Quadruple collocation analysis of in-situ, scatterometer, and NWP winds

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Abstract

Triple collocation is an established technique for retrieving linear calibration coefficients and observation error variances of a physical quantity observed simultaneously by three different observation systems. The formalism is extended to an arbitrary number of systems, and representativeness errors and associated cross-covariances are included in a natural way. It is applied to quadruple collocations of ocean surface vector winds from two scatterometers (ASCAT-A, ASCAT-B, or ScatSat), buoy measurements, and NWP model forecasts. There are fifteen possible sets of quadruple collocation equations, twelve of which are solvable for the essential variables (calibration coefficients, observation error variances, and common variance) as well as two additional error covariances, each set leading to a different solution. A remarkable property of the quadruple collocation equations is proven: when the two additional error covariances from a particular solution are used to correct the corresponding observed covariances, all sets yield the same solution. Therefore the quadruple collocation equations by themselves give no information on the representativeness errors involved; these have to be estimated using other methods. The spreading in the solutions is a measure of the accuracy of the underlying error model. Variation of the scale at which the spatial variances are evaluated yields an optimal scale of 100 to 200 km. For the datasets used in this study the error in the scatterometer error variances is 0.03 to 0.05 ms^{-1}, more than expected on statistical grounds. A more precise determination requires an error model better describing the data.

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Key Points:

- Triple and quadruple collocation analyses show consistent results to a high degree.
- Scatterometer error estimates from triple collocation are well within 0.05 m/s.
- Using prior information on error variances, quadruple collocation analyses can provide limited information on representativeness error.

Abstract

Triple collocation is an established technique for retrieving linear calibration coefficients and observation error variances of a physical quantity observed simultaneously by three different observation systems. The formalism is extended to an arbitrary number of systems, and representativeness errors and associated cross-covariances are included in a natural way. It is applied to quadruple collocations of ocean surface vector winds from two scatterometers (ASCAT-A, ASCAT-B, or ScatSat), buoy measurements, and NWP model forecasts. There are fifteen possible sets of quadruple collocation equations, twelve of which are solvable for the essential variables (calibration coefficients, observation error variances, and common variance) as well as two additional error covariances, each set leading to a different solution. A remarkable property of the quadruple collocation equations is proven: when the two additional error covariances from a particular solution are used to correct the corresponding observed covariances, all sets yield the same solution. Therefore the quadruple collocation equations by themselves give no information on the representativeness errors involved; these have to be estimated using other methods. The spreading in the solutions is a measure of the accuracy of the underlying error model. Variation of the scale at which the spatial variances are evaluated yields an optimal scale of 100 to 200 km. For the datasets used in this study the error in the scatterometer error variances is 0.03 to 0.05 ms^{-1}, more than expected on statistical grounds. A more precise determination requires an error model better describing the data.

Plain Language Summary

When a quantity like wind speed over the ocean is measured at (almost) the same time and place by three different measuring systems, it is possible to calculate the calibration of two systems with respect to the third as well as the measurement errors in each of the three systems. This is not possible if the measurements are made by only two systems. In case of quadruple collocations there are four measurement systems, and besides the calibrations and the measurement errors also two additional error correlations can be obtained. The advent of new satellite systems makes it possible to perform quadruple collocation analyses of the wind speed at the ocean surface. Triple and quadruple collocation analyses give no clue on how to improve the error model; such improvements must be found using other techniques. However, they do show the weaknesses of the error model. In particular, they show that the scatterometer error estimates are less precise than previously thought, but it should be remembered that this is “the error in the error”: the scatterometer errors in the wind components are around 0.5 m/s, and the accuracy of this estimate is 0.05 m/s - an order of magnitude smaller, so quite useful.

1 Introduction

The triple collocation method, introduced by Stoffelen (1998), is a well-established method for calculating the relative linear calibration coefficients and absolute error variances of a data set consisting of triplets of in space and time collocated measurements. The method that simultaneously evaluates three geophysical measurement systems has, for example, been applied to ocean vector winds measured by scatterometers (Stoffelen, 1998; Vogelzang et al., 2011; McColl et al., 2014), to ocean surface wind speed from scatterometer and altimeter (Abdalla and De Chiara, 2017), and soil moisture from scatterometer (Gruber et al., 2016). The method can be readily extended to quadruple and higher-order collocations. This has been done for ocean wave height by Janssen et al., (2007) and for ocean surface currents by Danielson et al. (2018).

The multi-collocation problem is cast in an elegant form by the covariance equations. The diagonal terms yield the error variances, while the other essential unknowns (the calibration scalings and the variance common to all systems) are obtained by setting the necessary number of off-diagonal error covariances to zero. For triple collocation there are six equations with six unknowns and all off-diagonal error covariances must be neglected. For quadruple collocation there are ten equations with eight unknowns, so two off-diagonal error covariances can be solved in addition. There are fifteen possible pairs of off-diagonal error covariances, and therefore fifteen possible ways to solve the covariance equations, of which twelve have a solution.

As stated above, the triple collocation equations are solved assuming that the error covariances are zero. In most cases this is not the case, because error covariances originate not only from correlated measurement errors, but also from differences in resolution between the various observing systems involved. The latter error covariances are known as representativeness errors, and they can easily be included in the multi-collocation formalism by correcting the observed covariances for them. The first estimate of representativeness errors was given by Stoffelen (1998) in the spectral domain assuming a $k^{-5/3}$ spectrum. This was refined by Vogelzang et al. (2011) using spectra calculated from scatterometer data. A direct approach in the spatial domain was developed by Vogelzang et al. (2015). Finally Lin et al. (2015) used a method based on the triple collocation analysis itself, in order to obtain representativeness errors for extreme conditions where spectral and spatial methods are inapplicable. In many studies representativeness errors are simply neglected or circumvented by averaging all systems to a common scale (Abdalla and De Chiara, 2017). The latter approach yields the error characteristics of the products at some average resolution, rather than at the original resolutions.

The Indian Space Research Organisation (ISRO) launched the ScatSat satellite carrying a K_u-band pencil-beam scatterometer on September 26, 2016. ScatSat was launched in the same orbital plane as ASCAT-A and ASCAT-B, so quadruple collocations of ScatSat and ASCAT winds combined with observations from moored buoys and ECMWF model forecasts are available.

The twelve soluble quadruple collocation equations (further referred to as models) all have different values for the essential unknowns and for the two additional off-diagonal error covariances. One can interpret the additional error covariances as extra information or as a measure of how well the error model satisfies the underlying assumptions (sufficiency of linear calibrations and independence of the measurement error from the magnitude of the wind component). The latter view is to be preferred. When representativeness errors are neglected, all models yield additional error covariances of the order of 0.1 m^2s^{-2}, though their signs may differ. They can't be used to estimate the representativeness errors, as this would require the values of three additional off-diagonal covariances. Increasing the representativeness errors diminishes the additional covariances and brings the essential unknowns closer together until an optimum value is found. This optimal value of the representativeness errors agrees with those from earlier studies.

The additional error covariances from a particular model can be made to vanish by first determining them and then solve the covariance equations again with the additional error covariances subtracted from the corresponding observed covariances. A remarkable phenomenon is proven: if the observed covariances are corrected in this way, all models yield the same solution and all additional error covariances vanish. In that case the covariance equations are called mathematically consistent. Numerical experiments show that mathematical consistency can also be achieved with a linear combination of additional off-diagonal error covariances from different models. This implies that there is an infinite number of ways to make the covariance equations mathematically consistent. Only one of them is physically consistent, i.e., the covariances are corrected in such a way that the covariance equations yield the right solution. The quadruple collocation method itself gives no clue on what choice should be made, so this information must come from external sources.

It is possible to reformulate the quadruple collocation error model in order to directly incorporate two unknown representativeness errors. The resulting solution is numerically highly unstable and can be used for huge collocation data sets only.

In section 2 the multi-collocation formalism is shortly presented. The covariance equations are derived and representativeness errors are included in the formalism. The solution method is presented. Mathematical and physical consistency are introduced and discussed. In section 3 the quadruple collocation data sets are presented. Section 4 contains the results for a simulated dataset. Section 5 contains the results of the real quadruple collocation data sets. The paper ends with conclusions in section 6. Some technical details are presented in Appendices A, B, and C.

2 Multi collocation formalism

2.1 Covariance equations

Suppose we have a set of K collocated measurements made by n observation systems, $\left\{x_i^{(k)}\right\}$, with k the collocation index, $k = 1, \ldots, K$, and i the observation system index, $i = 1, \ldots, n$. Assuming that linear calibration is sufficient for intercalibration and omitting the collocation index k, we can pose the following simplified observation error model:

$$x_i = a_i(t + \varepsilon_i) + b_i \tag{1}$$

where t is the signal common to all observation systems (also referred to as the truth), a_i the calibration scaling, b_i the calibration bias, and ε_i a random measurement error with zero average and variance σ_i^2. It is also assumed that ε_i is uncorrelated with the common signal t, $\langle t\varepsilon_i \rangle = 0$, where the brackets $\langle\ \rangle$ stand for averaging over all measurements k made by system i, for instance

$$\langle t\varepsilon_i \rangle = \frac{1}{K}\sum_{k=1}^{K} t^{(k)}\varepsilon_i^{(k)} \tag{2}$$

Of course, the assumptions made should be checked first by inspecting scatter plots. Note that x_i is uncalibrated and t is calibrated, so (1) actually constitutes an inverse calibration transformation.

Without loss of generality we can select the first observation system as calibration reference, so $a_1 = 1$ and $b_1 = 0$. Forming first moments $M_i = \langle x_i \rangle$ one readily finds that $M_i = a_i\langle t \rangle + b_i$. For $i = 1$ this yields $\langle t \rangle = M_1$ and the calibration biases for all i are given by

$$b_i = M_i - a_i M_1 \tag{3}$$

The second moments $M_{ij} = \langle x_i x_j \rangle$ satisfy

$$M_{ij} = a_i a_j \big(\langle t^2 \rangle - M_1^2 + \langle \varepsilon_i \varepsilon_j \rangle\big) + M_i M_j \tag{4}$$

where (3) was used to get rid of the biases. Forming covariances $C_{ij} = M_{ij} - M_i M_j$, introducing the common variance $T = \langle t^2 \rangle - M_1^2$, and writing $e_{ij} = \langle \varepsilon_i \varepsilon_j \rangle$ this reduces to the covariance equations

$$C_{ij} = a_i a_j \left(T + e_{ij}\right) \tag{5}$$

Note that C_{ij} and e_{ij} are symmetric in their indices.

Equations (3) and (5) completely define the multi collocation problem for error model (1). The covariances C_{ij} are calculated from the observed, uncalibrated data. Since a_i is the scaling of the inverse calibration transformation as remarked above, T and e_{ij} are in terms of the calibrated data. The calibrated covariances are given by $a_i^{-1} a_j^{-1} C_{ij}$, and the error variances by $\sigma_i^2 = e_{ii} = a_i^{-2} C_{ii} - T$.

2.2 Essential and additional unknowns

Equation (5) is symmetric in i and j, so for n collocated measurements there are $n(n+1)/2$ equations. These have to be solved for $2n$ essential unknowns: n error variances $\sigma_i^2 = e_{ii}$, $(n-1)$ calibration scalings $a_i, i = 2, \dots, n$, and the common variance T. The error variances must be obtained from the diagonal covariance equations of (5), leaving $n(n-1)/2$ off-diagonal equations to solve for the n remaining essential unknowns a_i and T.

For double collocation, $n = 2$, there are more unknowns than equations, and further assumptions must be made to obtain a solution. If the reference system is assumed to be free of errors, $\sigma_1^2 = 0$, the covariance equations can be solved as

$$T = C_{11}, \;\; a_2 = \frac{C_{12}}{C_{11}}, \;\; \sigma_2^2 = \frac{C_{22}}{a_2^2} - C_{11} \tag{6}$$

which is the well-known linear regression result. Note that alternatively one may for example assume equal errors, $\sigma_1^2 = \sigma_2^2 = \sigma^2$, such that $a_2 = \sqrt{C_{22}/C_{11}}$, representing a symmetric linear regression. In this case the value of σ^2 and hence that of T can be approximated by estimating the covariance of $x_1 - x_2$ following (1). It is clear that the results of a linear regression depend on the assumptions in the two underlying observation error models. Also in triple and quadruple collocation the results will depend on the appropriateness of the underlying error model, though more advanced error models may be tested.

In the case of triple collocation, $n = 3$, there are three off-diagonal equations and three remaining essential unknowns a_2, a_3, and T. By setting $e_{i,j} = 0$ for $i \neq j$ the covariance equations are readily solved in terms of the uncalibrated covariances as

$$T = \frac{C_{12} C_{13}}{C_{23}}, \;\; a_2 = \frac{C_{23}}{C_{13}}, \;\; a_3 = \frac{C_{23}}{C_{12}} \tag{7}$$

Note that (7) implies that $T = a_2^{-1} C_{12} = a_3^{-1} C_{13} = a_2^{-1} a_3^{-1} C_{23}$, so the calibrated off-diagonal covariances are all equal to the common variance, as can be expected from (5).

For quadruple collocation, $n = 4$, there are six off-diagonal equations and four remaining essential unknowns. Four error covariances e_{ij} must be set to zero to solve the covariance equations for a_i and T; the remaining two can easily be solved to obtain two additional error covariances e_{ij} as

$$e_{ij} = \frac{C_{ij}}{a_i a_j} - T \tag{8}$$

Alternatively, one could pose assumptions on the partial correlation between errors of different systems, e.g., due to equal spatial representation error between 2 or 3 systems (e.g., all scatterometers); see next section. Solution closure is also possible by assuming known or equal parameters of a_i or σ_i^2 for several systems. Obviously, in all cases the number of unknowns in the equations should not exceed six.

