Supporting Information for "Unravelling the kinematics of the Brewer-Dobson circulation change"

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Introduction This supporting information contains a detailed derivation of the decomposition method and a specific form of the numerical implementation is outlined. Schematic visualization of the acting mechanisms connected with individual terms of the decomposition is included, as well as more information about analyzed CMIP6 models.

Text S1. Having defined the upwelling across a material line in eq. (2) in the main text, we now want to differentiate it with respect to the time change. First, we use the Leibniz integral rule to capture the contribution of the variable bounds of integration, i.e. the effect of a net widening of the upwelling region as well as meridional shifts of individual boundaries.

$$\delta U = \int_{\varphi_2(t)}^{\varphi_2(t+\delta t)} \mathrm{d}T(\overline{z}(t^*,\varphi),t^*,\varphi) - \int_{\varphi_1(t)}^{\varphi_1(t+\delta t)} \mathrm{d}T(\overline{z}(t^*,\varphi),t^*,\varphi)$$
$$+ \int_{\max(\varphi_1(t),\varphi_1(t+\delta t))}^{\min(\varphi_2(t),\varphi_2(t+\delta t))} \mathrm{d}T(\overline{z}(t+\delta t,\varphi),t+\delta t,\varphi) - \mathrm{d}T(\overline{z}(t,\varphi),t,\varphi), \quad (1)$$

where t^* is either $t + \delta t$ (when the upwelling region is widening) or t (when the upwelling region is tapering to subtract the contribution to the change from the no-longer existing upwelling region). In the process, we assume that the center of the upwelling region is shifting only negligibly in the meridional direction compared to the width of the upwelling region. This is well justified for the annual mean upwelling in the stratosphere, where the core of the upwelling region is located around the equator (e.g. see Fig. 4 in Stiller et al., 2017). In more general instances, relative meridional coordinates following the center of the upwelling region would have to be used at this stage and also for further partitioning to separate the effect of a net meridional shift of the upwelling region.

The latter integral is taken over a domain, where upwelling is defined at both time instants, and quantifies the difference of upwelling without the widening contribution. This term is hiding five additional contributions to the net upwelling change (local accelerations of the vertical and meridional residual mean circulation components, vertical shift of the material line, changes in the shape of the material line and the changing density). These can be made explicit by realizing that evaluating the change of upwelling following the material line is akin to the concept of material derivative, hence drawing an analogy between the remaining term and the reconstruction of a material derivative in the Eulerian frame in a limit $\delta t \to 0$. From equation (1) we have:

$$\frac{\mathrm{D}\mathrm{d}T}{\mathrm{D}t}(\overline{z}(t,\varphi),t,\varphi) = 2\pi a \cos\varphi \frac{\mathrm{D}(\overline{\rho}(\overline{v}^*,\overline{w}^*)\cdot\vec{n}\mathrm{d}l)}{\mathrm{D}t}$$
$$= 2\pi a \cos\varphi[\frac{\partial(\overline{\rho}(\overline{v}^*,\overline{w}^*)\cdot\vec{n}\mathrm{d}l)}{\partial t} + \frac{\partial \overline{z}}{\partial t}\frac{\partial(\overline{\rho}(\overline{v}^*,\overline{w}^*)\cdot\vec{n}\mathrm{d}l)}{\partial z}], \tag{2}$$

where both the local derivative and partial derivative with respect to z are evaluated at $\overline{z}(t,\varphi)$, for the former we keep z and for the latter t constant.

The last term of the equation (2) gives us the contribution of the vertical shift of the material line to the net upwelling change.

