tag{25} \\ & \left[ - \frac{\Delta t_p}{\Delta \phi} r \cos(\phi + \Delta \phi) v(\phi + \Delta \phi, z) - \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} \cdot \frac{-\Delta t_p}{\Delta \phi} r \cos(\phi + \Delta \phi) v(\phi + \Delta \phi, z) \right. \\ & \left. - \frac{\Delta t}{\Delta z} w(\phi, z) \frac{-\Delta t_p}{\Delta \phi} r \cos(\phi + \Delta \phi) v(\phi + \Delta \phi, z) \right] = \\ & \frac{1}{2 \cos(\phi)} \left[ - \frac{\Delta t_p}{\Delta \phi} \cos(\phi + \Delta \phi) \frac{v(\phi + \Delta \phi, z)}{r} + \frac{(\Delta t_p)^2}{(\Delta \phi)^2} \frac{v(\phi, z)}{r} \cos(\phi + \Delta \phi) \frac{v(\phi + \Delta \phi, z)}{r} + \right. \\ & \left. \frac{(\Delta t_p)^2}{\Delta z \Delta \phi} w(\phi, z) \frac{v(\phi + \Delta \phi, z)}{r} \cos(\phi + \Delta \phi) \right] = \\ & - \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi + \Delta \phi, z)}{r} \cdot \frac{\cos(\phi + \Delta \phi)}{\cos(\phi)} \left( 1 - \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} - \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \end{aligned}$$

As a next step we differentiate predicted air densities (Eq. 22) with respect to air densities at the next higher altitude but the same latitude.

$$\begin{aligned} & \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z + \Delta z)} = - \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \right. \tag{26} \\ & \left. - \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \right] \end{aligned}$$

$$\begin{aligned}
& -\frac{\Delta t_p}{\Delta z} w(\phi, z) \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \Big] = \\
& -\frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \left( 1 - \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} - \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right]
\end{aligned}$$

Then we differentiate predicted air densities (Eq. 22) with respect to air densities at the next lower altitude but the same latitude.

$$\begin{aligned}
\frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z - \Delta z)} &= \frac{1}{2r^2 \cos(\phi)} \left[ \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \left( (r - \Delta z)^2 \cos(\phi) \right. \right. & (27) \\
& \left. \left. + \frac{\Delta t_p}{\Delta \phi} \left( (r - \Delta z) \cos(\phi) v(\phi, z - \Delta z) \right) + \frac{\Delta t_p}{\Delta z} \left( (r - \Delta z)^2 \cos(\phi) w(\phi, z - \Delta z) \right) \right) \right] = \\
& \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \left( \frac{(r - \Delta z)^2}{r^2} \right. \right. \\
& \left. \left. + \frac{\Delta t_p}{\Delta \phi} \left( \frac{(r - \Delta z)}{r} \cdot \frac{v(\phi, z - \Delta z)}{r} \right) + \frac{\Delta t_p}{\Delta z} \left( \frac{(r - \Delta z)^2}{r^2} w(\phi, z - \Delta z) \right) \right) \right] = \\
& \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \frac{(r - \Delta z)^2}{r^2} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z - \Delta z)}{r - \Delta z} + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right) \right]
\end{aligned}$$

Finally, we differentiate the predicted air densities (Eq. 22) with respect to air densities at the adjacent southern latitude and higher altitude

$$\begin{aligned}
\frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi - \Delta \phi, z + \Delta z)} &= & (28) \\
& -\frac{1}{2r^2 \cos(\phi)} \left[ \frac{v(\phi - \Delta \phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} (r + \Delta z)^2 \cos(\phi - \Delta \phi) w(\phi - \Delta \phi, z + \Delta z) = \right. \\
& \left. -\frac{1}{2} \left[ \frac{v(\phi - \Delta \phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} w(\phi - \Delta \phi, z + \Delta z) \right] \right]
\end{aligned}$$

and vice versa

$$\begin{aligned}
\frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta \phi, z - \Delta z)} &= & (29) \\
& -\frac{1}{2} \left[ w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{r - \Delta z}{r} \cdot \frac{\cos(\phi + \Delta \phi)}{\cos(\phi)} \cdot \frac{v(\phi + \Delta \phi, z - \Delta z)}{r} \right] = \\
& -\frac{1}{2} \left[ w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)^2}{r^2} \cdot \frac{\cos(\phi + \Delta \phi)}{\cos(\phi)} \cdot \frac{v(\phi + \Delta \phi, z - \Delta z)}{r - \Delta z} \right]
\end{aligned}$$

## 5 Integration of VMR tendencies

We start from Eq. (15) but we replace  $\rho$  by  $\rho vmr$  to get the tendency of partial density (with source term S):

$$\frac{\partial r^2 \cos(\phi) \rho vmr}{\partial t} + r \cos(\phi) \frac{\partial \rho vmr}{\partial \phi} v - r \sin(\phi) \rho vmr v + r^2 \cos(\phi) \frac{\partial \rho vmr}{\partial r} w + 2r \rho vmr w \cos(\phi) = (30)$$

$$Sr^2 \cos(\phi)$$

Application of the product rule gives:

$$r^2 \cos(\phi) \rho \frac{\partial vmr}{\partial t} + r \cos(\phi) \rho v \frac{\partial vmr}{\partial \phi} + r^2 \cos(\phi) \rho w \frac{\partial vmr}{\partial r} - Sr^2 \cos(\phi) = (31)$$

$$-vmr \frac{\partial r^2 \cos(\phi) \rho}{\partial t} - r \cos(\phi) vmr \frac{\partial \rho v}{\partial \phi} + r \sin(\phi) \rho vmr v - r^2 \cos(\phi) vmr \frac{\partial \rho w}{\partial r} - 2r \rho vmr w \cos(\phi)$$

The right-hand side of this is zero, because it is just  $vmr$  times the continuity equation of density. The remaining equation is, after cancellation of  $\rho$ :

$$r^2 \cos(\phi) \frac{\partial vmr}{\partial t} + r \cos(\phi) v \frac{\partial vmr}{\partial \phi} + r^2 \cos(\phi) w \frac{\partial vmr}{\partial r} = \frac{Sr^2 \cos(\phi)}{\rho} \quad (32)$$