As n increases, the number of additional variables that can be solved grows. For quintuple collocation, $n = 5$, there are ten off-diagonal equations with five remaining essential unknowns and five additional ones.

For collocation data sets with $n > 3$ there is freedom in which off-diagonal equations to choose for solving a_i and T. For quadruple collocation there are $\binom{6}{4} = 15$ possible combinations. Each particular combination of off-diagonal covariance equations will further be referred to as a model, and all quadruple model solutions are listed in Appendix A. It appears that three models have no solution: those for which the unused off-diagonal terms C_{ij} and C_{kl} have indices $\{i, j, k, l\}$ that are a permutation of $\{1,2,3,4\}$. For quintuple collocation the number of models is $\binom{10}{5} = 252$.

2.3 Representativeness errors

As stated above, the covariance equations are solved assuming that a sufficient number of error covariances are zero, so it is important to know which off-diagonal error covariances e_{ij} can be safely neglected. This is not an easy problem since nonzero off-diagonal error covariances can be caused not only by correlated measurement errors but also by differences in resolution between the various observation systems. The latter error covariances are known as representativeness errors, which may be of spatial, temporal, or geophysical origin. For triple collocation this happens when systems 1 and 2 (say buoys and scatterometer) have better resolution than system 3 (say Numerical Weather Prediction (NWP) model background). In such a case systems 1 and 2 share a common signal that is not resolved by system 3, and this shared signal expresses itself as an error covariance between systems 1 and 2 – hence the name representativeness error (Stoffelen, 1998; Vogelzang et al., 2011).

Suppose that in a triple collocation analysis the representativeness error is known as r_2^2 (the meaning of the subscript will be made clear below). Denoting $\bar{C}_{ij}$ as the covariances corrected for the representativeness error and C_{ij} the uncorrected ones, the correction reads

$$\bar{C}_{ij} = \begin{cases} C_{ij} - r_2^2, & i,j = 1,2 \\ C_{ij}, & i = 3 \vee j = 3 \end{cases} \tag{9}$$

This relation is obtained when assuming that a common signal ρ_2 with zero average and variance r_2^2 is part of the errors in systems 1 and 2 in (1), but not of system 3. In such a case, the solution of the off-diagonal covariance equations from (7) reads

$$\bar{T} = T - \frac{C_{13}}{C_{23}} r_2^2, \;\; \bar{a}_2 = a_2, \;\; \bar{a}_3 = \frac{C_{23}}{C_{12} - r_2^2} \tag{10}$$

where the bar denotes correction for the representativeness error. Consequently, the error variances follow from (8) as

$$\bar{\sigma}_1^2 = \sigma_1^2 + r_2^2\left(\frac{C_{13}}{C_{23}} - 1\right) \tag{11a}$$

$$\bar{\sigma}_2^2 = \sigma_2^2 + r_2^2\frac{C_{13}}{C_{23}}\left(1 - \frac{C_{13}}{C_{23}}\right) \tag{11b}$$

$$\bar{\sigma}_3^2 = \sigma_3^2 + r_2^2\left(\frac{C_{13}}{C_{23}} - 2\frac{C_{12}C_{33}}{C_{23}^2}\right) + r_2^4\frac{C_{33}}{C_{23}^2} \tag{11c}$$

In the practical cases considered in this work the off-diagonal uncalibrated covariances differ little among themselves and are larger than the representativeness error by at least an order of magnitude. Therefore correction of the representativeness error only reduces the error variance of system 3 and increases its calibration scaling. Note that Lin et al. (2015) find the representativeness error from (10) by demanding that $\bar{a}_3$ has a reasonable, pre-defined value.

If the variance of the signal in system 1 that is not measured by the other systems is known as r_1^2, equation (9) can be extended for C_{11} as $\bar{C}_{11} = C_{11} - r_1^2 - r_2^2$, leaving the other covariances unaltered. This only decreases $\bar{\sigma}_1^2$ by r_1^2; the other essential variables remain the same. Assuming that the systems are ordered in decreasing resolution, this suggest a general form with representativeness errors $r_k^2, k = 1, n-1$ that give the signal contained in system k but not measured by system $k+1$. A representativeness error r_k^2 is taken into account by subtracting it from all C_{ij} with $i \leq k$ and $j \leq k$, and (9) becomes

$$\bar{C}_{ij} = C_{ij} - \sum_{k=max(i,j)}^{n-1} r_k^2 \tag{12}$$

Note that this leaves the structure of the covariance equations (5) unaltered.

2.4 Mathematical and physical consistency

If in a quadruple collocation analysis a substitution $C_{ij} \to C_{ij} - E_{ij}$, with E_{ij} an external correction to the observed covariance, leads to a solution with error covariances $e_{ij} \equiv 0$ $(i \neq j)$ for all solvable models, the correction E_{ij} is said to make the covariance equations mathematically consistent. If, in addition, the corrections E_{ij} are equal to the true error correlations and/or representativeness errors, the covariance equations are also physically consistent. It is shown below for quadruple collocations that physical consistency is a much stronger requirement than mathematical consistency.

Suppose one runs the quadruple collocation analysis without any correction for representativeness or error correlations. For a specific model M between 1 and 12 this yields an error covariance matrix $e_{ij}^{(M)}$ with two nonzero additional error covariances, see (8). Redoing the analysis for model M with transformed covariances $C_{ij} \to C_{ij} - E_{ij}$, where

$$E_{ij} = a_i^{(M)} e_{ij}^{(M)} a_j^{(M)} \tag{13}$$

will yield the same solution for the essential unknowns as before, but the additional error covariances e_{ij} will now all become zero, because they were incorporated in the covariances. Now the following remarkable property holds: if one solves any other model with transformation (13), the solution becomes the same as that for model M. Therefore it no longer matters which model is used to solve the covariance equations in such a case: all models yield the same solution. The authors conjecture that this is a mathematical property of the covariance equations that also holds for higher order collocations.

In Appendix B this is shown explicitly for quadruple collocation models model 12 and 1. All other cases were checked in the same way using FORM, a program for algebraic manipulation (Vermaseren et al., 2018). Moreover, numerical experiments showed that the transformation (13) can be generalized to

$$E_{ij} = \sum_M w_M \, a_i^{(M)} e_{ij}^{(M)} a_j^{(M)} \tag{14}$$

where the summation is over an arbitrary number of models M. The weights w_M may take any value, also negative ones, but their sum should be between zero and two to ensure convergence of the calculation, with optimal convergence when the sum of the weights equals one.

This implies that there is an infinite number of ways to make the covariance equations mathematically consistent. Therefore mathematical consistency does not ensure physical consistency.

It is possible to retrieve representativeness errors r_2^3 and r_3^2 in a quadruple collocation analysis by adjusting the error model (1). The details are given in Appendix C. Unfortunately, the solution is numerically highly unstable.

2.5 Method of solution

The covariance equations are solved iteratively, thus enabling detection and removal of outliers. The iteration starts with assuming that the systems are perfectly calibrated, so $a_i = 1$ and $b_i = 0$ for all i. The first and second moments are calculated with the input data, covariances are formed, and equations (3) and (5) are solved analytically for calibration coefficients $\tilde{a}_i$ and $\tilde{b}_i$. These are used to update $a_i \rightarrow a_i \tilde{a}_i$ and $b_i \rightarrow b_i + \tilde{b}_i$. In each iteration also $std(d_{ij})$, the standard deviation of the difference between each pair of measurements is calculated. When during calculation of the moments it is found that d_{ij} for a particular measurement exceeds four times $std(d_{ij})$ from the previous iteration, that collocation is excluded – also known as four-sigma test. The iteration has converged when both $|1 - \tilde{a}_i| < \epsilon$ and $|\tilde{b}_i| < \epsilon$, with ϵ the required precision. Then the common variance T can be calculated, as well as all other unknowns.

In this study the calculations are done in double precision. Starting with $std(d_{ij}) = 3$, which is sufficiently large, the iteration converges within 10 iterations to a precision $\epsilon = 10^{-9}$.

3 Data

3.1 Collocation data

In order to distinguish easily between the quadruple collocation data sets and the triple collocation subsets that can be formed from them, “b” will stand for the buoys, “A” for ASCAT-A, “B” for ASCAT-B, “S” for Scatsat, and “E” for the ECMWF forecast.

In this paper three quadruple collocation data sets are studied:

1. buoys – ASCAT-A – ASCAT-B – ECMWF (bABE)
2. buoys – ASCAT-A – ScatSat – ECMWF (bASE)

3. buoys – ASCAT-B – ScatSat – ECMWF (bBSE)

3.1.1 Buoy data

The buoy measurements are obtained from ECMWFs Meteorological Archival and Retrieval System (MARS) at www.ecmwf.int/services/archive. Only data from buoys not blacklisted by ECMWF are used. Buoys are blacklisted by ECMWF when they show large differences with the model fields over prolonged periods (Bidlot et al., 2002). Most of the accepted buoy data is from the buoy arrays in the Tropics and from buoys off the coasts of the U.S.A. and Europe. The buoy measurements are point measurements averaged over 10 minutes time issued once per hour. At a typical wind speed of 7 m/s this corresponds to a scale of 4.2 km, making the buoys the measurement system with highest spatial resolution. Effects of air mass density and stability that affect the dispersion of the 10-m wind for given sea surface roughness are taken out by using the so-called stress-equivalent wind (de Kloe et al., 2017).

3.1.2 ASCAT data

ASCAT is a C-band scatterometer that measures the Normalized Radar Cross Section (NRCS, denoted as σ^0, with six fan beam antennas at VV polarization (Figa-Saldaña et al., 2002). Two antennas look forward to either side of the satellite track, two antennas look sideward, and two antennas look backward. ASCAT is mounted on the MetOp series of satellites operated by EUMETSAT. ASCAT-A was launched 19 October 2006 and ASCAT-B on 17 September 2012, both in a polar orbit with an altitude of 817 km and in the same orbital plane.

The σ^0 values over the open ocean are processed with the ASCAT Wind Data Processor (AWDP) to ocean surface vector winds (Verhoef et al., 2020). First, a Geophysical Model Function (GMF) giving radar cross section as a function of wind speed and direction, observation geometry, and radar frequency and polarization (Stoffelen et al., 2017) is inverted numerically. This procedure generally yields two to four solutions. After quality control, a preferred solution is selected in the ambiguity removal step. AWDP uses Two-Dimensional Variational Ambiguity Removal (2DVAR), see (Vogelzang et al., 2007) for more details.

In this study ASCAT-25 data on a 25 km grid are used. These data have a true spatial resolution of about 50 km.

3.1.3 ScatSat data

ScatSat is an Indian satellite launched on 26 September 2016 by the Indian Space Research Organization (ISRO) in a polar orbit at a height of 720 km in the same orbital plane as ASCAT-A and ASCAT-B. It carries a Ku-band scatterometer measuring σ^0, the radar cross section of the Earth's surface with a rotating pencil-beam antenna operating at HH and VV polarization [*Bhowmick et al*., 2019].

In this study 25-km sampled ScatSat data from 6 October 2016 to 22 July 2017 were used, because these were generated using version 1.1.3 of the ISRO L1B processor. The L1B σ^0 values were processed with the Pencil beam Wind Data Processor (PenWP) (Verhoef et al., 2018a). The inversion step in PenWP is similar to that in AWDP, but ambiguity removal is different. Wind data from rotating pencil beam scatterometers are noisy in the nadir part of the swath because of the unfavourable observation geometry. This noise can be reduced by the so-called Multi Solution Scheme (MSS) that takes the full wind pdf into account rather than only up to four local minima in the inversion residual. The empirical ECMWF background error covariances used in 2DVAR spatially filter the noisy local wind inversion pdfs and hence somewhat degrade spatial resolution (Vogelzang and Stoffelen, 2018).

ScatSat product verification for the 25-km winds by triple collocation shows that on the scatterometer scale the wind vector error of ScatSat, ECMWF and buoys is resp. 0.98 m/s, 1.58 m/s and 1.96 m/s (Verhoef et al., 2018b). Recent verification shows wind vector errors of ASCAT-B, ECMWF and buoys of resp. 0.69 m/s, 1.74 m/s and 1.83 m/s (Verspeek et al., 2019). Although different weather samples were used in these two triple collocations, it illustrates that 1) ASCAT winds are more accurate than ScatSat winds, 2) ECMWF wind vector errors are much larger than scatterometer wind vector errors, 3) ScatSat 25-km winds have somewhat lower spatial resolution than ASCAT 25-km winds. The latter assertion refers to the larger buoy error variance on the ScatSat scatterometer scale as compared to the buoy error variance on the ASCAT scatterometer scale. Since buoy wind measurements are very accurate, most of the buoy error variance in triple collocation is due to true wind variance within the scatterometer spatial resolution cell. This is further corroborated by verifications of scatterometer winds at varying spatial resolutions (Verhoef et al., 2018b; Verspeek et al., 2019).

3.1.4 ECMWF data

NWP forecasts from the Integrated Forecast System (IFS) of ECMWF are contained in the ASCAT and ScatSat wind products, since they are used as background for the ambiguity removal in AWDP and PenWP. The ECMWF forecasts are interpolated quadratic in time and bilinear in space to the time and position of the scatterometer measurement. The forecast lead is three hours at least to prevent that any collocated wind may have been assimilated by the IFS. Over the ocean ECMWF stress-equivalent winds are relatively smooth and prone to certain systematic errors (Vogelzang et al., 2011, Belmonte and Stoffelen, 2019; Trindade et al., 2020).

