

1 **Modelling the electrical conductivity of soil in the Yangtze**
2 **delta in three dimensions**

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20 ABSTRACT

21 Numerous processes, past and present, have given rise to lateral and vertical variation
22 in the soil and to its individual properties such as its salinity and electrical
23 conductivity. The resulting patterns of variation are complex and appear to comprise
24 both random and deterministic components. The latter dominates vertically as
25 trends in most soil profiles, and in the situation we describe it is prominent in the
26 horizontal plane, too. Describing this variation requires flexible choice of covariance
27 function. The processes of model estimation and prediction by kriging in three
28 dimensions are similar to those in two dimensions. The extra complexity of the
29 three-dimensional variation requires practitioners to appreciate fully the assumptions
30 that their choices of model imply and to establish ways of testing the validity of these
31 assumptions. We have examined several covariance functions more commonly used to
32 describe simultaneously variation in space and time and adapted them to model
33 three-dimensional variation in soil. We have applied these covariance functions to
34 model the variation in salinity in reclaimed land in the Yangtze delta of China where
35 the apparent electrical conductivity (EC_a) has been measured at numerous points
36 down to 1.1 m. The models take into account random and deterministic components
37 in both the horizontal and vertical dimensions. The most suitable mixed model was
38 then used to kriging the EC_a on a fine grid from which three-dimensional diagrams of
39 the salinity are displayed.

40

41 **1. Introduction**

42 It is now common practice to use geostatistical methods to model the horizontal
43 variation of soil properties and to predict values at unvisited sites by some form of
44 kriging (Webster and Oliver, 2007). In many instances one can treat the variation as
45 the outcomes of intrinsically stationary correlated random processes and model the

46 variation satisfactorily with one or other of the popular authorized variogram
47 functions. The random variation may be isotropic, so that one may disregard
48 direction. Alternatively where the spatial correlation evidently varies with changes in
49 direction one can often treat the anisotropy as geometric and elaborate the model in
50 the form of a geometric anisotropic variogram function. Such a function permits the
51 distance parameter(s) in the model to vary according to direction. If the variogram is
52 bounded its sill is the same in all directions.

53 In three dimensions this assumption of a constant sill is much less likely to be
54 appropriate for soil. The processes such as differential weathering, leaching and
55 fluctuating ground water which lead to vertical variation differ substantially from the
56 earth surface processes that act horizontally and on quite different spatial scales.
57 This can lead to quite different horizontal and vertical sill variances, even after the
58 removal of any trend components. More complex variograms or spatial covariance
59 functions are required.

60 An analogous problem occurs when we model the variation of a property in both
61 space and time, and several spatio-temporal correlation functions have been proposed
62 (De Cesare et al., 2001; Kyriakidis et al., 1999).

63 In this paper we demonstrate that such functions can be used to represent the
64 three-dimensional variation of a soil property, namely the soil's apparent electrical
65 conductivity (EC_a) which is commonly used as a proxy for soil salinity. We do so
66 with sample data on EC_a recorded in an ongoing investigation into the salinity in the
67 Yangtze delta (Li et al., 2013; 2015).

68 **2. The setting**

69 The land in the coastal zone of Zhejiang Province south of China's Hangzhou
70 Gulf of the Yangtze delta is formed of recent marine and fluvial deposits. Huge
71 quantities of sediment are deposited in the delta each year, and as the delta builds so
72 more of it can be empoldered and claimed for agriculture, in particular, for paddy
73 rice. Rice will not grow well, if at all, in salty soil, however. Farmers, therefore, wish

74 to be sure before they plant their rice that salt will not impair its growth. Farmers
75 therefore wish to know that the soil is effectively free of salt before they attempt to
76 grow the crop. They want accurate estimates of the soil's salinity, both laterally from
77 place to place within their new fields and down the profile because the rice plants are
78 susceptible to salt in the root zone from the surface to at least 1 m. Ideally they
79 would like three-dimensional maps of the salinity in their fields.

80 One can now monitor the soil's salinity using electromagnetic induction
81 equipment such as the Geonics EM31 and EM38 instruments (McNeill, 1980). These
82 devices measure the EC_a of the soil, which is closely related to the soil's salinity. The
83 EM38 is especially useful in that it can measure the EC_a to approximately 1.5 m
84 depth from the surface. One can use it therefore to obtain measures of the soil's
85 salinity throughout the root zone of the rice without having to dig or bore into the
86 soil to take samples.