Division by  $r^2 \cos(\phi)$  gives

$$\frac{\partial vmr}{\partial t} = -\frac{v}{r} \frac{\partial vmr}{\partial \phi} - w \frac{\partial vmr}{\partial r} + \frac{S}{\rho} \quad (33)$$

which is the usual 2D-continuity equation for mixing ratios in geographical coordinates (c.f., e.g. Brasseur and Solomon). After process splitting (since/sinks, horizontal advection and vertical advection, and mixing, hitherto not considered, are integrated independently. Advection terms can be brought into a MacCormack integrable form:

$$\left( \frac{\partial^r vmr}{\partial t} \right)_{hor.advection} = \frac{\partial vmr}{\partial \phi} \quad (34)$$

and

$$\left( \frac{\partial vmr}{\partial t} \right)_{vert.advection} = \frac{\partial vmr}{\partial r} \quad (35)$$

The preliminary prediction of the horizontal advection part of the change of vmr at  $\phi$  and  $z$  is:

$$\frac{r vmr_{i+1}(\phi, z)^*}{v(\phi, z)} = \frac{r vmr_i(\phi, z)}{v(\phi, z)} - \frac{\Delta t_p}{\Delta \phi} \left( vmr_i(\phi + \Delta \phi, z) - vmr_i(\phi, z) \right) \quad (36)$$

$$vmr_{i+1}(\phi, z)^* = vmr_i(\phi, z) - \frac{v(\phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta \phi} \left( vmr_i(\phi + \Delta \phi, z) - vmr_i(\phi, z) \right) \quad (37)$$

The prediction at  $\phi - \Delta \phi$  and  $z$  is

$$\frac{r vmr_{i+1}(\phi - \Delta \phi, z)^*}{v(\phi - \Delta \phi, z)} = \frac{r vmr_i(\phi - \Delta \phi, z)}{v(\phi - \Delta \phi, z)} - \frac{\Delta t_p}{\Delta \phi} \left( vmr_i(\phi, z) - vmr_i(\phi - \Delta \phi, z) \right) \quad (38)$$

$$vmr_{i+1}(\phi - \Delta\phi, z)^* = vmr_i(\phi - \Delta\phi, z) - \frac{v(\phi - \Delta\phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( vmr_i(\phi, z) - vmr_i(\phi - \Delta\phi, z) \right) \quad (39)$$

MacCormack integration of this gives the following corrected prediction for the change due to horizontal advection:

$$\begin{aligned} & \left[ vmr_{i+1}(\phi, z) \right]_{horizontal.advection} = \quad (40) \\ & \frac{v(\phi, z)}{2r} \left[ \frac{r vmr_i(\phi, z)}{v(\phi, z)} + \frac{r vmr_i(\phi, z)}{v(\phi, z)} - \frac{\Delta t_p}{\Delta\phi} \left( vmr_i(\phi + \Delta\phi, z) - vmr_i(\phi, z) \right) \right. \\ & \quad \left. - \frac{\Delta t_p}{\Delta\phi} \left( \frac{v(\phi, z)}{r} \left[ \frac{r vmr_i(\phi, z)}{v(\phi, z)} - \frac{\Delta t_p}{\Delta\phi} \left( vmr_i(\phi + \Delta\phi, z) - vmr_i(\phi, z) \right) \right] \right) \right. \\ & \quad \left. - \frac{v(\phi - \Delta\phi, z)}{r} \left[ \frac{r vmr_i(\phi - \Delta\phi, z)}{v(\phi - \Delta\phi, z)} - \frac{\Delta t_p}{\Delta\phi} \left( vmr_i(\phi, z) - vmr_i(\phi - \Delta\phi, z) \right) \right] \right] = \\ & vmr_i(\phi, z) + \frac{v(\phi, z)}{2r} \left[ -\frac{\Delta t_p}{\Delta\phi} \left( vmr_i(\phi + \Delta\phi, z) - vmr_i(\phi, z) \right) \right. \\ & \quad \left. - \frac{\Delta t_p}{\Delta\phi} \left( \left[ vmr_i(\phi, z) - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \left( vmr_i(\phi + \Delta\phi, z) - vmr_i(\phi, z) \right) \right] \right) \right. \\ & \quad \left. - \left[ vmr_i(\phi - \Delta\phi, z) - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \left( vmr_i(\phi, z) - vmr_i(\phi - \Delta\phi, z) \right) \right] \right] \end{aligned}$$

For vertical advection we have the preliminary predictions

$$\frac{vmr_{i+1}(\phi, z)^*}{w(\phi, z)} = \frac{vmr_i(\phi, z)}{w(\phi, z)} - \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \quad (41)$$

$$vmr_{i+1}(\phi, z)^* = vmr_i(\phi, z) - w(\phi, z) \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \quad (42)$$

$$\frac{vmr_{i+1}(\phi, z - \Delta z)^*}{w(\phi, z - \Delta z)} = \frac{vmr_i(\phi, z - \Delta z)}{w(\phi, z - \Delta z)} - \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z) - vmr_i(\phi, z - \Delta z) \right) \quad (43)$$

$$\begin{aligned} vmr_{i+1}(\phi, z - \Delta z)^* = \quad (44) \\ vmr_i(\phi, z - \Delta z) - w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z) - vmr_i(\phi, z - \Delta z) \right) \end{aligned}$$

With this we get the corrected prediction of vertical advection:

$$\begin{aligned} & \left[ vmr_{i+1}(\phi, z) \right]_{vertical.advection} = \quad (45) \\ & \frac{w(\phi, z)}{2} \left[ \frac{vmr_i(\phi, z)}{w(\phi, z)} + \frac{vmr_i(\phi, z)}{w(\phi, z)} - \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \right. \end{aligned}$$



$$\begin{aligned}
& -\frac{\Delta t_p}{\Delta z} \left( w(\phi, z) \left[ \frac{vmr_i(\phi, z)}{w(\phi, z)} - \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \right] \right. \\
& \left. - w(\phi, z - \Delta z) \left[ \frac{vmr_i(\phi, z - \Delta z)}{w(\phi, z - \Delta z)} - \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z) - vmr_i(\phi, z - \Delta z) \right) \right] \right) = \\
& = vmr_i(\phi, z) + \frac{1}{2} \left[ -w(\phi, z) \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \right. \\
& \left. - \frac{\Delta t_p}{\Delta z} \left( \left[ \frac{w(\phi, z)^2 vmr_i(\phi, z)}{w(\phi, z)} - w(\phi, z)^2 \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \right] \right. \right. \\
& \left. \left. - w(\phi, z - \Delta z) w(\phi, z) \left[ \frac{vmr_i(\phi, z - \Delta z)}{w(\phi, z - \Delta z)} - \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z) - vmr_i(\phi, z - \Delta z) \right) \right] \right) \right] \\
& = vmr_i(\phi, z) - \frac{1}{2} \left[ w(\phi, z) \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \right. \\
& \left. + \frac{\Delta t_p}{\Delta z} \left( \left[ w(\phi, z) vmr_i(\phi, z) - w(\phi, z)^2 \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z) \right) \right] \right. \right. \\
& \left. \left. - w(\phi, z) \left[ vmr_i(\phi, z - \Delta z) - w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \left( vmr_i(\phi, z) - vmr_i(\phi, z - \Delta z) \right) \right] \right) \right]
\end{aligned}$$