3.1.5 Data preparation

First three triple collocation files of buoys, scatterometer, and ECMWF forecast were made with a maximum distance between the buoy and the center of the scatterometer wind vector cell of 17.7 km and a maximum time difference of 30 minutes. Next, each pair of triple collocation files was merged into a quadruple collocation file, by searching for the same buoy (using the buoy identification number) at the same date and time plus or minus one hour. If the buoy measurement times differed by one hour, then the one closest in time to the two scatterometer measurements was selected. The maximum time difference between scatterometer measurements in the quadruple collocation files was set to one hour. The ECMWF wind forecast associated with ASCAT-A or ASCAT-B (in order of preference) was added to the quadruple collocation file. The number of collocations is 4034 for bASE, 3976 for bBSE, and 10083 for bABE.

3.2 Scatterometer resolution and representativeness errors

As argued in the previous subsection, ScatSat has a poorer resolution than ASCAT because of the use of 2DVAR in combination with MSS in ScatSat processing. As an example, figure 1 shows a wind front observed simultaneously by ASCAT and ScatSat on October 24, 2016 around 17:00. Winds flagged by the AWDP and PenWP quality control are depicted in grey. The ScatSat wind field is smooth, in particular in the nadir part of the swath and broadens the frontal zone, while the front is very sharp in ASCAT.

Figure 2 shows the difference in spatial variance of scatterometer and ECMWF, $\Delta V(s) = V_{scat}(s) - V_{ECMWF}(s)$, as a function of separation distance s for ASCAT-A, ASCAT-B, and ScatSat. In the terminology of equation (12), the ScatSat representativeness error with respect to the ECMWF model in bASE or bBSE collocations, r_3^2, is defined as $r_3^2 = V_{ScatSat}(s) - V_{ECMWF}(s)$, the height of the dotted curve. The representativeness error r_2^2 of ASCAT-A or ASCAT-B relative to ScatSat equals the vertical distance between the dotted curve on one hand and the solid or dashed curve on the other. This is rather small for the zonal wind component u. The ASCAT representativeness error with respect to the ECMWF background equals $r_2^2 + r_3^2$.

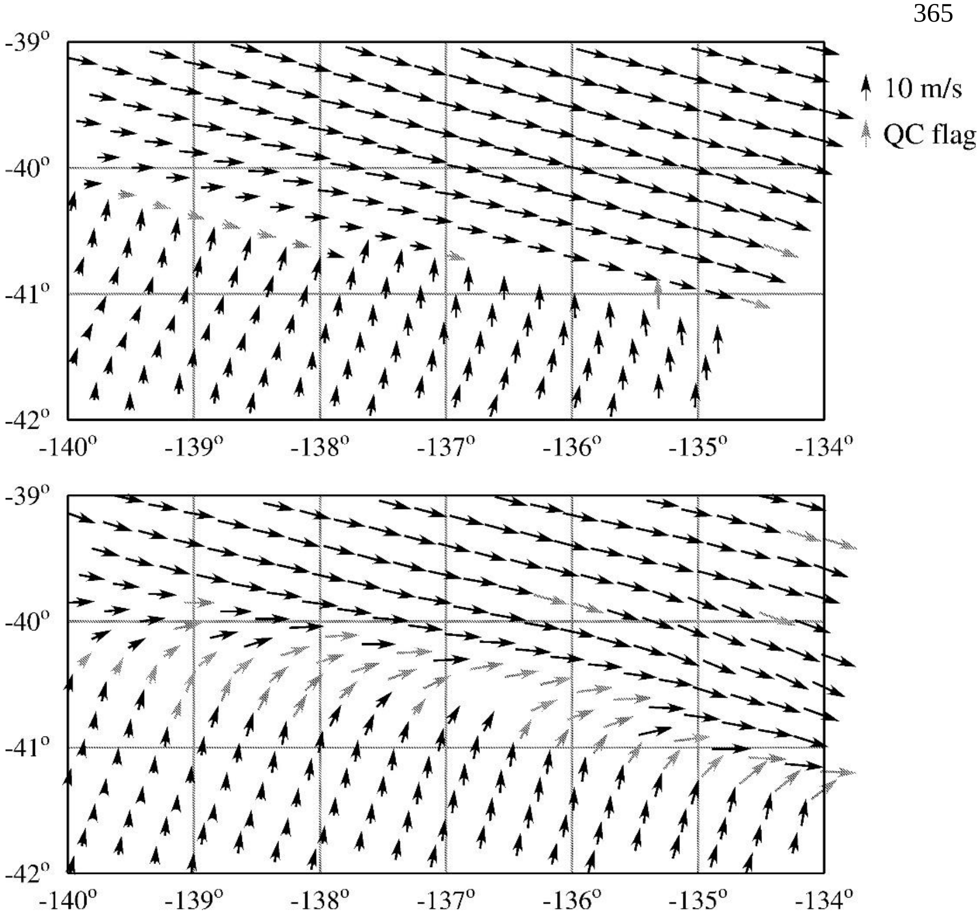

Figure 1. Wind field observed simultaneously by ASCAT (upper panel) and ScatSat (lower panel) on October 24, 2016 around 17:00.

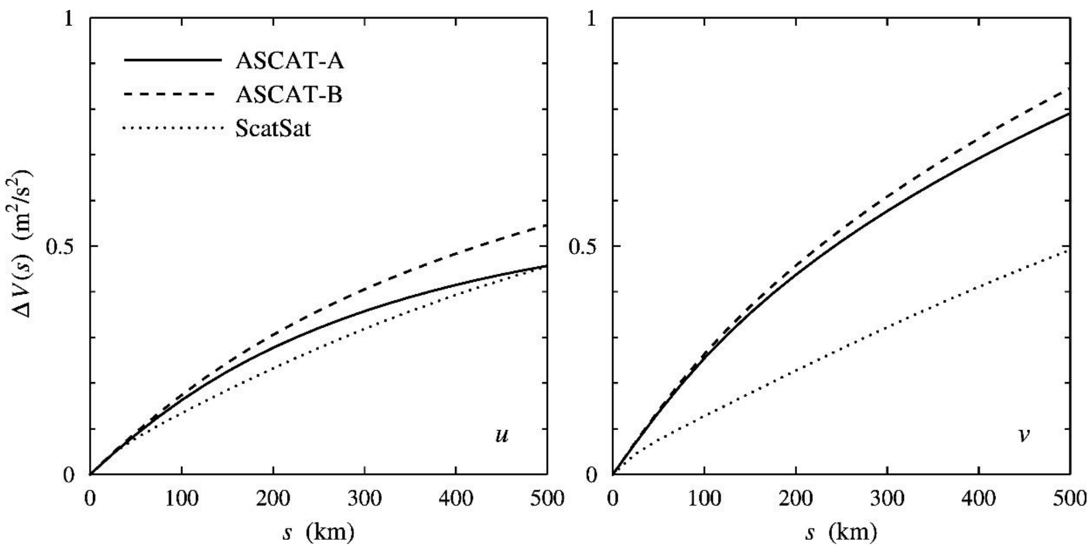

Figure 2. Difference between the spatial variance of ASCAT-A, ASCAT-B, and ScatSat and that of ECMWF, $\Delta V(s)$, as a function of s for the zonal and meridional wind components, u and v.

The scale s at which the representativeness errors are evaluated is defined in (Vogelzang et al., 2015) as s equal to 200 km, the estimated real spatial resolution of the ECMWF model over the open ocean. Since the representativeness errors will be used with quadruple collocations including buoys, the spatial variances were calculated for the Northern Hemisphere and the Tropics only (latitude > -30°) because the data sets contain no buoys in the Southern Hemisphere.

3.3 Simulated data

The simulated data are constructed from the ASCAT-A measurements in the bABE collocation data set. In principle, any wind data set could be chosen, but this choice has the advantage that statistical errors caused by the limited number of observations are equal for real and simulated data.

The u and v components of these data are considered as the true signal to which linear calibrations with known coefficients may be applied and to which Gaussian errors with known spread may be added. There are two ways of introducing representativeness errors: by explicitly adding the same Gaussian error of known amplitude to two or more systems, or by running with a certain stride through the data and taking averages. The second method comes closer to what happens in reality, but has the disadvantage that the averaging procedure introduces a calibration shift which complicates interpretation of the results. Moreover, the averaging requires a large data set. Therefore the first method is chosen.

4 Simulations

Solving the quadruple collocations using simulated data with known characteristics yields insight in the behavior of the solutions. In this section the effect of representativeness errors that are not explicitly accounted for is studied. From (12) the full error model reads

$$x_1 = a_1(t + \varepsilon_1) + b_1 + \rho_2 + \rho_3 \tag{15a}$$

$$x_2 = a_2(t + \varepsilon_2) + b_2 + \rho_2 + \rho_3 \tag{15b}$$

$$x_3 = a_3(t + \varepsilon_3) + b_3 + \rho_3 \tag{15c}$$

$$x_3 = a_4(t + \varepsilon_4) + b_4 \tag{15d}$$

with $a_1 = 1$, $b_1 = 0$, and ρ_2 and ρ_3 are Gaussian random signals with zero average and variances r_2^2 and r_3^2, respectively. This model will be solved neglecting representativeness errors, despite the fact that they are included in the collocation data. The simulated data in this section have error variances $\sigma_1^2 = 0.6$ m^{2}s^{-2}, $\sigma_2^2 = 0.8$ m^{2}s^{-2}, $\sigma_3^2 = 1.0$ m^{2}s^{-2}, and $\sigma_4^2 = 1.2$ m^{2}s^{-2}. The calibration scalings are $a_2 = 0.99$, $a_3 = 0.98$, and $a_4 = 0.95$. The error correlations can be included by adding ρ_2 and ρ_3 to the collocation data or, easier, to add the resulting error covariances e_{ij} at the appropriate place in the covariance equations (5).

The first simulation addresses the case of only a representativeness error r_2^2, corresponding to a situation in which systems 1 and 2 have high resolution while systems 3 and 4 have poor resolution, so $r_3^2 = 0$. This is accomplished by setting $e_{12} = r_2^2$, and the representativeness error only affects covariance C_{12}. Figure 3 shows the resulting error variances as a function of r_2^2 for each of the twelve solvable models listed in Appendix A.

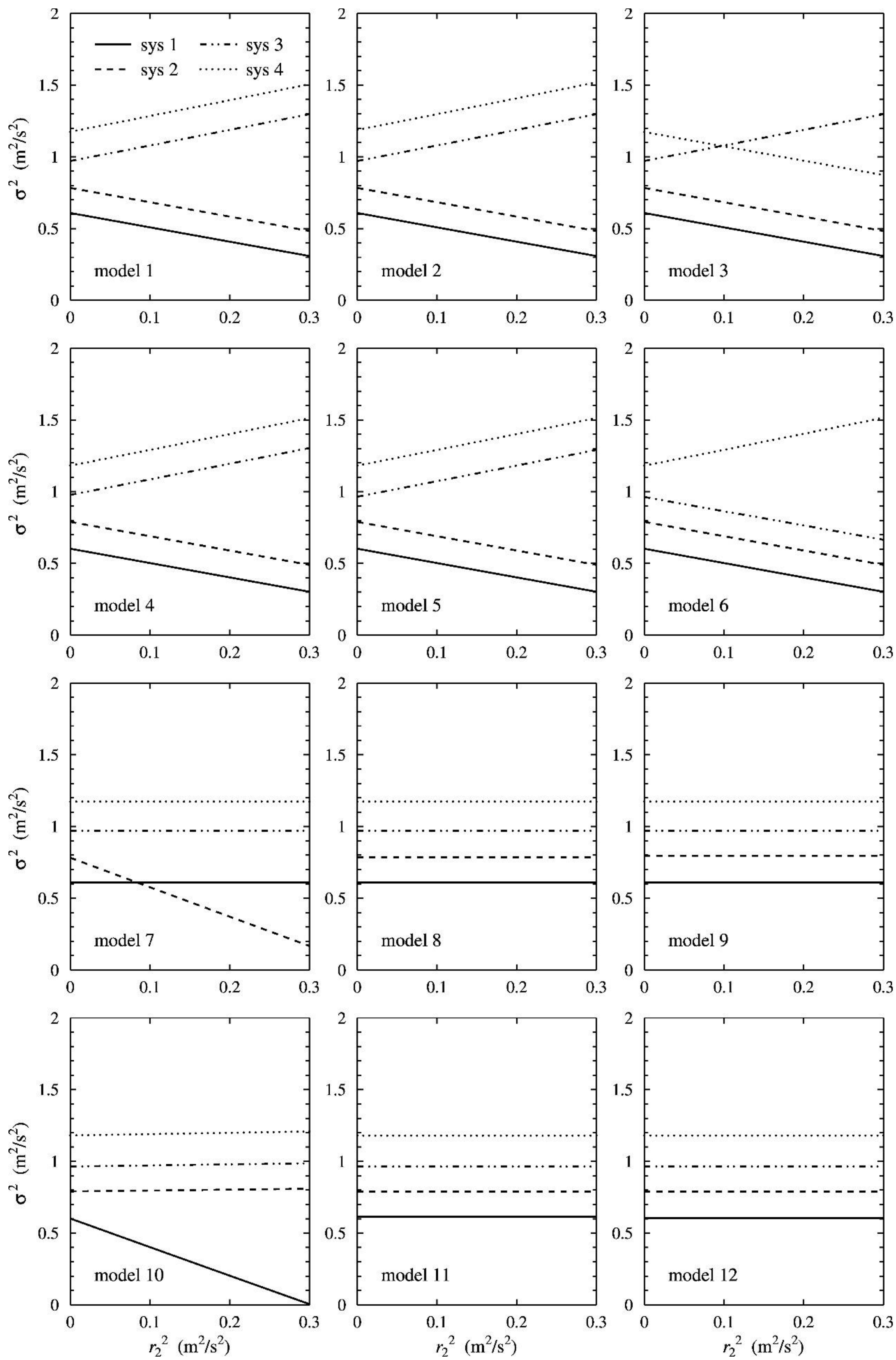

Figure 3. Error variances as a function of representativeness error r_2^2 for the twelve quadruple collocation models.