87 In an earlier paper (Li et al., 2013) we described the Tikhonov regularization for
88 converting the instrumental responses of the EM38 to EC_a at ten depths in the soil in
89 a 2.2-ha field that had been empoldered in 1996. We then modelled the
90 three-dimensional variation in EC_a as a series of correlated two-dimensional
91 regionalized variables, one variable for each of the ten depths down to 1.1 m, and
92 kriged the EC_a on a fine grid at those depths. We displayed the kriged predictions as
93 a series of maps of EC, and built from the bottom upwards a three-dimensional block
94 diagram. Since measurements from different depths were treated as different
95 variables, discontinuities were evident in the predicted vertical profiles and EC_a could
96 not be predicted at depths where it was not measured.

97 The results revealed a trend in salinity across the field. In a second paper (Li et
98 al., 2105), for which we had many more measurements in the topsoil, we were able to
99 treat the data as the outcome of a linear mixed model (LMM) comprising both a
100 fixed effect of the trend and a random residual from it and to estimate the
101 parameters of the model by residual maximum likelihood (REML). Then by universal

102 kriging we predicted the salinity at the nodes of a fine grid for mapping.

103 Figure 7 of the paper by Li et al. (2013) also showed what appeared to be a
104 general increase in salinity with increasing depth. In an independent study in an
105 adjacent field the authors found that in five of the nine profiles they measured there
106 was indeed a steady increase in conductivity.

107 Our aim now is to model the full three-dimensional variation in salinity, taking
108 into account both the lateral and vertical trends, and to use whatever models we fit
109 to predict the salinity in the three dimensions by kriging.

110 3. The data

111 The field has an area of approximately 2.2 ha. The electrical conductivity of soil,
112 recorded as EC_a , was measured with a Geonics EM38 conductivity meter at 56 nodes,
113 approximately on a 20 m \times 20 m grid (Figure 1).

114 At each position, the readings were made using EM38 instruments with the coil
115 configured both horizontally and vertically. The first EC_a measurements were made
116 on the ground surface to provide values of the soils EC_a to theoretical depths of 0.75
117 and 1.5 m, respectively. Then, the EM38 instrument was raised in increments of 0.1
118 m and readings were taken up to 0.6 m. Further readings were taken at heights of
119 0.75, 0.9, 1.1, 1.2 and 1.5 m above the surface. The linear model described by
120 Borchers et al. (1997) was applied to this set of measurements to estimate EC_a at ten
121 depths, namely 0.05, 0.15, 0.25, 0.35, 0.45, 0.55, 0.675, 0.825, 0.95 and 1.05 m, by
122 second-order Tikhonov regularization. The diameters of the white circles in Figure 1
123 are proportional to the mean EC_a across all ten depths. These values of EC_a and
124 their spatial coordinates comprise the data for our study. We use the following
125 notation in referring them.

126 We denote by the vector \mathbf{z} of length n the full set of $n = 560$ observations from
127 $n_s = 56$ sites at $n_d = 10$ depths. We denote the spatial coordinates at which the
128 observations were made by $\mathbf{x} \equiv \{x, y, d\}$ in which x and y are the two lateral
129 dimensions and d is depth.

130 We draw attention here to two features of the data, displayed in Figure 2, and to
 131 the nature of the problem. Figure 2 shows (a) that there is a gradually increasing
 132 trend in EC_a with increasing depth and (b) that the variance is not constant; the
 133 standard deviation is fairly constant down to 55 cm, but increases thereafter down
 134 the profile. With these preliminary results in mind we nevertheless, proceed in stages,
 135 as follows.

136 4. The general model

137 We assume that the observed EC_a can be represented by a linear mixed model
 138 (LMM):

$$\mathbf{z} = \mathbf{M}\boldsymbol{\beta} + \mathbf{u} . \quad (1)$$

139 As above, \mathbf{z} denotes the vector of the $n = 560$ observations. In addition \mathbf{M} is the
 140 design matrix of the fixed effects; $\boldsymbol{\beta}$ is the parameter vector for those effects and \mathbf{u} is
 141 the vector of random effects which are realizations of a multivariate Gaussian random
 142 process with mean zero and covariance matrix \mathbf{C} .

143 In the two-dimensional LMM of Li et al. (2015) for salinity in the top 10 cm of
 144 soil the best-fitting model had a quadratic spatial trend in the fixed effects (i.e. the
 145 columns of the \mathbf{M} matrix were $1s$, x , y , x^2 , y^2 and xy , as displayed in Figure 1), and
 146 an isotropic two-dimensional spatial covariance function, $C(h)$, in which h is a lag in
 147 horizontal distance only. Our aim here is to extend that model to describe
 148 quantitatively the variation in three dimensions. We might succeed by including
 149 depth, d , in the fixed effects or by estimating a covariance matrix that is a function of
 150 the three-dimensional lag vector separating the pairs of observations (i.e. $C = C(h, v)$
 151 for vertical lag v), or a combination of the two. We itemize some of the possible
 152 extended models in the appendix below.