The horizontal diffusion operator is

$$\begin{aligned}
[vmr_{i+1}(\phi, z) - vmr_i\phi, z]_{diff.horizontal} &= \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \times \\
& \left[ (K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi)) \cos(\phi + \frac{\Delta\phi}{2}) (vmr_i(\phi + \Delta\phi, z) - vmr_i(\phi, z)) \right. \\
& \left. - (K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi)) \cos(\phi - \frac{\Delta\phi}{2}) (vmr_i(\phi, z) - vmr_i(\phi - \Delta\phi, z)) \right]
\end{aligned} \tag{46}$$

The vertical diffusion operator is

$$\begin{aligned}
[vmr_{i+1}(\phi, z) - vmr_i\phi, z]_{diff.vertical} &= +\frac{\Delta t_p}{2r^2(\Delta z)^2} \times \\
& \left[ \left( r + \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z + \Delta z)) (vmr_i(\phi, z + \Delta z) - vmr_i(\phi, z)) - \right. \\
& \left. \left( r - \frac{\Delta z}{2} \right)^2 \times (K_z(\phi, z) + K_z(\phi, z - \Delta z)) (vmr_i(\phi, z) - vmr_i(\phi, z - \Delta z)) \right]
\end{aligned} \tag{47}$$

For sinks due to unimolecular chemical processes like photolysis we have

$$\rho_{g;i+1} = \rho_{g,i} e^{-j_g \Delta t_p} \tag{48}$$

$$vmr_{g;i+1} = vmr_{g,i} \frac{\rho_i}{\rho_{i+1}} e^{-j_g \Delta t_p} \tag{49}$$

Process splitting simplifies this in approximation to

$$vmr_{g;i+1} = vmr_{g,i} e^{-j_g \Delta t_p} \tag{50}$$

From this the derivatives of the predicted mixing ratios with respect to the initial mixing ratios can be calculated:

$$\begin{aligned}
\frac{\partial vmr_{i+1}(\phi, z)}{\partial vmr_i(\phi, z)} &= 1 + \frac{v(\phi, z)}{2r} \left[ -\frac{\Delta t_p}{\Delta \phi} (-1) - \frac{\Delta t_p}{\Delta \phi} \left( \left[ 1 - \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} (-1) \right] \right. \right. \\
&\quad \left. \left. - \left[ -\frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} (1) \right] \right) \right] - \frac{1}{2} \left[ w(\phi, z) \frac{\Delta t_p}{\Delta z} (-1) + \frac{\Delta t_p}{\Delta z} \left( \left[ w(\phi, z) - w(\phi, z)^2 \frac{\Delta t_p}{\Delta z} (-1) \right] \right. \right. \\
&\quad \left. \left. - w(\phi, z) \left[ -w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} (1) \right] \right) \right] + \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \times \\
&\quad \left[ (K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi, z)) \cos\left(\phi + \frac{\Delta \phi}{2}\right) (-1) - (K_\phi(\phi, z) + K_\phi(\phi - \Delta \phi, z)) \cos\left(\phi - \frac{\Delta \phi}{2}\right) (1) \right] + \\
&\quad + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z + \Delta z)) (-1) - \left( r - \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z - \Delta z)) (1) \right] = \\
&= 1 + \frac{v(\phi, z)}{2r} \left[ \frac{\Delta t_p}{\Delta \phi} - \frac{\Delta t_p}{\Delta \phi} \left( \left[ 1 + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} \right] + \right. \right. \\
&\quad \left. \left. \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} \right] \right) \right] + \frac{1}{2} \left[ w(\phi, z) \frac{\Delta t_p}{\Delta z} - \frac{\Delta t_p}{\Delta z} \left( \left[ w(\phi, z) + w(\phi, z)^2 \frac{\Delta t_p}{\Delta z} \right] \right. \right. \\
&\quad \left. \left. - w(\phi, z) \left[ -w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} (1) \right] \right) \right] + \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \times \\
&\quad \left[ - (K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi, z)) \cos\left(\phi + \frac{\Delta \phi}{2}\right) - (K_\phi(\phi, z) + K_\phi(\phi - \Delta \phi, z)) \cos\left(\phi - \frac{\Delta \phi}{2}\right) \right] + \\
&\quad + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ - \left( r + \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z + \Delta z)) - \left( r - \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z - \Delta z)) \right] = \\
&= 1 + \frac{v(\phi, z)}{2r} \left[ \frac{\Delta t_p}{\Delta \phi} - \frac{\Delta t_p}{\Delta \phi} \left( \left[ 1 + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} \right] + \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} \right] \right) \right] \\
&\quad + \frac{1}{2} \left[ w(\phi, z) \frac{\Delta t_p}{\Delta z} - \frac{\Delta t_p}{\Delta z} \left( \left[ w(\phi, z) + w(\phi, z)^2 \frac{\Delta t_p}{\Delta z} \right] + w(\phi, z) \left[ w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \right) \right] \\
&\quad - \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ (K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi, z)) \cos\left(\phi + \frac{\Delta \phi}{2}\right) + (K_\phi(\phi, z) + K_\phi(\phi - \Delta \phi, z)) \cos\left(\phi - \frac{\Delta \phi}{2}\right) \right] \\
&\quad - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z + \Delta z)) + \left( r - \frac{\Delta z}{2} \right)^2 (K_z(\phi, z) + K_z(\phi, z - \Delta z)) \right] = \\
&= 1 + \frac{v(\phi, z)}{2r} \left[ \frac{\Delta t_p}{\Delta \phi} - \frac{\Delta t_p}{\Delta \phi} \left( \cancel{1} + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} \right) \right] \\
&\quad + \frac{w(\phi, z)}{2} \left[ \frac{\Delta t_p}{\Delta z} - \frac{\Delta t_p}{\Delta z} \left( \cancel{1} + w(\phi, z) \frac{\Delta t_p}{\Delta z} + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right) \right] - \\
&\quad \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi, z) \right) \cos\left(\phi + \frac{\Delta \phi}{2}\right) + \right.
\end{aligned}
\tag{51}$$