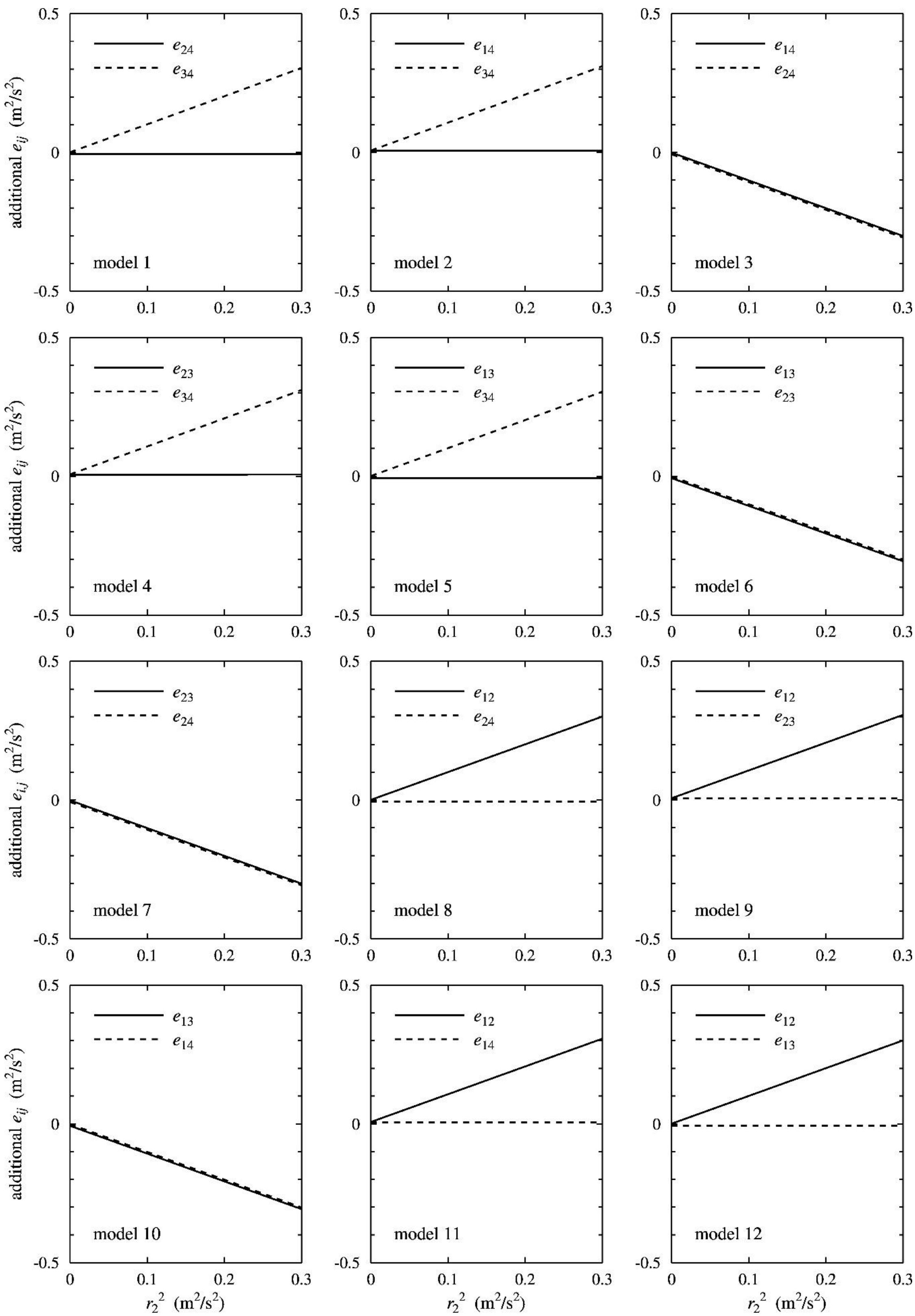

Figure 4. Additional error covariances as a function of representativeness error r_2^2 for the twelve quadruple collocation models.

As can be seen from the figure and understood from the equations in appendix A, only models 8, 9, 11, and 12 give the correct constant error variances for all systems, as these models have e_{12} as additional estimated covariance, so the value of C_{12} and hence r_2^2 does not affect the solution. If r_2^2 were corrected for, σ_1^2 and σ_2^2 would both be diminished by r_2^2. All other models give incorrect estimates for the error variances, because these assume that $e_{12} = 0$. There is a clear similarity between the solutions of the various models. This is because systems 1, 2, and 3 form a triple collocation subset in models 1 - 3. Therefore only system 4 has a different solution in these models. In the same way, systems 1, 2, and 4 form a triple collocation subset in models 4 - 6, systems 1, 3, and 4 a triple collocation subset in models 7 - 9, and systems 2, 3, and 4 a subset in models 10 - 12. Being the only model for which all a_i and T depend on C_{12}, model 10 is an exception: here all four error variances deviate from their correct value, though the deviation is small for systems 2, 3, and 4. Figure 3 makes clear that incorrect assumptions on system covariances or error models invalidate quadruple collocation results, while correct assumptions lead to the desired result.

Figure 4 shows the additional error covariances e_{ij} resulting from each of the models. As can be seen from the figure and understood from the equations in appendix A, only models 8, 9, 11, and 12 give the correct results as these have e_{12} as additional covariance. Hence, quadruple collocation is able to estimate the representativeness error common to systems 1 and 2, but only when the other off-diagonal error covariances are zero. All other models give incorrect estimates for the additional error covariances, because of the assumption that $e_{12} = 0$. Note that the additional error covariances e_{ij} take only a limited number of values among the models.

In the second simulation r_3^2 is set to 0.3 m^2s^{-2}, while r_2^2 is varied from 0 to 0.3 m^2s^{-2}. This is achieved by setting $e_{12} = r_2^2 + r_3^2$ and $e_{13} = e_{23} = r_3^2$. When r_2^2 equals zero, systems 1, 2, and 3 all have the same representativeness error r_3^2 relative to system 4, as one would expect for bABE collocations. When $r_2^2 = 0.3$ m^2s^{-2} system 3 has a finer resolution than system 4, and systems 1 and 2 have finer resolution than system 3. This corresponds to bASE and bBSE collocations of the meridional wind v as can be inferred from Figure 2.

Figure 5 shows the resulting error variances. For $r_2^2 = 0$, when systems 1, 2, and 3 have the same representativeness error, all models give the same solution. Models 8,9, 11, and 12 again yield constant error variances, though that of systems 1 and 3 is lower by about 0.3 m^2s^{-2} and that of systems 2 and 4 higher by about 0.35 m^2s^{-2}. The curves in figure 5 resemble those in figure 3, except for shifts in the ordinates.

Figure 6 shows the free error covariances for the second simulation. Figure 6 very much resembles figure 4, except for a small shift in ordinates. At $r_2^2 = 0$ all models yield zero free error covariances. This indicates statistical consistency, and all models will give the same solution as shown in Figure 5. Note that models 8, 9, 11, and 12 give a value of e_{12} that is remarkably close to the value of r_2^2. This suggests that the value of the free error covariance e_{12} may be a good approximation of the value of r_2^2, provided that the error model sufficiently describes the data.

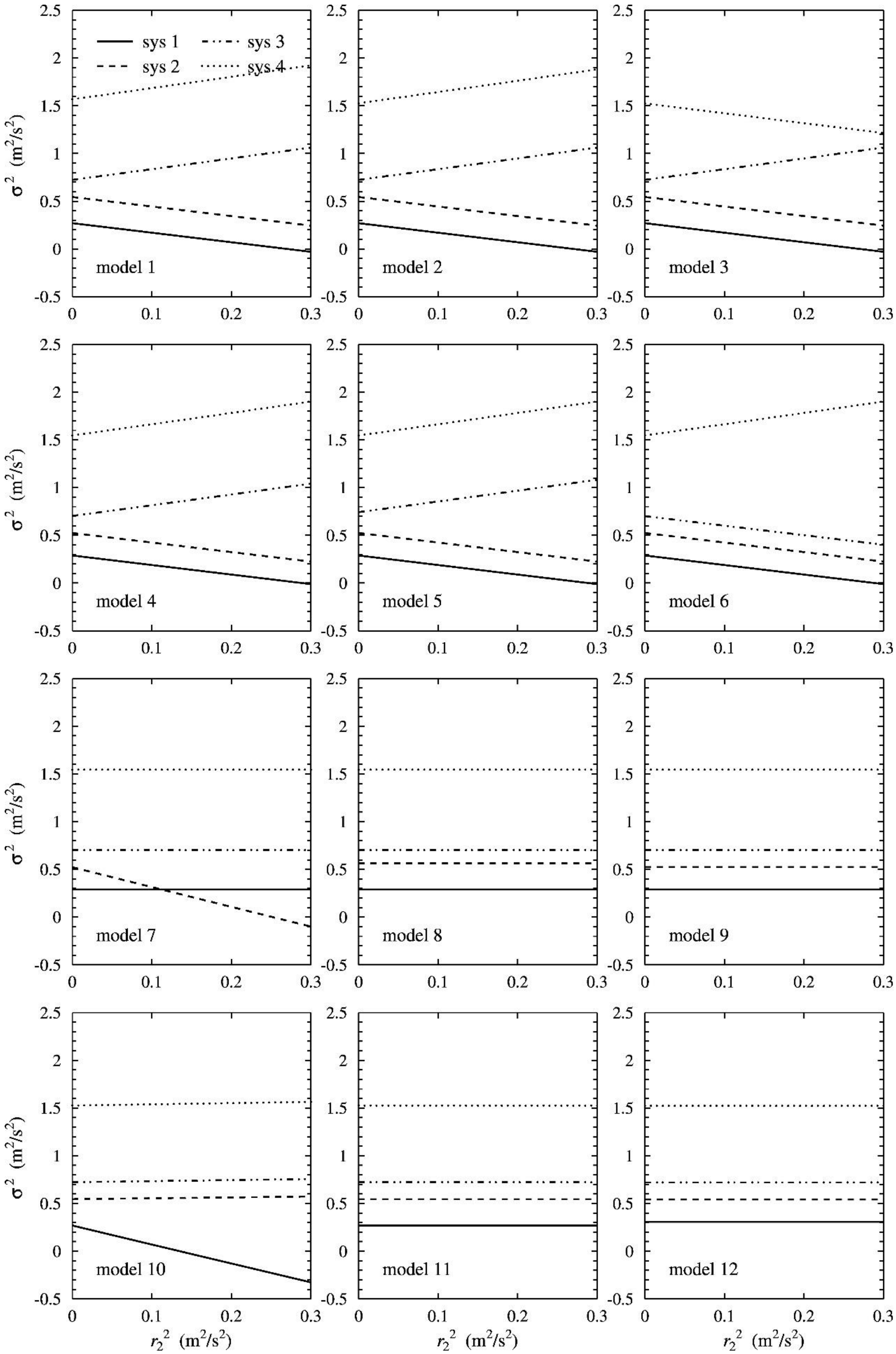

Figure 5. Error variances as a function of representativeness error r_2^2 with constant $r_3^2 = 0.3$ m^{2}s^{-2} for the twelve quadruple collocation models.