In previous studies, only the vertical residual mean velocity component has been considered to contribute to the upwelling. However, due to the slope of the material line $\alpha(\overline{z}(t,\varphi),t,\varphi)$, the normal vector to it is frequently not strictly vertical. The effect of the slope is twofold - it allows contributions from the meridional residual mean velocity component to the upwelling and also affects the length of the integration path $\mathrm{d}l(\overline{z}(t,\varphi),t,\varphi)$. Hence, we can rewrite the partial derivative as:

$$\frac{\partial(\overline{\rho}(\overline{v}^*,\overline{w}^*)\cdot\vec{n}\mathrm{d}l)}{\partial t} = \frac{\partial}{\partial t}[\overline{\rho}(\overline{w}^*\cos\alpha + \overline{v}^*\sin\alpha)\frac{a\mathrm{d}\varphi}{\cos\alpha}]$$
$$= (\frac{\partial\overline{\rho w}^*}{\partial t} + \frac{\partial\overline{\rho v}^*\tan\alpha}{\partial t})a\mathrm{d}\varphi, \tag{3}$$

where the first term gives the traditional vertical mass flux change and the latter gives the joint effect of the changing slope, both evaluated at fixed $\overline{z}(t,\varphi)$. Further, we decompose the slope term to distinguish between contributions from the accelerating meridional mass flux keeping the slope constant and directly from local changes of the slope.

$$\frac{\partial \overline{\rho v}^* \tan\alpha}{\partial t} = \tan\alpha \frac{\partial \overline{\rho v}^*}{\partial t} + \frac{\overline{\rho v}^*}{\cos^2\alpha}\frac{\partial \alpha}{\partial t}, \tag{4}$$

Text S2. To get an accurate discrete form of the decomposition, we need to start with a discrete derivative of the product of several functions. For two functions we have (notation $x^+ = x(t+1)$ and $x = x(t)$):

$$\begin{aligned} f^+g^+ - fg &= a(f^+g^+ - f^+g + f^+g - fg) + (1-a)(f^+g^+ - fg^+ + fg^+ - fg) \\ &= (f^+ - f)[ag + (1-a)g^+] + (g^+ - g)[af^+ + (1-a)f], \end{aligned} \tag{5}$$

where a is an arbitrary real number. For symmetry between functions f and g we choose $a = 0.5$. For the product of three functions, it is convenient to arrange the definition of the derivative into a symmetric form for all three functions as follows:

$$f^+g^+h^+ - fgh = \frac{1}{3}[(fg)^+h^+ - (fg)h] + \frac{1}{3}[(fh)^+g^+ - (fh)g] + \frac{1}{3}[(gh)^+f^+ - (gh)f]. \tag{6}$$

Next we can use the relation for two functions for the respective terms in the equation above, which we illustrate for the first left-hand side term only:

$$\begin{aligned} \frac{1}{3}((fg)^+h^+ - fgh) = \frac{1}{6}(f^+g^+ - fg)(h + h^+) + \frac{1}{6}(h^+ - h)(f^+g^+ + fg) = \\ = \frac{1}{12}[(f^+ - f)(g + g^+) + (g^+ - g)(f^+ + f)](h + h^+) + \frac{1}{6}(h^+ - h)(f^+g^+ + fg) = \\ = \frac{1}{12}(f^+ - f)(g^+h^+ + g^+h + gh^+ + gh) + \\ + \frac{1}{12}(g^+ - g)(f^+h^+ + f^+h + fh^+ + fh) + \\ + \frac{1}{12}(h^+ - h)(2f^+g^+ + 2fg). \end{aligned} \tag{7}$$

For the remaining terms we can get analogous relations by cyclic substitution of functions. Finally, for the product of the three functions, we can obtain after summation a symmetric discrete derivative of the form:

$$\begin{aligned} f^+g^+h^+ - fgh = \\ \frac{1}{6}(h^+ - h)(2f^+g^+ + f^+g + fg^+ + 2fg) + \\ +\frac{1}{6}(g^+ - g)(2f^+h^+ + f^+h + fh^+ + 2fh) + \\ +\frac{1}{6}(f^+ - f)(2g^+h^+ + g^+h + gh^+ + 2gh). \end{aligned} \tag{8}$$