$$\begin{aligned}
& \left[ \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi, z) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) \right] \\
& - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] \\
& = 1 - \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta\phi, z)] - \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] - \\
& \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi, z) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right) + \right. \\
& \left. \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi, z) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) \right] \\
& - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right].
\end{aligned}$$

$$\begin{aligned}
\frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi + \Delta\phi, z)} &= \frac{v(\phi, z)}{2r} \left[ -\frac{\Delta t_p}{\Delta\phi} - \frac{\Delta t_p}{\Delta\phi} \left( -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right) \right] \quad (52) \\
&+ \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi, z) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right) = \\
&= -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{2r} \left( 1 - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right) \\
&+ \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi, z) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi - \Delta\phi, z)} &= \frac{v(\phi, z)}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \right) \quad (53) \\
&+ \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi, z) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z + \Delta z)} &= -\frac{1}{2} \cdot w(\phi, z) \cdot \frac{\Delta t_p}{\Delta z} \left( 1 - \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \quad (54) \\
&+ \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z - \Delta z)} &= \frac{\Delta t_p}{\Delta z} \cdot \frac{1}{2} \cdot w(\phi, z) \left[ 1 + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \quad (55) \\
&+ \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right)
\end{aligned}$$

## 6 Second derivatives of air density with respect to velocities

### 6.1 Derivatives of Equation (23)

Equation (37) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z)} \right) = \tag{56} \\
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{1}{2} \left[ 2 - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi - \Delta \phi, z)v(\phi, z)}{r^2} \right] \right. \right. \\
& \left. \left. - \frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z)w(\phi, z) \right] \right] \right) = \\
& \frac{1}{2} \left[ - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{1}{r} \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{v(\phi, z)}{r^2} \cdot \frac{\Delta t_p}{\Delta \phi} + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r^2} \right] - \frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{\Delta t_p}{\Delta \phi} \frac{1}{r} \right) \right] \right] = \\
& \frac{1}{2} \left[ - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{2\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r^2} + \frac{\Delta t_p}{\Delta z} \frac{w(\phi, z)}{r} + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r^2} \right] - \frac{\Delta t_p}{\Delta z} \cdot \frac{w(\phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta \phi} \right] = \\
& - \frac{1}{2} \left[ \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \frac{2v(\phi, z)}{r^2} + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{w(\phi, z)}{r} + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r^2} + \frac{\Delta t_p}{\Delta z} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{w(\phi, z)}{r} \right] = \\
& - \frac{\Delta t_p}{2\Delta \phi} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{2v(\phi, z)}{r^2} + \frac{v(\phi - \Delta \phi, z)}{r^2} + 2 \frac{\Delta t_p}{\Delta z} \cdot \frac{w(\phi, z)}{r} \right]
\end{aligned}$$

Equation (38) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z)} \right) = \tag{57} \\
& \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( \frac{1}{2} \left[ 2 - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi - \Delta \phi, z)v(\phi, z)}{r^2} \right] \right. \right. \\
& \left. \left. - \frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z)w(\phi, z) \right] \right] \right) = \\
& \frac{1}{2} \left[ - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r^2} \right] \right] = - \frac{1}{2} \cdot \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{v(\phi, z)}{r^2}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi + \Delta \phi, z)}{\partial \rho_i(\phi + \Delta \phi, z)} \right) = - \frac{1}{2} \cdot \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{v(\phi + \Delta \phi, z)}{r^2} \tag{58}$$

Equation (51) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z)} \right) = \tag{59} \\
& \frac{\partial}{\partial w(\phi, z)} \left( \frac{1}{2} \left[ 2 - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi - \Delta \phi, z)v(\phi, z)}{r^2} \right] \right. \right.
\end{aligned}$$

$$\begin{aligned}
& -\frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{\Delta t_p v(\phi, z)}{\Delta \phi r} + \frac{\Delta t_p w(\phi, z)}{\Delta z} \right) + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) w(\phi, z) \right] \Bigg] = \\
& -\frac{1}{2} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta z} + \frac{\Delta t_p}{\Delta z} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) + \frac{\Delta t_p}{\Delta z} w(\phi, z) + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right] \right] = \\
& -\frac{1}{2} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi, z)}{r} + 2 \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) + \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z - \Delta z) \right] = \\
& -\frac{1}{2} \left[ 2 \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{v(\phi, z)}{r} + 2 \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) + \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z - \Delta z) \right] = \\
& -\frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{v(\phi, z)}{r} - \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) - \frac{1}{2} \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z - \Delta z)
\end{aligned}$$

Equation (52) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z)} \right) = \tag{60} \\
& \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{1}{2} \left[ 2 - \frac{\Delta t_p}{\Delta \phi} \left[ \frac{v(\phi, z)}{r} \left( \frac{\Delta t_p v(\phi, z)}{\Delta \phi r} + \frac{\Delta t_p w(\phi, z)}{\Delta z} \right) + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi - \Delta \phi, z) v(\phi, z)}{r^2} \right] \right. \right. \\
& \left. \left. - \frac{\Delta t_p}{\Delta z} \left[ w(\phi, z) \left( \frac{\Delta t_p v(\phi, z)}{\Delta \phi r} + \frac{\Delta t_p w(\phi, z)}{\Delta z} \right) + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) w(\phi, z) \right] \right] \right) = \\
& -\frac{1}{2} \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z)
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z + \Delta z)}{\partial \rho_i(\phi, z + \Delta z)} \right) = -\frac{1}{2} \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z + \Delta z) \tag{61}$$

The density at  $(\phi, z)$  does not depend on any other velocities.