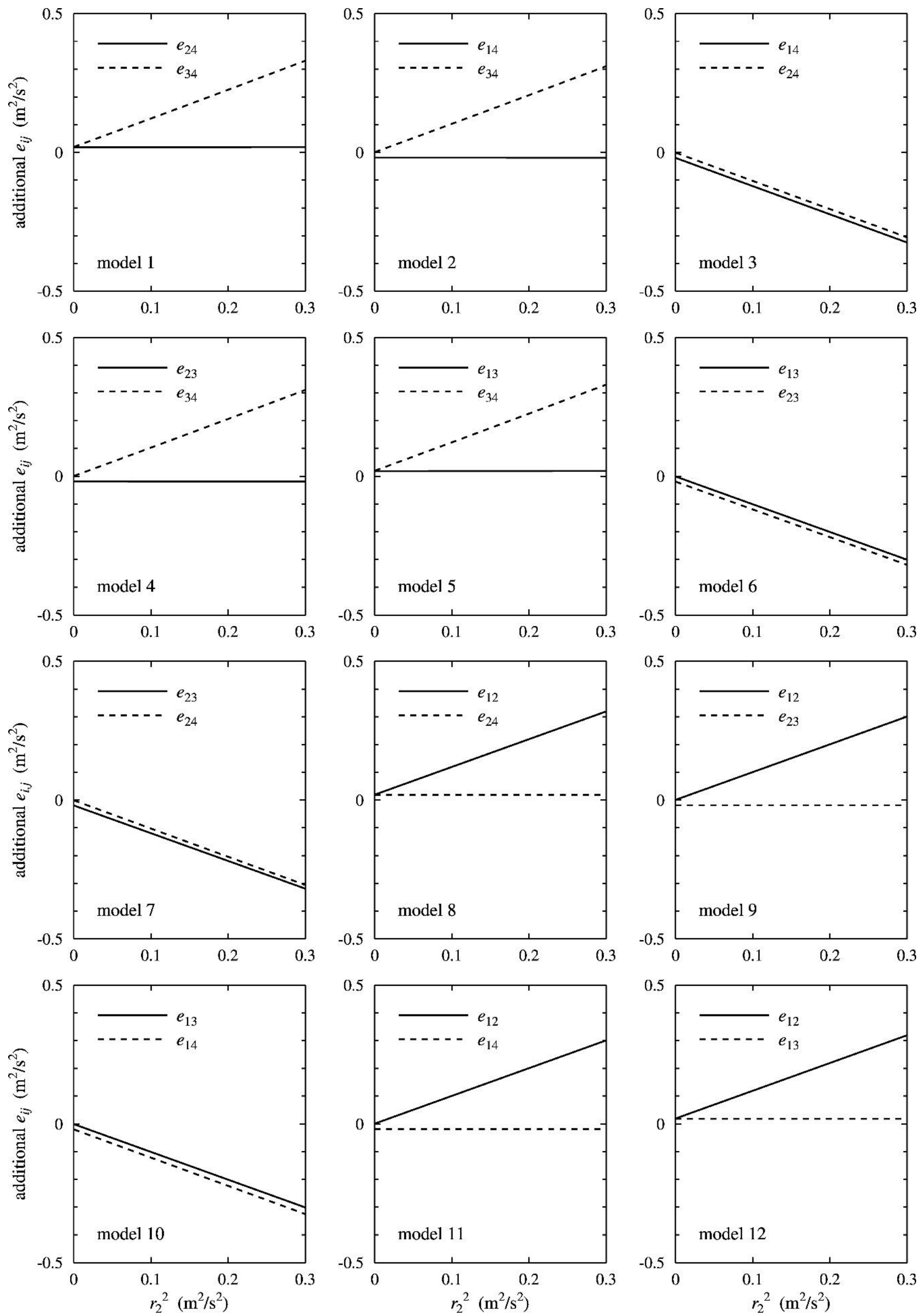

Figure 6. Additional error covariances as a function of representativeness error r_2^2 with constant $r_3^2 = 0.3$ m^{2}s^{-2} for the twelve quadruple collocation models.

5 Results and discussion

5.1 Observation error covariances

The simulations in the previous section showed that representativeness error variances are important for understanding the results of quadruple collocation analyses. The free error covariance e_{12} might be used to infer the value of r_2^2 (this will be addressed further in section 5.3), but the value of r_3^2 is not determined. Therefore estimates based on differences in spatial variances as presented in section 3.2 and figure 2 are used. To further illustrate the importance of representativeness, results will be shown as a function of the scale s (in km) at which the differences are evaluated.

As mentioned before, the buoys (system 1) have the finest resolution, followed by ASCAT-B (system 2 in bBSE and system 2 in bABE) and ASCAT-A (system 2 in bASE and system 3 in bABE). Note that ScatSat (system 3) has a coarser resolution than ASCAT, in particular for the meridional wind component v, while the ECMWF background field (system 4) has the coarsest resolution. Thus $r_2^2(s) = V_2(s) - V_3(s)$ and $r_3^2(s) = V_3(s) - V_4(s)$, $V_i(s)$ being the spatial variance of system i at scale s.

Figure 7 shows the bASE error variances for each of the four systems and each of the 12 solvable models as a function of scale s. The systems are, from top panels to bottom panels, buoys, ASCAT-A, ScatSat, and ECMWF. Left hand panels give results for the zonal wind component u, right hand panels for the meridional wind component v. Note that some variances are the same for different models, because the solution of the covariance equations is the same, see table A.1 in Appendix A. This is because the systems involved form a triple collocation subset: bAS in models 1 - 3, bAE in models 4 – 6, bSE in models 7 – 9, and ASE in models 10 – 12. A similar situation occurred in the simulations of section 4.

Figure 7 shows that at $s = 0$ (no correction for representativeness errors) the error variances from the various models differ considerably, a clear indication that representativeness is important. With increasing scale the results come closer together, in particular for v. The smallest variation is for scales around 200 km for u and 100 km for v. This is consistent with earlier findings [*Vogelzang et al*., 2015] when taking into account that the true spatial resolution of the ECMWF model over the open ocean improves over time because of model development. Nevertheless, the spreading among the models is considerable, notably for u, indicating that the representativeness errors used do not lead to mathematical consistency.

Figure 8 is similar to figure 7, but now for bBSE collocations. The minimum spreading in error variances for v occurs even below 100 km, so for lower representativeness errors than for bASE. The spreading in v is smaller than for bASE, but for u it is larger.

Figure 9 shows the error variances for bABE collocations. Here the value of the representativeness errors have little effect on the error variances of buoys and scatterometers, and only affect those of the ECMWF background. Moreover, the results of all models are close together. This is because the representativeness errors of ASCAT-A and ASCAT-B are almost the same, so the covariance equations are close to mathematical consistency, in agreement with the simulations (figure 6). Note that the spreading in the error variances is slightly larger for ASCAT-A than for ASCAT-B, while the error variances themselves are slightly larger for ASCAT-B than for ASCAT-A.

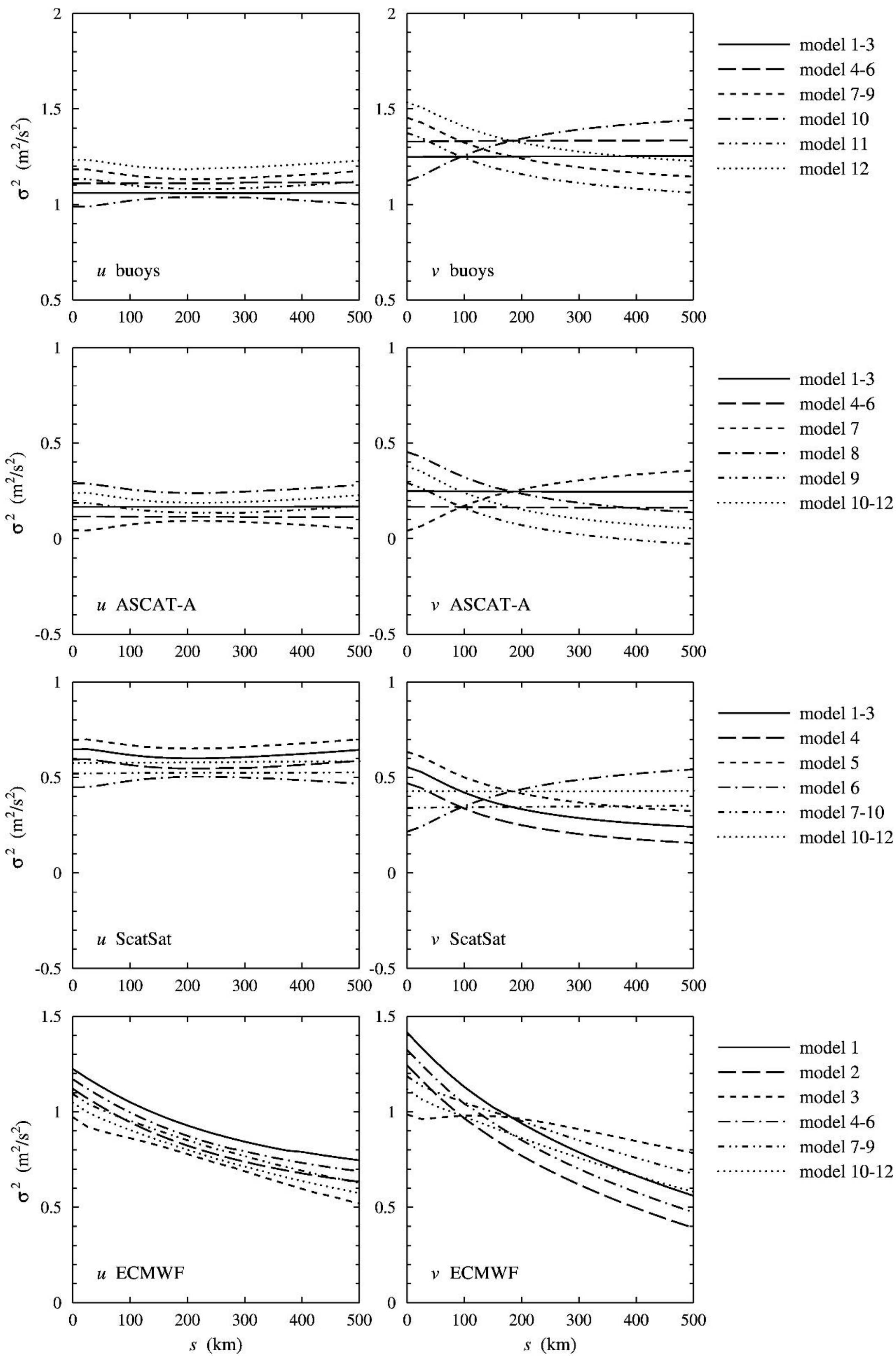

Figure 7. Error variances for bASE quadruple collocation analyses as a function of scale.

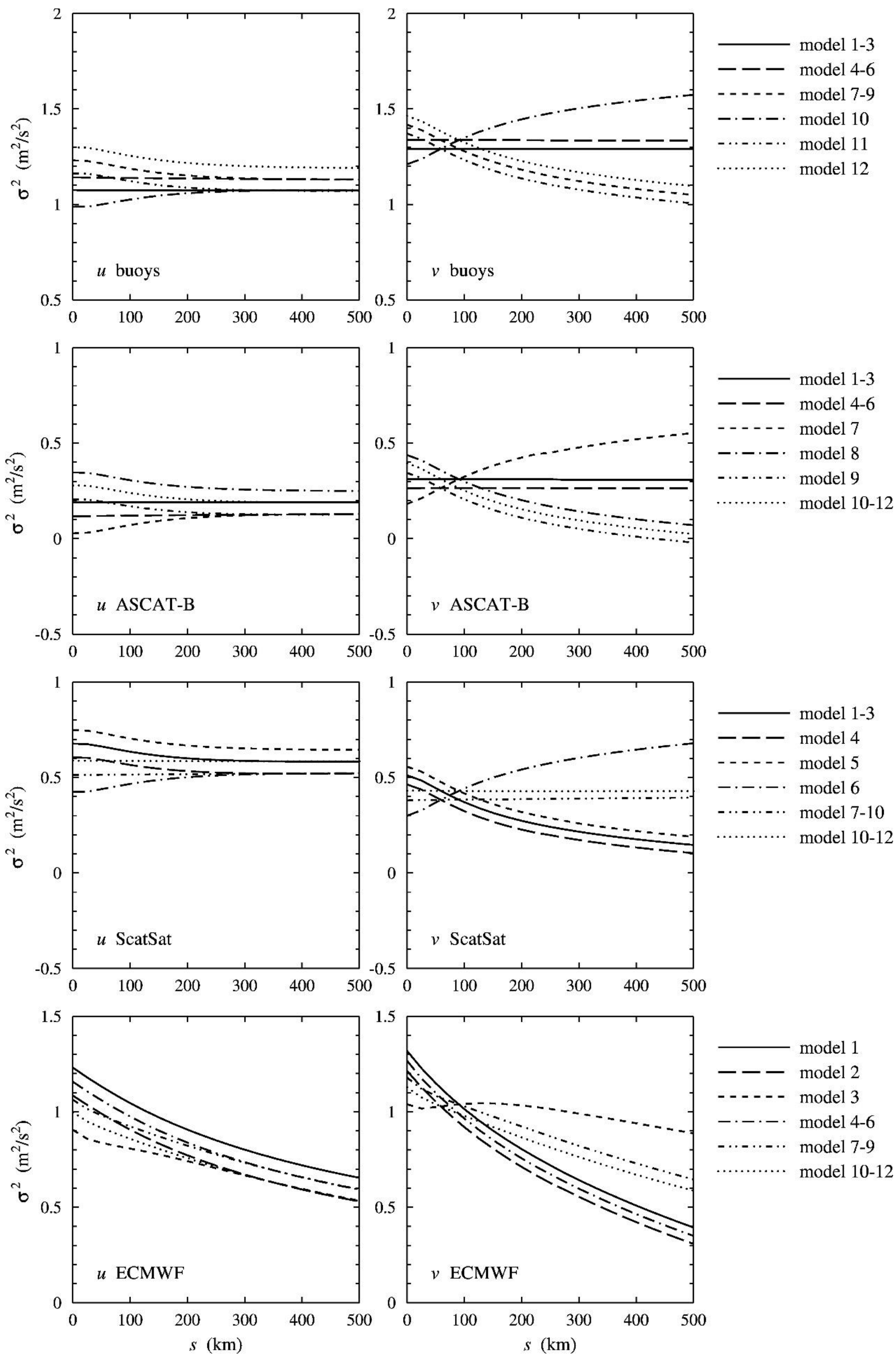

Figure 8. As figure 7, but for bBSE.