Now we can use the definitions to rewrite the change of transport U between two discrete times t and t^+:

$$\begin{aligned} \delta U = \int_{\varphi_2(t)}^{\varphi_2(t^+)} \mathrm{d}T(\overline{z}(t^*,\varphi),t^*,\varphi) - \int_{\varphi_1(t)}^{\varphi_1(t^+)} \mathrm{d}T(\overline{z}(t^*,\varphi),t^*,\varphi) + \\ + \int_{\max(\varphi_1(t),\varphi_1(t^+))}^{\min(\varphi_2(t),\varphi_2(t^+))} \mathrm{d}T(\overline{z}(t^+,\varphi),t^+,\varphi) - \mathrm{d}T(\overline{z}(t,\varphi),t,\varphi), \end{aligned} \tag{9}$$

where t^* has the same meaning as in the continuous case. The first two integrals correspond to the change in the width of the upwelling region. This change can be discretized straightforwardly, as it is nothing else than a sum of upwelling increments over the newly emerging regions, or subtraction of the upwelling increments at a preceeding time from regions no longer located in the upwelling region.

The latter term for changes at a constant height can be rewritten as follows (the dependence on φ is omitted here for the sake of space):

$$\begin{aligned} \mathrm{d}T(z(t^+),t^+) - \mathrm{d}T(z(t),t) = \\ = [\mathrm{d}T(z(t^+),t^+) - \mathrm{d}T(z(t),t^+)] + [\mathrm{d}T(z(t),t^+) - \mathrm{d}T(z(t),t)] \end{aligned} \tag{10}$$

Here, the first term is the discrete version of the vertical shift term and the second term corresponds to the changes at a fixed height. The vertical shift term is discretized as follows:

$$\frac{1}{2\pi a^2}[\mathrm{d}T(z(t^+),t^+) - \mathrm{d}T(z(t),t^+)] =$$
$$= \rho(z(t^+),t^+)\overline{w}^*(z(t^+),t^+) - \rho(z(t),t^+)\overline{w}^*(z(t),t^+) +$$
$$+\rho(z(t^+),t^+)\overline{v}^*(z(t^+),t^+)\tan\alpha(t^+) - \rho(z(t),t^+)\overline{v}^*(z(t),t^+)\tan\alpha(t^+). \tag{11}$$

The second term in the equation (10) then contains the remaining components of the upwelling decomposition. Using the form of the derivative of the product of the two (for the vertical component) and three functions (for the meridional mass flux component) we obtain their numerical implementation (shortening $z(t)$ to z):

$$\frac{1}{2\pi a^2}[\mathrm{d}T(z,t^+) - \mathrm{d}T(z,t)] = \overbrace{\frac{1}{2}[\rho(z,t^+)+\rho(z,t)][\overline{w}^*(z,t^+) - \overline{w}^*(z,t)}^{\overline{w}^*\text{ term}} +$$
$$+\overbrace{\frac{1}{6}[\rho(z,t^+)\tan\alpha(t) + 2\rho(z,t^+)\tan\alpha(t^+) + 2\rho(z,t)\tan\alpha(t) + \rho(z,t)\tan\alpha(t^+)][\overline{v}^*(z,t^+) - \overline{v}^*(z,t)]}^{\overline{v}^*\text{ term}} +$$
$$+\overbrace{\frac{1}{6}[\rho(z,t^+)\overline{v}^*(z,t) + 2\rho(z,t^+)\overline{v}^*(z,t^+) + 2\rho(z,t)\overline{v}^*(z,t) + \rho(z,t)\overline{v}^*(z,t^+)][\tan\alpha(t^+) - \tan\alpha(t)]}^{\text{shape term}} +$$
$$+\overbrace{\frac{1}{2}[\overline{w}^*(z,t^+) + \overline{w}^*(z,t)][\rho(z,t^+) - \rho(z,t)]}^{\rho\text{ term}} +$$
$$+\overbrace{\frac{1}{6}[\overline{v}^*(z,t^+)\tan\alpha(t) + 2\overline{v}^*(z,t^+)\tan\alpha(t^+) + 2\overline{v}^*(z,t)\tan\alpha(t) + \overline{v}^*(z,t)\tan\alpha(t^+)][\rho(z,t^+) - \rho(z,t)]}^{\rho\text{ term}}. \tag{12}$$

Table S1. List of the models used for CMIP6. For CESM2-WACCM SSP370 simulation, only one realisation was available for the whole period, two realisations were only until 2055.