## 6.2 Derivatives of Equation (24)

Equation (39) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi - \Delta \phi, z)} \right) = \tag{62} \\
& \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi - \Delta \phi, z) \right) \right] \right) = \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{1}{r} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi - \Delta \phi, z) \right) + \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} \left( \frac{\Delta t_p}{\Delta \phi} \cdot \frac{1}{r} \right) = \\
& \frac{1}{2r} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} \left( 1 + 2 \frac{\Delta t_p}{\Delta \phi} \cdot \frac{v(\phi - \Delta \phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi - \Delta \phi, z) \right)
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi + \Delta\phi, z)}{\partial \rho_i(\phi, z)} \right) = \frac{1}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\cos(\phi)}{\cos(\phi + \Delta\phi)} \left( 1 + 2 \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \quad (63)$$

Equation (54) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial w(\phi - \Delta\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z - \Delta z)} \right) = \\ & \frac{\partial}{\partial w(\phi - \Delta\phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \cdot \frac{\cos(\phi - \Delta\phi)}{\cos(\phi)} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi - \Delta\phi, z) \right) \right] \right) = \\ & \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \cdot \frac{\cos(\phi - \Delta\phi)}{\cos(\phi)} \end{aligned} \quad (64)$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi + \Delta\phi, z)}{\partial \rho_i(\phi + \Delta\phi, z - \Delta z)} \right) = \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{v(\phi, z)}{r} \cdot \frac{\cos(\phi)}{\cos(\phi + \Delta\phi)} \quad (65)$$

### 6.3 Derivatives of Equation (25)

Equation (40) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta\phi, z)} \right) = \\ & \frac{\partial}{\partial v(\phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi + \Delta\phi, z)}{r} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \right) = \\ & \frac{1}{2} \cdot \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \cdot \frac{v(\phi + \Delta\phi, z)}{r^2} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \end{aligned} \quad (66)$$

Equation (41) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial v(\phi + \Delta\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta\phi, z)} \right) = \\ & \frac{\partial}{\partial v(\phi + \Delta\phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi + \Delta\phi, z)}{r} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \right) = \\ & \frac{1}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \end{aligned} \quad (67)$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi - \Delta\phi, z)}{\partial \rho_i(\phi, z)} \right) = \frac{1}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\cos(\phi)}{\cos(\phi - \Delta\phi)} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \frac{v(\phi - \Delta\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi - \Delta\phi, z) \right) \quad (68)$$

Equation (53) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta\phi, z)} \right) = \tag{69} \\
& \frac{\partial}{\partial w(\phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi + \Delta\phi, z)}{r} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \right) = \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{v(\phi + \Delta\phi, z)}{r} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)}
\end{aligned}$$

#### 6.4 Derivatives of Equation (26)

Equation (43) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z + \Delta z)} \right) = \tag{70} \\
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \left( -1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \right) = \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{(r + \Delta z)^2}{r^3} w(\phi, z + \Delta z)
\end{aligned}$$

Equation (56) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z + \Delta z)} \right) = \tag{71} \\
& \frac{\partial}{\partial w(\phi, z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \left( -1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \right) = \\
& \frac{1}{2} \left( \frac{\Delta t_p}{\Delta z} \right)^2 \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z)
\end{aligned}$$

Equation (57) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial w(\phi, z + \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z + \Delta z)} \right) = \tag{72} \\
& \frac{\partial}{\partial w(\phi, z + \Delta z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} w(\phi, z + \Delta z) \left( -1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \right] \right) = \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} + \frac{\Delta t_p}{\Delta z} w(\phi, z) \right)
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z - \Delta z)}{\partial \rho_i(\phi, z)} \right) = \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{r^2}{(r - \Delta z)^2} \left( -1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z - \Delta z)}{r - \Delta z} + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right) \tag{73}$$

## 6.5 Derivatives of Equation (27)

Equation (42) of the main manuscript:

$$\begin{aligned} \frac{\partial}{\partial v(\phi, z - \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z - \Delta z)} \right) &= \\ \frac{\partial}{\partial v(\phi, z - \Delta z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \frac{(r - \Delta z)^2}{r^2} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z - \Delta z)}{r - \Delta z} + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right) \right] \right) &= \\ \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{(r - \Delta z)^2}{r^2} \frac{w(\phi, z - \Delta z)}{r - \Delta z} & \end{aligned} \quad (74)$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z + \Delta z)}{\partial \rho_i(\phi, z)} \right) = \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{r^2}{(r + \Delta z)^2} \frac{w(\phi, z)}{r} \quad (75)$$

Equation (55) of the main manuscript:

$$\begin{aligned} \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi, z - \Delta z)} \right) &= \\ \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \frac{(r - \Delta z)^2}{r^2} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z - \Delta z)}{r - \Delta z} + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right) \right] \right) &= \\ \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)^2}{r^2} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z - \Delta z)}{r - \Delta z} + \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right) + & \\ \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \frac{(r - \Delta z)^2}{r^2} \cdot \frac{\Delta t_p}{\Delta z} = & \\ \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)^2}{r^2} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z - \Delta z)}{r - \Delta z} + 2 \frac{\Delta t_p}{\Delta z} w(\phi, z - \Delta z) \right) & \end{aligned} \quad (76)$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z + \Delta z)}{\partial \rho_i(\phi, z)} \right) = \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{r^2}{(r + \Delta z)^2} \left( 1 + \frac{\Delta t_p}{\Delta \phi} \frac{v(\phi, z)}{r} + 2 \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) \quad (77)$$

## 6.6 Derivatives of Equation (28)

Equation (44) of the main manuscript:

$$\begin{aligned} \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi - \Delta \phi, z + \Delta z)} \right) &= \\ \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( -\frac{1}{2} \left[ \frac{v(\phi - \Delta \phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} w(\phi - \Delta \phi, z + \Delta z) \right] \right) &= \\ -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta \phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^3} \cdot \frac{\cos(\phi - \Delta \phi)}{\cos(\phi)} w(\phi - \Delta \phi, z + \Delta z) & \end{aligned} \quad (78)$$



This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi + \Delta\phi, z)}{\partial \rho_i(\phi, z + \Delta z)} \right) = -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^3} \cdot \frac{\cos(\phi)}{\cos(\phi + \Delta\phi)} w(\phi, z + \Delta z) \quad (79)$$