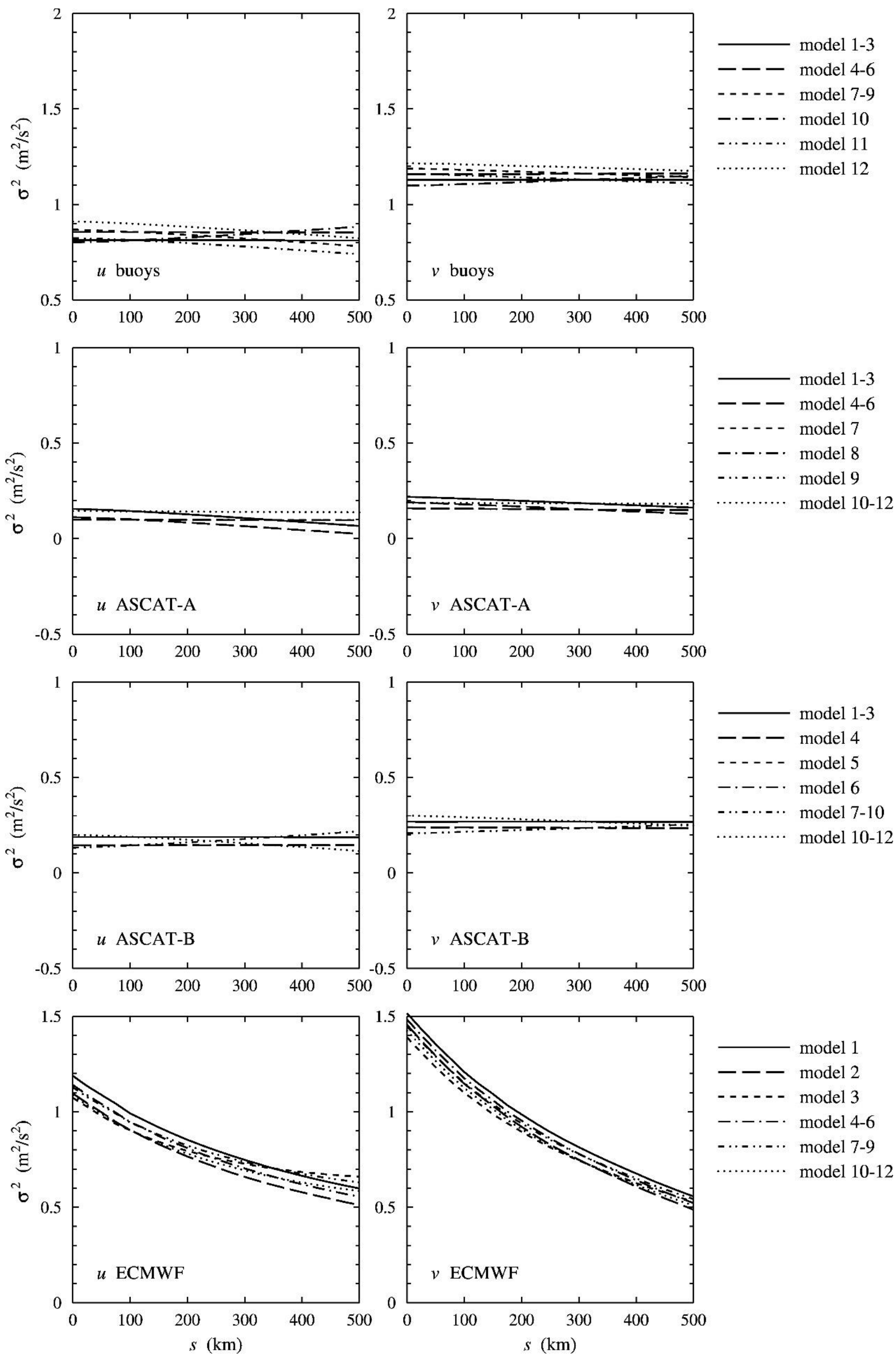

Figure 9. As figure 7, but for bABE.

From figure 3 one expects about the same reprentativness errors in u for ASCAT-A, ASCAT-B, and ScatSat. The results for σ_u^2 in figures 7 – 9 indeed resemble each other. However, at a scale of 500 km the representativeness errors for ASCAT-A and ScatSat become equal, while this is not visible in figure 7 as a convergence in the results. The fact that the representativeness errors are calculated from spatial variances over all of the Tropics and the Northern Hemisphere and may therefore not be representative for the specific locations of the buoys can only partly explain this, because the bABE collocations give consistent results. It is most likely caused by deficiencies in the error model.

5.2 Common variance

Figure 10 shows the common variance as a function of scale. The results resemble those for the error variances: for bASE and bABE the spreading in T_v has a minimum, for s around 100 km, while the minimum is weak or absent in T_u. For bABE the values of T_u and T_v are close together and slightly diverge for large scales. Note that the common variances for bABE (bottom panels of figure 10) are substantially lower than those for bASE and bBSE (top and middle panels). This is due to sampling effects: 45 % of the bASE and bBSE collocations are outside the Tropics, and only 26% of the bABE collocations. The bABE collocations are therefore dominated by the Tropics where high winds are much less frequent than in the Extratropics.

For all three quadruple collocation data sets the values of the additional error covariances found for the various models appear as differences in the common variances and propagate into differences between error covariances. Moreover, the additional error covariances are very similar among the models, as shown in the simulations, figures 4 and 6. This explains the similarity in the results for error variances, common variance, and additional error covariances.

5.3 Estimation of representativeness errors

Table 1 gives the values of the free error covariance e_{12} from models 8, 9, 11, and 12 in case no correction for representativeness error is made. Models 8 and 12 give almost the same result, as indicated in the table, and the same applies to models 9 and 11, though for a different value. The last row in table 1 gives the representativeness error derived from spatial variance differences, at 200 km for u and at 200 km for v.

quantity	bASE		bBSE		bABE	
(m^2s^{-2})	$\boldsymbol{u}$	$\boldsymbol{v}$	$\boldsymbol{u}$	$\boldsymbol{v}$	$\boldsymbol{u}$	$\boldsymbol{v}$
e_{12} (8 & 12)	0.122	0.205	0.160	0.126	0.055	0.059
e_{12} (9 & 11)	0.072	0.125	0.089	0.080	0.012	0.031
r_2^2	0.045	0.127	0.074	0.136	0.028	0.009

Table 1. Representativeness error estimates

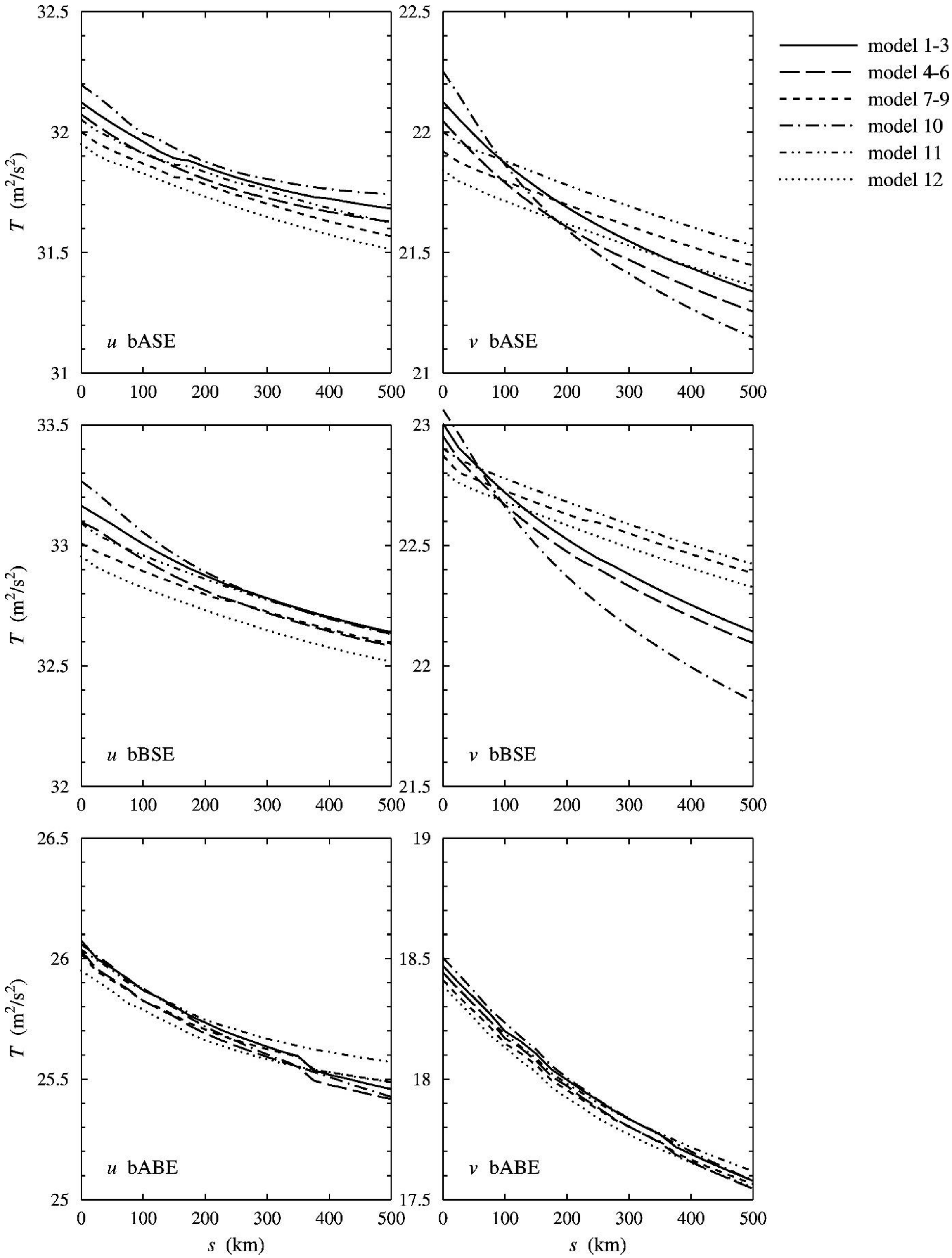

Figure 10. Spreading in the common variance as function of scale for the three quadruple collocation datasets.

Table 1 shows that e_{12} is of the same order of magnitude as r_2^2, with accidental good agreement either with models 9 and 11 (meridional wind component of bASE) or models 8 and 12 (meridional wind component of bBSE). The simulation results do not appear in the real data, so apparently the error model used is not fully appropriate.

One may speculate on what causes the difference between the different quadruple collocation models. For bASE and bBSE retrieval problems in ScatSat may play a role, while for bABE it may be caused by the relatively large time difference of 50 minutes between the ASCAT-A and ASCAT-B overpasses. It has been shown that the meteorological situation can change significantly in this period, even on the ASCAT resolution scale (King et al., 2017). Other possible causes are insufficiency of linear calibration w.r.t. buoys for one or more observation systems, error covariances between some of the systems, or observation errors that are not independent of the common signal.

5.4 Triple collocation

In order to further investigate the differences between the various quadruple collocation runs, attention is focused on the triple collocation subsets. From each quadrupole collocation data set one can form four triple collocation subsets. Tables 2, 3, and 4 show the error standard deviations (in ms^{-1}) for all triple collocation subsets of the bASE, bBSE, and bABE data sets, respectively, with representativeness errors at a scale of 200 km for u and 100 km for v. The first column characterizes the triple collocation subset for later reference. The second last row of each table, labeled "range" gives the range of values (maximum minus minimum) in each column, while the last row labeled "2σ", gives twice the precision estimate assuming that the errors are Gaussian (Vogelzang et al., 2011).

Subset	Buoy		ASCAT-A		ScatSat		ECMWF	
	σ_u	σ_v	σ_u	σ_v	σ_u	σ_v	σ_u	σ_v
bAS	1.03	1.12	0.41	0.49	0.78	0.65	--	--
bAE	1.06	1.15	0.34	0.41	--	--	0.94	1.03
bSE	1.09	1.21	--	--	0.72	0.59	0.92	1.03
ASE	--	--	0.43	0.49	0.76	0.65	0.90	0.98
range	0.06	0.09	0.09	0.08	0.06	0.06	0.04	0.05
2σ	0.04	0.04	0.02	0.02	0.03	0.02	0.04	0.04

Table 2. Triple collocation error standard deviations (in ms^{-1}) for the bASE collocations.

Subset	**Buoy**		**ASCAT-B**		**ScatSat**		**ECMWF**	
	σ_u	σ_v	σ_u	σ_v	σ_u	σ_v	σ_u	σ_v
bBS	1.04	1.14	0.44	0.56	0.78	0.61	--	--
bBE	1.07	1.16	0.35	0.51	--	--	0.92	0.99
bSE	1.11	1.19	--	--	0.72	0.62	0.91	1.02
BSE	--	--	0.46	0.50	0.78	0.66	0.89	0.99
range	0.07	0.05	0.11	0.06	0.06	0.05	0.03	0.03
2σ	0.04	0.05	0.02	0.02	0.03	0.02	0.04	0.04

Table 3. Triple collocation error standard deviations (in ms^{-1}) for the bBSE collocations.

Subset	Buoy		ASCAT-A		ASCAT-B		ECMWF	
	σ_u	σ_v	σ_u	σ_v	σ_u	σ_v	σ_u	σ_v
bAB	0.90	1.06	0.40	0.47	0.47	0.53	--	--
bAE	0.93	1.09	0.31	0.39	--	--	0.91	1.08
bBE	0.93	1.08	--	--	0.38	0.49	0.90	1.09
ABE	--	--	0.41	0.44	0.45	0.54	0.86	1.04
range	0.03	0.03	0.09	0.08	0.09	0.05	0.05	0.05
2σ	0.02	0.03	0.01	0.01	0.01	0.01	0.02	0.02

Table 4. Triple collocation error standard deviations (in ms^{-1}) for the bABE collocations.

The spread in values is quite similar for the bASE, bBSE, and bABE collocations, as expressed by the range in tables 2, 3, and 4, indicating that the scatterometer error variances are reliable within 0.05 m^2s^{-2}, and that the error variances of buoys and ECMWF background are even more precise. The range in values for the meridional wind component v is slightly smaller than that for the zonal wind component u, in particular for the scatterometers. The 2σ accuracy estimate agrees quite well with the range for the buoys and the ECMWF background, but is substantially smaller for the scatterometers.

