Table 4
Error subspace initialization (index $k=0$ is omitted)

Tracer horizontal covariance eigendecomposition		
Normalized variability covariance matrix:	$\mathbf{C}_{\mathrm{trc}}^{r*}=\mathbf{E}_{\mathrm{trc}}^{r*}\Pi_{\mathrm{trc}}^{r*}\mathbf{E}_{\mathrm{trc}}^{r*T}$.	(A5)
Tracer vertical covariance eigendecomposition		
Historical (past synoptic) tracer residuals:	$\mathrm{d}_{\mathrm{r}}^{i}=\mathrm{d}^{i}-\mathrm{C}^{i}\hat{\psi}_{\mathrm{trc}},\ i=1,\ldots,s$.	(A6)
Remove horizontal average, normalize:	$\mathrm{d}_{\mathrm{r}}^{i*}=N_{\mathrm{r}}^{-1}(\mathrm{d}_{\mathrm{r}}^{i}-\bar{\mathrm{d}}_{\mathrm{r}})$.	(A7)
SVD of the matrix of normalized tracer residuals:	$\mathrm{SVD}([\mathrm{d}_{\mathrm{r}}^{1*},\ldots,\mathrm{d}_{\mathrm{r}}^{s*}])=\mathbf{E}_{\mathrm{r}}^{*}\Sigma_{\mathrm{r}}^{*}\mathbf{V}_{\mathrm{r}}^{*T}$.	(A8)
Tracer variability covariance matrix:	$\mathrm{C}_{\mathrm{trc}}^{z}=\mathbf{E}_{\mathrm{trc}}^{z}\Pi_{\mathrm{trc}}^{z}\mathbf{E}_{\mathrm{trc}}^{zT}$, where $\Pi_{\mathrm{trc}}^{z}=\Sigma_{\mathrm{r}}^{*2}/s$.	(A9)
Tracer 3D variability covariance eigendecomposition		
Kronecker product:	$\mathbf{P}_{\mathrm{trc}}=\mathrm{C}_{\mathrm{trc}}^{z}\otimes\mathrm{C}_{\mathrm{trc}}^{r*}$.	(A10)
Sort eigenvalues and truncate to subspace:	$\mathbf{P}_{\mathrm{trc}}^{p}=\mathbf{E}_{\mathrm{trc}}\Pi_{\mathrm{trc}}\mathbf{E}_{\mathrm{trc}}^{T}$.	(A11)
Primitive Equation Based Error Subspace		
Ensemble of perturbed initial tracer fields:	$\hat{\psi}_{\mathrm{trc}}^{j}=\hat{\psi}_{\mathrm{trc}}+\mathbf{E}_{\mathrm{trc}}\Pi_{\mathrm{trc}}^{\frac{1}{2}}\sqrt{q}\,\mathrm{e}^{j},\quad j=1,\ldots,q$.	(A12)
Differences of PE adjusted fields, normalize:	$\mathbf{M}=[\hat{\psi}_{0}^{1}-\Psi_{0},\ldots,\hat{\psi}_{0}^{q}-\Psi_{0}];\quad M=NM^{*}$.	(A13)
SVD of normalized PE variability:	$\mathrm{SVD}(\mathbf{M}^{*})=\mathrm{E}^{*}\Sigma^{*}\mathbf{V}^{*T}$	(A14)
Initial principal error covariance matrix estimate:	$\mathbf{P}^{p}=\gamma^{2}\mathrm{E}\,\Pi\,\mathrm{E}^{T}$, with $\Pi=\Sigma^{*2}/q$.	(A15)

covariance of the tracer variability (Eqs. (A12), (A13), (A14) and (A15)). A factor scales the variability to an error variance.

In the first stage, the tracer variability covariance function is assumed separable in the horizontal and vertical. In the horizontal, the variability covariance matrices of $\boldsymbol{T}$ and $\boldsymbol{S}$, when normalized by their total variances, are presumed equal: $\mathbf{C}_{TT}^{\mathbf{r}*}=\mathbf{C}_{TS}^{\mathbf{r}*}=\mathbf{C}_{SS}^{\mathbf{r}*}=\mathbf{C}_{\mathrm{trc}}^{\mathbf{r}*}$, using a notation similar to that of Daley (1991), with the superscript $\mathbf{r}$ denoting the horizontal separation vector. In the present study, [4] the matrix $\mathbf{C}_{\mathrm{trc}}^{\mathbf{r}*}\in\mathbb{R}^{l_h\times l_h}$ is specified analytically, in accord with the horizontal scales seen in the data (Fig. 4a). Its eigende-composition (Eq. (A5)) is feasible and simply carried out. In the vertical, the decomposition of the dimensional tracer covariance matrix, $C_{\mathrm{trc}}^{z}\in\mathbb{R}^{2l_v\times 2l_v}$, is computed from EOFs of data residuals. The misfits between the initial profiles (Fig. 4a) and objectively analyzed tracers $\hat{\psi}_{\mathrm{trc}}$ are evaluated at data-points Eq. (A6). In Eq. (A6), the $\mathbf{d}^{i}$ contain the $i=1,\ldots,s$ profiles linearly interpolated onto the l_{v} model levels. The $\mathbf{C}^{i}$ consist of horizontal bilinear interpolators. The horizontal averages $\bar{d}_{\mathrm{r}}$ of the residuals $\mathbf{d}_{\mathrm{r}}^{i}$ are then removed and the resulting zero-mean residuals normalized by their sample and

[4] The number of horizontal, vertical and total grid points are l_{h}, l_{v} and $l\doteq l_{\mathrm{h}}l_{\mathrm{v}}$, respectively.