Equation (58) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial w(\phi - \Delta\phi, z + \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi - \Delta\phi, z + \Delta z)} \right) = \quad (80) \\ & \frac{\partial}{\partial w(\phi - \Delta\phi, z + \Delta z)} \left( -\frac{1}{2} \left[ \frac{v(\phi - \Delta\phi, z)}{r} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} \cdot \frac{\cos(\phi - \Delta\phi)}{\cos(\phi)} w(\phi - \Delta\phi, z + \Delta z) \right] \right) = \\ & -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r + \Delta z)^2}{r^2} \cdot \frac{\cos(\phi - \Delta\phi)}{\cos(\phi)} \frac{v(\phi - \Delta\phi, z)}{r} \end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi + \Delta\phi, z - \Delta z)}{\partial \rho_i(\phi, z)} \right) = -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{r^2}{(r - \Delta z)^2} \cdot \frac{\cos(\phi)}{\cos(\phi + \Delta\phi)} \frac{v(\phi, z - \Delta z)}{r - \Delta z} \quad (81)$$

## 6.7 Derivatives of Equation (29)

Equation (45) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial v(\phi + \Delta\phi, z - \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta\phi, z - \Delta z)} \right) = \quad (82) \\ & \frac{\partial}{\partial v(\phi + \Delta\phi, z - \Delta z)} \left( -\frac{1}{2} \left[ w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)^2}{r^2} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \cdot \frac{v(\phi + \Delta\phi, z - \Delta z)}{r - \Delta z} \right] \right) = \\ & -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)}{r^2} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \cdot w(\phi, z - \Delta z) \end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial \rho_{i+1}(\phi - \Delta\phi, z + \Delta z)}{\partial \rho_i(\phi, z)} \right) = -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{r}{(r + \Delta z)^2} \cdot \frac{\cos(\phi)}{\cos(\phi - \Delta\phi)} \cdot w(\phi - \Delta\phi, z) \quad (83)$$

Equation (59) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{\partial \rho_{i+1}(\phi, z)}{\partial \rho_i(\phi + \Delta\phi, z - \Delta z)} \right) = \quad (84) \\ & \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( -\frac{1}{2} \left[ w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)^2}{r^2} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \cdot \frac{v(\phi + \Delta\phi, z - \Delta z)}{r - \Delta z} \right] \right) = \\ & -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta\phi} \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{(r - \Delta z)^2}{r^2} \cdot \frac{\cos(\phi + \Delta\phi)}{\cos(\phi)} \cdot \frac{v(\phi + \Delta\phi, z - \Delta z)}{r - \Delta z} \end{aligned}$$

## 7 Second derivatives of volume mixing ratios with respect to velocities, and mixing coefficients

### 7.1 Derivatives of Equation (51)

Equation (46) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \tag{85} \\
& \frac{\partial}{\partial v(\phi, z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta \phi, z)] \right. \\
& \quad - \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] \\
& \quad - \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi) \right) \cos \left( \phi + \frac{\Delta \phi}{2} \right) \right. \\
& \quad \left. + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta \phi) \right) \cos \left( \phi - \frac{\Delta \phi}{2} \right) \right] \\
& \quad - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \\
& \quad \left. + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] \Bigg) = \\
& - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{1}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta \phi, z)] - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} \cdot \mathbf{1} = \\
& - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{1}{r^2} \cdot \left( v(\phi, z) + \frac{v(\phi - \Delta \phi, z)}{2} \right)
\end{aligned}$$

Equation (47) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \tag{86} \\
& \frac{\partial}{\partial v(\phi - \Delta \phi, z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta \phi, z)] \right. \\
& \quad - \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] - \\
& \quad \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi) \right) \cos \left( \phi + \frac{\Delta \phi}{2} \right) + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta \phi) \right) \cos \left( \phi - \frac{\Delta \phi}{2} \right) \right] \\
& \quad - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] \Bigg) = \\
& - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \cdot \frac{v(\phi, z)}{2r^2}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi + \Delta\phi, z)}{\partial v m r_i(\phi + \Delta\phi, z)} \right) = - \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \cdot \frac{v(\phi + \Delta\phi, z)}{2r^2} \quad (87)$$

Equation (60) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \quad (88) \\ & \frac{\partial}{\partial w(\phi, z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta\phi, z)] \right. \\ & - \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] \\ & - \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos \left( \phi + \frac{\Delta\phi}{2} \right) \right. \\ & \left. + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos \left( \phi - \frac{\Delta\phi}{2} \right) \right] \\ & - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \\ & \left. + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] \Big) = \\ & - \left( \frac{\Delta t_p}{\Delta z} \right)^2 \cdot 1 \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] - \left( \frac{\Delta t_p}{\Delta z} \right)^2 \cdot w(\phi, z) \cdot \frac{1}{2} \cdot 1 = \\ & - \left( \frac{\Delta t_p}{\Delta z} \right)^2 \left( w(\phi, z) + \frac{w(\phi, z - \Delta z)}{2} \right) \end{aligned}$$

Equation (61) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \quad (89) \\ & \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta\phi, z)] \right. \\ & - \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] \\ & - \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos \left( \phi + \frac{\Delta\phi}{2} \right) \right. \\ & \left. + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos \left( \phi - \frac{\Delta\phi}{2} \right) \right] \\ & - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \end{aligned}$$

$$\begin{aligned}
& + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \Big] \Big) = \\
& - \left( \frac{\Delta t_p}{\Delta z} \right)^2 \frac{w(\phi, z)}{2}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z + \Delta z)}{\partial v m r_i(\phi, z + \Delta z)} \right) = - \left( \frac{\Delta t_p}{\Delta z} \right)^2 \frac{w(\phi, z + \Delta z)}{2} \quad (90)$$

Equation (65) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_\phi(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \quad (91) \\
& \frac{\partial}{\partial K_\phi(\phi, z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta \phi, z)] \right. \\
& - \left. \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] \right. \\
& - \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi) \right) \cos \left( \phi + \frac{\Delta \phi}{2} \right) \right. \\
& + \left. \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta \phi) \right) \cos \left( \phi - \frac{\Delta \phi}{2} \right) \right] \\
& - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \\
& + \left. \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] \Big) = \\
& - \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ \cos \left( \phi + \frac{\Delta \phi}{2} \right) + \cos \left( \phi - \frac{\Delta \phi}{2} \right) \right] = \\
& - \frac{\Delta t_p}{(\Delta \phi)^2} \cdot \frac{1}{2r^2} \cdot \frac{\cos \left( \phi + \frac{\Delta \phi}{2} \right) + \cos \left( \phi - \frac{\Delta \phi}{2} \right)}{\cos(\phi)}
\end{aligned}$$