Clearly, the interpretation of the error model and true variance are not identical in the different comparisons between the different systems. Again, one may speculate on what causes the modest differences between the different triple collocation models and may point to ScatSat retrieval problems (Ebuchi, 1999; Bhowmick et al., 2019) Other possible causes are the time difference of 50 minutes between the ASCAT-A and ASCAT-B overpasses, insufficiency of linear calibration w.r.t. buoys for one or more observation systems, mis-specified error covariances between some of the systems, or observation errors that are not independent of the common signal or not constant in expectation, such as ocean currents. Triple and quadruple collocation analyses provide little clue on how the error model can be improved, but help show the uncertainties involved .

5.5 Direct calculation of the representativeness errors

It is possible to extend the collocation model (1) in such a way that the two representativeness errors r_2^2 and r_3^2 appear as additional unknowns. The technical details are given in Appendix C. However, the solution is numerically highly unstable because it involves the quotient of two differences between quantities of almost equal magnitude. It gives no sensible results for the bABE, bASE, and bBSE collocations.

It is also shown in Appendix C that the solvability of the quadruple collocation model including representativeness depends critically on the precise formulation of the collocation model. It is therefore advisable to check the stability of solutions of any quadruple or higher collocation model, also when numerical solution methods are applied.

A way out for estimating representativeness errors may seem to construct a quintuple collocation data set with as fifth system the ECMWF forecast from one analysis earlier. This is named an instrumental variable (Su et al., 2014; Danielson et al., 2018). Now the covariance equations can be solved for five essential and five additional variables. One must also solve for the additional error covariances e_{12}, e_{13}, and e_{23} to find the representativeness errors, and for the

NWP model error correlation e_{45}. Then there are five possible sets of equations, each with one extra additional error correlation. Unfortunately no set has a solution.

6 Conclusions

The covariance equations give an elegant and concise formulation of the multi-collocation problem. Representativeness errors can be easily included. The formalism is applied to simulated data and to three quadruple collocation data sets, bASE, bBSE, and bASE, involving buoys (b), ASCAT-A (A), ASCAT-B (B), ScatSat (S), and ECMWF forecasts (E). For quadruple collocation there are fifteen ways to solve the covariance equations, referred to as models, only twelve of which have a solution. Besides the linear calibration coefficients and the error variances, a quadruple collocation analysis also yields two additional error covariances.

The covariance equations are named mathematically consistent if the observed covariances are corrected in such a way that the resulting additional error covariances vanish for all models. If the corrections to the covariances also equal the true error covariances and representativeness errors, the covariance equations are named physically consistent. Physical consistency is a much stronger requirement than mathematical consistency. From a linear combination of additional error covariances an infinite number of error covariance corrections can be constructed that make the quadruple covariance equations mathematically consistent. Therefore mathematical consistency gives no clue to the correct values of the error covariances.

Simulations suggest that the representativeness error r_2^2 equals the additional error covariance e_{12} for models 8, 9, 11, and 12. The additional error covariances take a limited number of values for the various models. The simulations indicate that the covariance equations also become mathematically consistent if two systems have the same representativeness error.

For the real data representativeness errors were obtained from differences in spatial variance. The scale at which these differences were evaluated was varied. For bASE and bBSE collocations, the smallest spread in observation error variances was obtained at scales around 200 km for the zonal wind component u and around 100 km for the meridional wind component v, in good agreement with earlier studies and the expected true spatial resolution of the ECMWF model over the open ocean. Comparison of the free error covariance e_{12} from models 8, 9, 10, and 12 with the optimum value of r_2^2 only showed agreement in order of magnitude. For bABE collocations the value of the representativeness error only affects the ECMWF results, in agreement with the simulations, because the ASCAT-A and ASCAT-B representativeness errors are almost the same. A similar remark holds for the zonal wind component in the bASE and bBSE collocations, where the difference between the scatterometer representativeness errors is also small.

For the buoys and the ECMWF background the spread in the error standard deviations agrees quite well with estimates assuming Gaussian error distributions, but for all scatterometers it is substantially larger. Apparently, the scatterometer errors are less accurate than previously thought, but their accuracy is well within 0.05 ms^{-1}.

The spread in the results is due to imperfections in the error model that may have various causes. For bASE and bBSE it may be caused by retrieval problems in the ScatSat winds, while for bABE the large time difference of 50 minutes between the scatterometer overpasses may play a role. Other possible causes are nonlinearities in one or more calibrations w.r.t. buoys and dependencies of one or more observation errors on the common signal However, the involved remaining uncertainties in the interpretation of true variance, collocation errors, representativeness errors, and other observation errors are rather modest. Triple and quadruple collocation analyses provide little clue on how the error model can be improved, but help show the uncertainties involved .

The quadruple collocation error model can be modified in order to directly incorporate representativeness errors. However, the resulting solution is numerically unstable and of no practical use. More generally speaking, solutions of higher-order collocation analyses should be carefully checked for their numerical stability.

Appendix A Quadruple collocation solutions

For quadruple collocation there are six off-diagonal equations to solve for four essential unknowns (three calibration scalings and one common variance). From the six off-diagonal equations one can form fifteen combinations of four equations. Table A.1 shows the solutions as well as the additional error covariances and the ones that are set to zero to solve the covariance equations.

From the table it is easily inferred that all models will give the same solution when all C_{ij} are equal for $i \neq j$. In that case all a_i equal one, so all systems are perfectly intercalibrated, and the error model completely describes the data.

Model	**Used (set to zero)**				**Additional**		$\boldsymbol{a_2}$	$\boldsymbol{a_3}$	$\boldsymbol{a_4}$	$\boldsymbol{T}$
1	e_{12}	e_{13}	e_{14}	e_{23}	e_{24}	e_{34}	$\frac{C_{23}}{C_{13}}$	$\frac{C_{23}}{C_{12}}$	$\frac{C_{14}C_{23}}{C_{12}C_{13}}$	$\frac{C_{12}C_{13}}{C_{23}}$
2	e_{12}	e_{13}	e_{23}	e_{24}	e_{14}	e_{34}	$\frac{C_{23}}{C_{13}}$	$\frac{C_{23}}{C_{12}}$	$\frac{C_{24}}{C_{12}}$	$\frac{C_{12}C_{13}}{C_{23}}$
3	e_{12}	e_{13}	e_{23}	e_{34}	e_{14}	e_{24}	$\frac{C_{23}}{C_{13}}$	$\frac{C_{23}}{C_{12}}$	$\frac{C_{34}}{C_{13}}$	$\frac{C_{12}C_{13}}{C_{23}}$
4	e_{12}	e_{13}	e_{14}	e_{24}	e_{23}	e_{34}	$\frac{C_{24}}{C_{14}}$	$\frac{C_{13}C_{24}}{C_{12}C_{14}}$	$\frac{C_{24}}{C_{12}}$	$\frac{C_{12}C_{14}}{C_{24}}$
5	e_{12}	e_{14}	e_{23}	e_{24}	e_{13}	e_{34}	$\frac{C_{24}}{C_{14}}$	$\frac{C_{23}}{C_{12}}$	$\frac{C_{24}}{C_{12}}$	$\frac{C_{12}C_{14}}{C_{24}}$
6	e_{12}	e_{14}	e_{24}	e_{34}	e_{13}	e_{23}	$\frac{C_{24}}{C_{14}}$	$\frac{C_{34}}{C_{14}}$	$\frac{C_{24}}{C_{12}}$	$\frac{C_{12}C_{14}}{C_{24}}$
7	e_{12}	e_{13}	e_{14}	e_{34}	e_{23}	e_{24}	$\frac{C_{12}C_{34}}{C_{13}C_{14}}$	$\frac{C_{34}}{C_{14}}$	$\frac{C_{34}}{C_{13}}$	$\frac{C_{13}C_{14}}{C_{34}}$
8	e_{13}	e_{14}	e_{23}	e_{34}	e_{12}	e_{24}	$\frac{C_{23}}{C_{13}}$	$\frac{C_{34}}{C_{14}}$	$\frac{C_{34}}{C_{13}}$	$\frac{C_{13}C_{14}}{C_{34}}$
9	e_{13}	e_{14}	e_{24}	e_{34}	e_{12}	e_{23}	$\frac{C_{24}}{C_{14}}$	$\frac{C_{34}}{C_{14}}$	$\frac{C_{34}}{C_{13}}$	$\frac{C_{13}C_{14}}{C_{34}}$
10	e_{12}	e_{23}	e_{24}	e_{34}	e_{13}	e_{14}	$\frac{C_{23}C_{24}}{C_{12}C_{34}}$	$\frac{C_{23}}{C_{12}}$	$\frac{C_{24}}{C_{12}}$	$\frac{C_{12}^2C_{34}}{C_{23}C_{24}}$

11	e_{13}	e_{23}	e_{24}	e_{34}	e_{12}	e_{14}	$\frac{C_{23}}{C_{13}}$	$\frac{C_{23}C_{34}}{C_{13}C_{24}}$	$\frac{C_{34}}{C_{13}}$	$\frac{C_{13}^2C_{24}}{C_{23}C_{34}}$
12	e_{14}	e_{23}	e_{24}	e_{34}	e_{12}	e_{13}	$\frac{C_{24}}{C_{14}}$	$\frac{C_{34}}{C_{14}}$	$\frac{C_{24}C_{34}}{C_{14}C_{23}}$	$\frac{C_{14}^2C_{23}}{C_{24}C_{34}}$
13	e_{12}	e_{13}	e_{14}	e_{24}	e_{14}	e_{23}	no solution			
14	e_{12}	e_{14}	e_{23}	e_{34}	e_{13}	e_{24}	no solution			
15	e_{13}	e_{14}	e_{23}	e_{24}	e_{12}	e_{34}	no solution			

Table A.1. All possible quadruple collocation solutions for the essential unknowns.

Appendix B. Quadruple covariance transformations

It will be shown here how the covariance equations can be made mathematically consistent for models 12 and 1 by applying the error covariance correction transformation $C_{ij} \rightarrow C_{ij} - E_{ij}$, where $E_{ij} = a_i^{(M)} e_{ij}^{(M)} a_j^{(M)}$, equation (13), with M the model number.

The model 12 solution reads (see Appendix A)

$$a_2^{(12)} = \frac{C_{24}}{C_{14}},\ \ a_3^{(12)} = \frac{C_{34}}{C_{14}},\ \ a_4^{(12)} = \frac{C_{24}C_{34}}{C_{14}C_{23}},\ \ T^{(12)} = \frac{C_{14}^2 C_{23}}{C_{24}C_{34}} \tag{B.1}$$

In obtaining this solution, the terms with C_{12} and C_{13} were not used. Therefore the residual errors $e_{12}^{(12)}$ and $e_{13}^{(12)}$ are nonzero; all others have been set to zero to solve the covariance equations. It readily follows from (8) and (B.1) that

$$e_{12}^{(12)} = \frac{C_{12}C_{14}}{C_{24}} - \frac{C_{14}^2 C_{23}}{C_{24}C_{34}},\ \ e_{13}^{(12)} = \frac{C_{13}C_{14}}{C_{34}} - \frac{C_{14}^2 C_{23}}{C_{24}C_{34}} \tag{B.2}$$

Now consider the solution for model 1 which reads

$$a_2^{(1)} = \frac{C_{23}}{C_{13}},\ \ a_3^{(1)} = \frac{C_{23}}{C_{12}},\ \ a_4^{(1)} = \frac{C_{14}C_{23}}{C_{12}C_{13}},\ \ T^{(1)} = \frac{C_{12}C_{13}}{C_{23}} \tag{B.3}$$

Applying the error covariance correction transformation (remember that $a_1^{(12)} = 1$)

$$C_{12} \rightarrow C_{12} - a_2^{(12)} e_{12}^{(12)} = \frac{C_{14}C_{23}}{C_{34}} \tag{B.4a}$$

$$C_{13} \rightarrow C_{13} - a_3^{(12)} e_{13}^{(12)} = \frac{C_{14}C_{23}}{C_{24}} \tag{B.4b}$$

one easily obtains

$$a_2^{(1)} \rightarrow \frac{C_{24}}{C_{14}} = a_2^{(12)} \tag{B.5a}$$

$$a_3^{(1)} \rightarrow \frac{C_{34}}{C_{14}} = a_3^{(12)} \tag{B.5b}$$

$$a_4^{(1)} \rightarrow \frac{C_{24}C_{34}}{C_{14}C_{23}} = a_4^{(12)} \tag{B.5c}$$

$$T^{(1)} \rightarrow \frac{C_{14}^2 C_{23}}{C_{24}C_{34}} = T^{(12)} \tag{B.5d}$$

This proves the proposition for models 12 and 1. For any other combination, the proof is analogous and has been checked using FORM, a program for algebraic manipulation (Vermaseren et al., 2018). From the solutions listed in Appendix A it is clear that a change in both C_{12} and C_{13} affects every solution except that of model 12.

All transformations of the form (B.4a) and (B.4b) are listed in table B.1. Each off-diagonal covariance $C_{i,j}$ can be transformed in two ways, and each transformation applies to two models. The general form is

$$C_{ij} \rightarrow \frac{C_{ik}C_{jl}}{C_{kl}} \tag{B.6}$$

with $\{i, j, k, l\}$ a permutation of $\{1,2,3,4\}$, taking into account the symmetry of the covariance matrix. The error covariance correction transformation (B.6) is nonlinear, because the substitutions may occur in the denominators of the solutions for the calibration scalings and the common variance. However, (8) implies that it is approximately linear when the off-diagonal error covariances are almost equal, which occurs when the systems are well intercalibrated, $a_i a_j \approx 1$, and when the error covariances are small, $e_{ij} \ll T$, conditions satisfied by the bASE, bBSE, and bABE collocation data sets.