Model	Hor. res. [km]	No. of realisations (AMIP & SSP370)	Vertical levels
CESM2	100	10 & 3	70
CESM2-WACCM	100	3 & 3*	70
MRI-ESM2-0	100	3 & 5	80
UKESM1-0-LL	250	- & 10	85

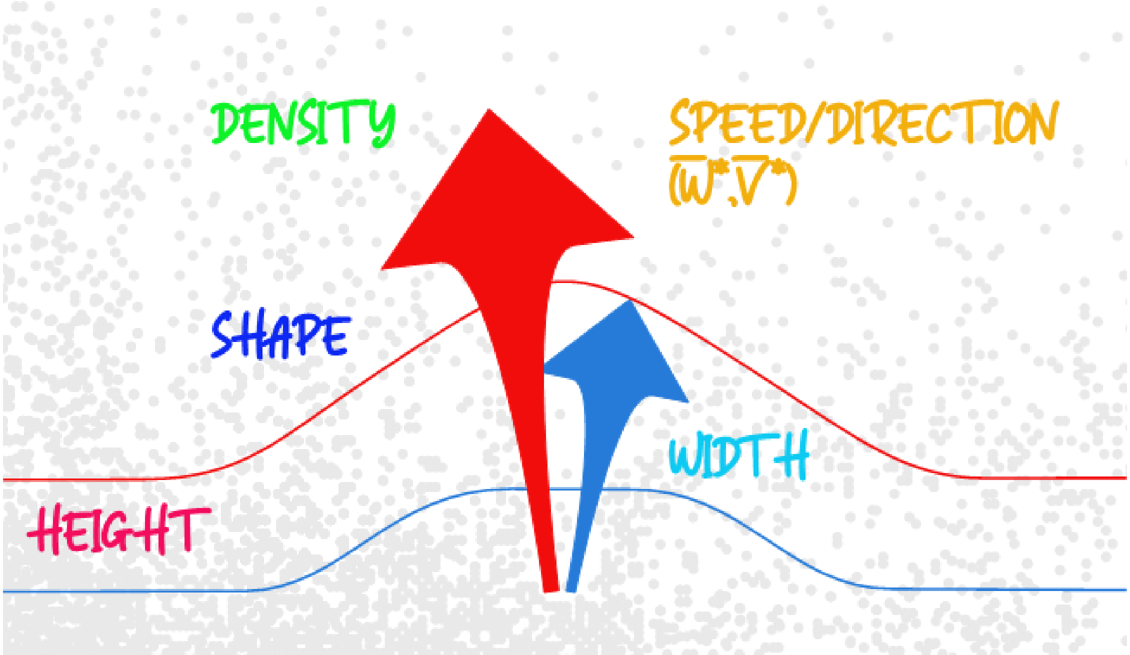

Figure S1. Schematic illustration of the contributions to the change of net upwelling across a material line A (blue line) and B (red line). The net change consists of contributions from changes of the speed (size of the arrow) and direction (inclination of the arrow) of the circulation, the width of the upwelling region, the vertical shift (height changes) of the material line, changes in the shape of the material line controlling the effectivity of meridional transport and of changing density of air that is connected with the spatially variable temperature trends (stippled background).

References

Stiller, G. P., Fierli, F., Ploeger, F., Cagnazzo, C., Funke, B., Haenel, F. J., … von Clarmann, T. (2017). Shift of subtropical transport barriers explains observed hemispheric asymmetry of decadal trends of age of air. *Atmospheric Chemistry and Physics*, *17*(18), 11177–11192. doi: 10.5194/acp-17-11177-2017