Equation (66) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_\phi(\phi \pm \Delta \phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \quad (92) \\
& \frac{\partial}{\partial K_\phi(\phi \pm \Delta \phi, z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta \phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta \phi, z)] \right. \\
& - \left. \left( \frac{\Delta t_p}{\Delta z} \right)^2 \cdot w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] \right. \\
& - \frac{\Delta t_p}{2r^2(\Delta \phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta \phi) \right) \cos \left( \phi + \frac{\Delta \phi}{2} \right) \right.
\end{aligned}$$

$$\begin{aligned}
& + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos \left( \phi - \frac{\Delta\phi}{2} \right) \Big] \\
& - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \\
& \left. + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] = \\
& - \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{1}{2r^2} \cdot \frac{\cos \left( \phi \pm \frac{\Delta\phi}{2} \right)}{\cos(\phi)}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial K_\phi(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi \pm \Delta\phi, z)}{\partial v m r_i(\phi \pm \Delta\phi, z)} \right) = - \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{1}{2r^2} \cdot \frac{\cos \left( \phi \mp \frac{\Delta\phi}{2} \right)}{\cos(\phi \mp \Delta\phi)} \quad (93)$$

Equation (71) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \\
& \frac{\partial}{\partial K_z(\phi, z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta\phi, z)] \right. \\
& - \left( \frac{\Delta t_p}{\Delta z} \right)^2 \cdot w(\phi, z) \cdot \frac{1}{2} [w(\phi, z) + w(\phi, z - \Delta z)] \\
& - \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos \left( \phi + \frac{\Delta\phi}{2} \right) \right. \\
& \left. + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos \left( \phi - \frac{\Delta\phi}{2} \right) \right] \\
& - \frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \\
& \left. + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] = \\
& - \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r + \frac{\Delta z}{2} \right)^2 + \left( r - \frac{\Delta z}{2} \right)^2}{2r^2}
\end{aligned} \quad (94)$$

Equation (72) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_z(\phi, z \pm \Delta z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z)} \right) = \\
& \frac{\partial}{\partial K_z(\phi, z \pm \Delta z)} \left( 1 - \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi, z)}{r^2} \cdot \frac{1}{2} [v(\phi, z) + v(\phi - \Delta\phi, z)] \right)
\end{aligned} \quad (95)$$

$$\begin{aligned}
& -\left(\frac{\Delta t_p}{\Delta z}\right)^2 \cdot w(\phi, z) \cdot \frac{1}{2}[w(\phi, z) + w(\phi, z - \Delta z)] \\
& -\frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left[ \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right) \right. \\
& \left. + \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) \right] \\
& -\frac{\Delta t_p}{2r^2(\Delta z)^2} \left[ \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right. \\
& \left. + \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right] = \\
& -\frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r \pm \frac{\Delta z}{2} \right)^2}{2r^2}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z \mp \Delta z)}{\partial v m r_i(\phi, z \mp \Delta z)} \right) = -\frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r \mp \frac{\Delta z}{2} \right)^2}{2\left( r \mp \Delta z \right)^2} \quad (96)$$

## 7.2 Derivatives of Equation (52)

Equation (50) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi + \Delta\phi, z)} \right) = \\
& \frac{\partial}{\partial v(\phi, z)} \left( -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{2r} \left( 1 - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right) \right. \\
& \left. + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right) \right) = \\
& -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{1}{2r} \left( 1 - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right) - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{2r} \left( -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{1}{r} \right) = \\
& -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{1}{r} \left( \frac{1}{2} - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right)
\end{aligned} \quad (97)$$

Equation (68) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi + \Delta\phi, z)} \right) = \\
& \frac{\partial}{\partial K_\phi(\phi, z)} \left( -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{2r} \left( 1 - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right) \right)
\end{aligned} \quad (98)$$

$$\begin{aligned}
& + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right) \Big) = \\
& \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \cos\left(\phi + \frac{\Delta\phi}{2}\right) = \\
& \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{1}{2r^2} \cdot \frac{\cos\left(\phi + \frac{\Delta\phi}{2}\right)}{\cos(\phi)}
\end{aligned}$$

Equation (70) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K(\phi + \Delta\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi + \Delta\phi, z)} \right) = \tag{99} \\
& \frac{\partial}{\partial K_\phi(\phi + \Delta\phi, z)} \left( -\frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{2r} \left( 1 - \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi, z)}{r} \right) \right) \\
& + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi + \Delta\phi) \right) \cos\left(\phi + \frac{\Delta\phi}{2}\right) \Big) = \\
& \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{1}{2r^2} \cdot \frac{\cos\left(\phi + \frac{\Delta\phi}{2}\right)}{\cos(\phi)}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial K(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi - \Delta\phi, z)}{\partial v m r_i(\phi, z)} \right) = \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{1}{2r^2} \cdot \frac{\cos\left(\phi - \frac{\Delta\phi}{2}\right)}{\cos(\phi - \Delta\phi)} \tag{100}$$

### 7.3 Derivatives of Equation (53)

Equation (48) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi - \Delta\phi, z)} \right) = \tag{101} \\
& \frac{\partial}{\partial v(\phi, z)} \left( \frac{v(\phi, z)}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \right) \right) \\
& + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) \Big) = \\
& \frac{1}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \right)
\end{aligned}$$

Equation (49) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial v(\phi - \Delta\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi - \Delta\phi, z)} \right) = \tag{102} \\
& \frac{\partial}{\partial v(\phi - \Delta\phi, z)} \left( \frac{v(\phi, z)}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \right) \right)
\end{aligned}$$

$$\begin{aligned}
& + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) = \\
& \frac{1}{2r} \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi, z)}{r}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial v(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi + \Delta\phi, z)}{\partial v m r_i(\phi, z)} \right) = \frac{1}{2r} \left( \frac{\Delta t_p}{\Delta\phi} \right)^2 \frac{v(\phi + \Delta\phi, z)}{r} \quad (103)$$

Equation (67) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_\phi(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi - \Delta\phi, z)} \right) = \\
& \frac{\partial}{\partial K_\phi(\phi, z)} \left( \frac{v(\phi, z)}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \right) \right. \\
& \left. + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) \right) = \\
& \frac{1}{2r^2} \cdot \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{\cos\left(\phi - \frac{\Delta\phi}{2}\right)}{\cos(\phi)}
\end{aligned} \quad (104)$$