Transformation	**models**		**Transformation**	**models**	
$C_{12} \rightarrow \frac{C_{14}C_{23}}{C_{34}}$	8	12	$C_{12} \rightarrow \frac{C_{13}C_{24}}{C_{34}}$	9	11
$C_{13} \rightarrow \frac{C_{14}C_{23}}{C_{24}}$	5	12	$C_{13} \rightarrow \frac{C_{12}C_{34}}{C_{24}}$	6	10
$C_{14} \rightarrow \frac{C_{13}C_{24}}{C_{23}}$	2	11	$C_{14} \rightarrow \frac{C_{12}C_{34}}{C_{23}}$	3	10
$C_{23} \rightarrow \frac{C_{13}C_{24}}{C_{14}}$	4	9	$C_{23} \rightarrow \frac{C_{12}C_{34}}{C_{14}}$	6	7
$C_{24} \rightarrow \frac{C_{14}C_{23}}{C_{13}}$	1	8	$C_{24} \rightarrow \frac{C_{12}C_{34}}{C_{13}}$	3	7
$C_{34} \rightarrow \frac{C_{14}C_{23}}{C_{12}}$	1	5	$C_{34} \rightarrow \frac{C_{13}C_{24}}{C_{12}}$	2	4

Table B.1. Covariance transformations.

Appendix C. Quadruple collocation with representativeness errors

In order to incorporate representativeness errors, the collocation model (1) may be extended as

$$x_1 = a_1(t + \varepsilon_1) + b_1 + \rho_2 + \rho_3 \tag{C.1a}$$

$$x_2 = a_2(t + \varepsilon_2) + b_2 + \rho_2 + \rho_3 \tag{C.1b}$$

$$x_3 = a_3(t + \varepsilon_3) + b_3 + \rho_3 \tag{C.1c}$$

$$x_3 = a_4(t + \varepsilon_4) + b_4 \tag{C.1d}$$

with $a_1 = 1$ and $b_1 = 0$. Here, ρ_3 is the signal detected by systems 1 – 3 but not by system 4 and ρ_2 is the signal detected by systems 1 and 2 but not by systems 3 and 4. Signal $\rho_i, i = 2, 3,$ has zero average and variance r_i^2. It is uncorrelated with t and ε_i, and $\langle \rho_2 \rho_3 \rangle = 0$. The covariance equations can now be formed as in section 2.1. The error variances σ_i^2 must be obtained from the diagonal covariance equations, the other unknowns from the off-diagonal equations which read

$$\begin{aligned} &C_{12} = a_2 T + r_2^2 + r_3^2 \quad C_{23} = a_2 a_3 T + r_3^2 \quad C_{34} = a_3 a_4 T \\ &C_{13} = a_3 T + r_3^2 \qquad C_{24} = a_2 a_4 T \\ &C_{14} = a_4 T \end{aligned} \tag{C.2}$$

From the term with C_{14} one obtains

$$a_4 = \frac{C_{14}}{T} \tag{C.3}$$

Substituting this in the terms with C_{24} and C_{34} yields

$$a_2 = \frac{C_{24}}{C_{14}} \quad a_3 = \frac{C_{34}}{C_{14}} \tag{C.4}$$

Substituting (C.4) in the term with C_{13} gives

$$r_3^2 = C_{13} - \frac{C_{34}}{C_{14}} T \tag{C.5}$$

Now T can be solved from (C.5) and the term with C_{23} as

$$T = \frac{C_{14}^2}{C_{34}} \frac{C_{13} - C_{23}}{C_{14} - C_{24}} \tag{C.6}$$

Finally a_4 is easily obtained from (C.3), r_3^2 from (C.5), and r_2^2 from the term in (C.2) with C_{12}.

Unfortunately, this solution is numerically highly unstable. The common variance is expected to have a value between 18 m^2s^{-2} and 32 m^2s^{-2}, see figure 10, so the covariances C_{ij} are of the same order of magnitude. Equation (C.6) shows that T is given by the product of two factors: the first one is of the order of C_{ij} and the second one is the quotient of the two differences $C_{13} - C_{23}$ and $C_{14} - C_{24}$, i.e., the quotient of two differences between quantities that are almost the same. The quotient should be close to 1, and if it is required to be precise by 2%, each of the differences should be precise by 1% or 0.01 as the differences are of order 1. This requires each of the covariances to be precise by 0.005, which can only be satisfied by a huge collocation dataset of at least 10 million points. This makes the solution unusable for the datasets considered in this paper.

Note that the precise formulation of the collocation model is quite critical: if the model (C.1) is changed into

$$x_1 = a_1(t + \varepsilon_1 + \rho_2 + \rho_3) + b_1 \tag{C.7a}$$

$$x_2 = a_2(t + \varepsilon_2 + \rho_2 + \rho_3) + b_2 \tag{C.7b}$$

$$x_3 = a_3(t + \varepsilon_3 + \rho_3) + b_3 \tag{C.7c}$$

$$x_3 = a_4(t + \varepsilon_4) + b_4 \tag{C.7d}$$

then the resulting covariance equations have no solution because T and r_3^2 can not be separated from each other in the terms with C_{13} and C_{23}.

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The ASCAT-A, ASCAT-B, and ScatSat data can be obtained from the EUMETSAT archive www.eumetsat.int/website/home/Data/DataDelivery/EUMETSATDataCentre (BUFR or NetCDF format). The ASCAT data can also be obtained from the Physical Oceanography Distributed Active Archive Centre podaac.jpl.nasa.gov (NetCDF format only). The ECMWF NWP forecasts are part of the scatterometer data. The collocation data can be obtained with doi TBD from TBD.

AWDP and PenWP are developed within the framework of the OSI SAF of EUMETSAT. These packages can be requested free of charge at the NWP SAF web page nwp-saf.eumetsat.int/site/software/scatterometer.

References

Abdalla, S., & De Chiara, G. (2017), Estimating random errors of scatterometer, altimeter, and model wind speed data. *IEEE JSTARS*, 10, 2406-2414. doi: 10.1109/JSTARS.2017.2659220.

Belmonte Rivas, M. & Stoffelen, A. (2019), Characterizing ERA-Interim and ERA5 surface wind biases using ASCAT, *Ocean Sci.*, 15, 831–852, doi: 10.5194/os-15-831-2019.

Bhowmick, S.A., Cotton, J., Fore, A., Kumar, R., Payan, C., Rodríguez, E., Sharma, A., Stiles, B., Stoffelen, A. & Verhoef, A. (2019), An assessment of the performance of ISRO's SCATSAT-1 Scatterometer, *Current Science* 117 (6), 959-972, doi: 10.18520/cs/v117/i6/959-972.

Bidlot, J., Holmes, D., Wittmann, P., Lalbeharry, R., & Chen, H. (2002), Intercomparison of the performance of operational ocean wave forecasting systems with buoy data, *Weather Forecast.*, 17, 287–310, doi:10.1175/1520-0434.

Danielson, R.E., Johannessen, J.A, Quartly, G.D., Rio, M-H., Chapron, B., Collard, F., & Donlon, C. (2018), Exploitation of error correlation in a large analysis validation: GlobCurrent case study. *Rem. Sens. Env.* 217, pp. 476-490, doi: 10.1016/j.rse.2018.07.016.

Ebuchi, N. (1999), Statistical distribution of wind speeds and directions globally observed by NSCAT, *J. Geophys. Res.*, 104(C5), 11393– 11403, doi:10.1029/98JC02061.

Figa-Saldaña, J., Wilson, J.J.W., Attema, E., Gelsthorpe, R., Drinkwater, M.R. & Stoffelen, A. (2002), The advanced scatterometer (ASCAT) on the meteorological operational (MetOp) platform: A follow on for European wind scatterometers, *Can. J. Remote Sensing* 28 (3), pp. 404–412, doi: 10.5589/m02-035.

Gruber, A., Su, C.-H, Zwieback, S., Crow, W., Dorigo, W. & Wagner, W. (2016), Recent advances in (soil moisture) triple collocation analysis, *Intern. J. of Appl. Earth Observation and Geoinformation*, 45 (B), pp. 200-211, doi: 10.1016/j.jag.2015.09.002.

Janssen, P.A.E.M, Abdalla, S., Hersbach, H. & Bidlot, J. (2007), Error estimation of buoy, satellite, and model wave height data. *J. Atm. Ocean. Tech*., 24, 1665-1677.

King, G.P., Portabella, M., Lin, W. & Stoffelen, A. (2017), *Correlating extremes in wind and stress divergence with extremes in rain over the Tropical Atlantic*. OSISAF Scientific Report OSI_AVS_15_02, www.osi-saf.org.

Kloe, J. de, Stoffelen, A. & Verhoef, A. (2017). Improved Use of Scatterometer Measurements by Using Stress-Equivalent Reference Winds, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing* 10(5): 2340-2347, doi: 10.1109/JSTARS.2017.2685242.

Lin, W., Portabella, M., Stoffelen, A., Vogelzang, J. & Verhoef, A. (2015). ASCAT wind quality under high sub-cell wind variability conditions. *J. Geophys. Res. Oceans* 120: 5804-5819, doi: 10.1002/2015JC010861.

McColl, K. A., Vogelzang, J., Konings, A.G., Entekhabi, D., Piles, M. & Stoffelen, A. (2014), Extended triple collocation: Estimating errors and correlation coefficients with respect to an unknown target, *Geophys. Res. Lett*., 41, 6229–6236, doi: 10.1002/2014GL061322.

Stoffelen, A., Verspeek, J., Vogelzang, J. & Verhoef, A. (2017), The CMOD7 Geophysical Model Function for ASCAT and ERS Wind Retrievals, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*. 10 (5), 2123-2134, doi:10.1109/JSTARS.2017.2681806.

Stoffelen, A. (1998), Toward the true near-surface wind speed: Error modelling and calibration using triple collocation. *J. Geophys. Res.* 103(C4), 7755-7766, doi: 10.1029/97JC03180.

Su, C.-H., Ryu, D., Crow, W.T. & Western, A.W. (2014), Beyond triple collocation: Applications to soil moisture monitoring. *J. Geophys. Res. Atm.*, 119, 6419-6439, doi: 10.1002/2013JD021043.

Trindade, A., Portabella, M., Stoffelen, A., Lin, W. & Verhoef, A. (2020), ERAstar: A High-Resolution Ocean Forcing Product, *IEEE Transactions on Geoscience and Remote Sensing*, 58(2), 1337-1347, doi: 10.1109/TGRS.2019.2946019.

Verhoef, A., Vogelzang, J., Verspeek, J. & Stoffelen, A. (2018a), PenWP User Manual and Reference Guide, EUMETSAT NWP Satellite Application Facility Document NWPSAF-KN-UD-009, Version 2.2, KNMI, De Bilt, the Netherlands, https://nwp-saf.eumetsat.int/site/download/documentation/scatterometer/penwp/NWPSAF-KN-UD-009_PenWP_User_Guide_v2.2.pdf.

Verhoef, A., Vogelzang, J. & Stoffelen, A. (2018b), ScatSat-1 wind validation report 25 km (OSI-112-a) and 50 km (OSI-112-b) wind products, EUMETSAT Ocean and Sea Ice Satellite Application Facility Document SAF/OSI/CDOP3/KNMI/TEC/RP/324, Version 1.0, KNMI, De Bilt, the Netherlands, projects.knmi.nl/scatterometer/publications/pdf/osisaf_cdop3_ss3_valrep_scatsat1_winds.pdf.

Verhoef, A., Vogelzang, J., Verspeek, J. & Stoffelen, A. (2020), AWDP User Manual and Reference Guide, EUMETSAT NWP Satellite Application Facility Document NWPSAF-KN-UD-005 Version 3.3, KNMI, De Bilt, the Netherlands, https://nwp-saf.eumetsat.int/site/download/ documentation/scatterometer/AWDP/NWPSAF-KN-UD-005_AWDP_User_Guide_v3.3.pdf.

Vermaseren, J.A.M., Taneko, T., Kuipers, J., Ruijl, B., Tentyuokov, M., Ueda, T. & Vollinga, J. (2018), FORM version 4.2 Reference manual, NIKHEF, The Netherlands. www.nikhef.nl/~form/maindir/documentation/reference/online/online.html.

Verspeek, J., Verhoef, A. & Stoffelen, A. (2019), ASCAT-C wind product calibration and validation Global OSI SAF 25 km wind product (OSI-102-c) Global OSI SAF coastal wind product (OSI-104-c) Regional EARS 25 km and coastal wind products, EUMETSAT Ocean and Sea Ice Satellite Application Facility Document SAF/OSI/CDOP3/KNMI/TEC/RP/345, Version: 1.3, projects.knmi.nl/scatterometer/publications/pdf/osisaf_cdop3_ss3_valrep_ascat_c_winds_1.3.pdf.

Vogelzang, J., Stoffelen, A., Verhoef, A. & Figa-Saldaña, J. (2011), On the quality of high-resolution scatterometer winds, *J. Geophys. Res*., 116, C10033, doi:10.1029/2010JC006640.

Vogelzang, J., King, G.P. & Stoffelen, A. (2015), Spatial variances of wind fields and their relation to second-order structure functions and spectra, *J. Geophys. Res. Oceans*, 120, 1048–1064, doi:10.1002/2014JC010239.

Vogelzang, J. & Stoffelen, A. (2018), Improvements in K_u-band scatterometer wind ambiguity removal using ASCAT-based empirical background error correlations. *Q J R Meteorol Soc.* 144, 2245– 2259, https://doi.org/10.1002/qj.3349.