Equation (69) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_\phi(\phi - \Delta\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi - \Delta\phi, z)} \right) = \\
& \frac{\partial}{\partial K_\phi(\phi - \Delta\phi, z)} \left( \frac{v(\phi, z)}{2r} \cdot \frac{\Delta t_p}{\Delta\phi} \left( 1 + \frac{\Delta t_p}{\Delta\phi} \cdot \frac{v(\phi - \Delta\phi, z)}{r} \right) \right. \\
& \left. + \frac{\Delta t_p}{2r^2(\Delta\phi)^2 \cos(\phi)} \left( K_\phi(\phi, z) + K_\phi(\phi - \Delta\phi) \right) \cos\left(\phi - \frac{\Delta\phi}{2}\right) \right) = \\
& \frac{1}{2r^2} \cdot \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{\cos\left(\phi - \frac{\Delta\phi}{2}\right)}{\cos(\phi)}
\end{aligned} \quad (105)$$

This is equivalent with

$$\frac{\partial}{\partial K_\phi(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi + \Delta\phi, z)}{\partial v m r_i(\phi, z)} \right) = \frac{1}{2r^2} \cdot \frac{\Delta t_p}{(\Delta\phi)^2} \cdot \frac{\cos\left(\phi + \frac{\Delta\phi}{2}\right)}{\cos(\phi + \Delta\phi)} \quad (106)$$

#### 7.4 Derivatives of Equation (54)

Equation (64) of the main manuscript:

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z + \Delta z)} \right) = \quad (107)$$



$$\begin{aligned}
& \frac{\partial}{\partial w(\phi, z)} \left( -\frac{1}{2} \cdot w(\phi, z) \cdot \frac{\Delta t_p}{\Delta z} \left( 1 - \frac{(\Delta t_p)}{(\Delta z)} w(\phi, z) \right) \right. \\
& \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right) = \\
& -\frac{1}{2} \left[ \frac{\Delta t_p}{\Delta z} \left( 1 - \frac{\Delta t_p}{\Delta z} w(\phi, z) \right) - w(\phi, z) \cdot \frac{\Delta t_p}{\Delta z} \cdot \frac{\Delta t_p}{\Delta z} \right] = \\
& -\frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \left[ 1 - 2 \frac{(\Delta t_p)}{(\Delta z)} w(\phi, z) \right]
\end{aligned}$$

Equation (75) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z + \Delta z)} \right) = \tag{108} \\
& \frac{\partial}{\partial K_z(\phi, z)} \left( -\frac{1}{2} w(\phi, z) \frac{\Delta t_p}{\Delta z} \left( 1 - \frac{(\Delta t_p)}{(\Delta z)} w(\phi, z) \right) \right. \\
& \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right) = \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r + \frac{\Delta z}{2} \right)^2}{r^2}
\end{aligned}$$

Equation (76) of the main manuscript:

$$\begin{aligned}
& \frac{\partial}{\partial K_z(\phi, z + \Delta z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z + \Delta z)} \right) = \tag{109} \\
& \frac{\partial}{\partial K_z(\phi, z + \Delta z)} \left( -\frac{1}{2} w(\phi, z) \frac{\Delta t_p}{\Delta z} \left( 1 - \frac{(\Delta t_p)}{(\Delta z)} w(\phi, z) \right) \right. \\
& \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r + \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z + \Delta z) \right) \right) = \\
& \frac{1}{2} \cdot \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r + \frac{\Delta z}{2} \right)^2}{r^2}
\end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z - \Delta z)}{\partial v m r_i(\phi, z)} \right) = \frac{1}{2} \cdot \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r - \frac{\Delta z}{2} \right)^2}{\left( r - \Delta z \right)^2} \tag{110}$$

## 7.5 Derivatives of Equation (55)

Equation (62) of the main manuscript:

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z - \Delta z)} \right) = \tag{111}$$

$$\begin{aligned} & \frac{\partial}{\partial w(\phi, z)} \left( \frac{\Delta t_p}{\Delta z} \cdot \frac{1}{2} \cdot w(\phi, z) \left[ 1 + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \right. \\ & \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right) = \\ & \frac{1}{2} \cdot \frac{\Delta t_p}{\Delta z} \left[ 1 + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \end{aligned}$$

Equation (63) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z - \Delta z)} \right) = \tag{112} \\ & \frac{\partial}{\partial w(\phi, z - \Delta z)} \left( \frac{\Delta t_p}{\Delta z} \cdot \frac{1}{2} \cdot w(\phi, z) \left[ 1 + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \right. \\ & \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right) = \\ & \frac{1}{2} \cdot \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z) \end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial w(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z + \Delta z)}{\partial v m r_i(\phi, z)} \right) = \frac{1}{2} \cdot \left( \frac{\Delta t_p}{\Delta z} \right)^2 w(\phi, z + \Delta z) \tag{113}$$

Equation (74) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z - \Delta z)} \right) = \tag{114} \\ & \frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\Delta t_p}{\Delta z} \cdot \frac{1}{2} w(\phi, z) \left[ 1 + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \right. \\ & \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right) = \\ & \frac{1}{2} \cdot \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r - \frac{\Delta z}{2} \right)^2}{r^2} \end{aligned}$$

Equation (73) of the main manuscript:

$$\begin{aligned} & \frac{\partial}{\partial K_z(\phi, z - \Delta z)} \left( \frac{\partial v m r_{i+1}(\phi, z)}{\partial v m r_i(\phi, z - \Delta z)} \right) = \tag{115} \\ & \frac{\partial}{\partial K_z(\phi, z - \Delta z)} \left( \frac{\Delta t_p}{\Delta z} \cdot \frac{1}{2} w(\phi, z) \left[ 1 + w(\phi, z - \Delta z) \frac{\Delta t_p}{\Delta z} \right] \right. \\ & \left. + \frac{\Delta t_p}{2r^2(\Delta z)^2} \left( r - \frac{\Delta z}{2} \right)^2 \left( K_z(\phi, z) + K_z(\phi, z - \Delta z) \right) \right) = \\ & \frac{1}{2} \cdot \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left( r - \frac{\Delta z}{2} \right)^2}{r^2} \end{aligned}$$

This is equivalent with

$$\frac{\partial}{\partial K_z(\phi, z)} \left( \frac{\partial v m r_{i+1}(\phi, z + \Delta z)}{\partial v m r_i(\phi, z)} \right) = \frac{1}{2} \cdot \frac{\Delta t_p}{(\Delta z)^2} \cdot \frac{\left(r + \frac{\Delta z}{2}\right)^2}{(r + \Delta z)^2} \quad (116)$$