153 The parameters of our covariance functions could be estimated by the
 154 method-of-moments (Webster and Oliver, 2007). In this approach, point estimates of
 155 the expected squared differences between pairs of observations are calculated for

156 several lags. Then the model parameters are selected such that there is a good match
 157 between the point estimates and the fitted covariance function. We previously used
 158 the method-of-moments to estimate our model which treated the EC_a measurements
 159 from different depths as a series of correlated two-dimensional regionalized variables
 160 (Li et al., 2013). In our later paper, however, which looked specifically at
 161 two-dimensional variation (Li et al., 2015), we found that better validation statistics
 162 resulted from models estimated by likelihood-based methods. This finding was not
 163 unexpected because the method-of-moments requires several subjective decisions. In
 164 particular, the practitioner must decide what lag bins to use and how to the allocate
 165 pairs of observations among them, and he or she must choose a suitable criterion to
 166 identify the best fitting model. Also, the method-of-moments does not account for
 167 the correlation between the different point estimates. In contrast, likelihood-based
 168 estimators estimate model parameters according to a statistical criterion that
 169 accounts fully for the correlations among the data.

170 Therefore, we estimate each model by maximum likelihood (ML) and compare
 171 the suitabilities of the models by calculating the Akaike Information Criterion (AIC):

$$AIC = 2k - 2 \ln L, \quad (2)$$

172 where L is the likelihood and k is the number of parameters in the model (Akaike,
 173 1973). The preferred model is the one with the smallest AIC; we consider it the best
 174 compromise between quality of fit to the data and the model's complexity (number of
 175 parameters).

176 We have cross-validated the models by the leave-one-out method and calculated
 177 the standardized prediction errors:

$$\theta_i = \frac{(z_i - \widehat{Z}_i)^2}{\sigma_K^2(i)}, \quad (3)$$

178 where z_i is the observation at site i , \widehat{Z}_i is the kriged prediction at site i when z_i is
 179 excluded from the kriging predictor, and $\sigma_K^2(i)$ is the corresponding kriging variance.
 180 If the errors are normally distributed then the θ_i will be a realization of a

181 standardized chi-squared distribution with one degree of freedom. The mean of the
 182 θ_i , say, $\bar{\theta}$, and usually reported as the mean squared deviation ratio (MSDR), then
 183 has expectation 1.0, and the median of θ_i , $\tilde{\theta}$ or medSDR, has the expected value
 184 0.455 for a standard chi-squared distribution.

185 We follow Li et al. (2015) and assume a quadratic horizontal spatial trend in the
 186 fixed effects. We add a linear trend with d which reflects the observed relationship
 187 between EC_a and d (Fig. 2). We compare various covariance functions. In the
 188 discussion below we denote authorized covariance functions of (i) horizontal lag, (ii)
 189 vertical lag and (iii) horizontal and vertical lag by C_H , C_V and C_{HV} respectively.

190 Our initial covariance model is a second-order stationary Matérn function
 191 (Matérn, 1960; Marchant and Lark, 2007):

$$\begin{aligned}
 C(h, v) &= c_1 \left\{ \frac{1}{2^{\nu-1}} \Gamma(\nu) \left(\frac{\sqrt{h^2 + v^2}}{a} \right)^\nu K_\nu \left(\frac{\sqrt{h^2 + v^2}}{a} \right) \right\} \text{ for } \sqrt{h^2 + v^2} > 0, \\
 C(h, v) &= c_0 \text{ for } \sqrt{h^2 + v^2} = 0,
 \end{aligned}
 \tag{4}$$

192 where c_0 is the nugget variance, c_1 is the sill variance of the correlated structure, a is
 193 a spatial parameter, ν is a smoothness parameter, K_ν is a modified Bessel function of
 194 the second kind of order ν (Abramowitz and Stegun, 1972) and Γ is the gamma
 195 function.

196 Though this isotropic model is our starting point, we recognize that it is highly
 197 unlikely to be optimal, for that would imply identical covariance functions for the
 198 horizontal and vertical dimensions. The variation is almost certain to be anisotropic.
 199 Anisotropy is commonly accommodated in covariance functions via an affine
 200 transformation:

$$C(h, v) = C_{HV} \left(\sqrt{h^2 + \alpha v^2} \right) .
 \tag{5}$$

201 Here, h and v are the lags in the horizontal and vertical dimensions, which are
 202 denoted by the subscripts H and V. The parameter α stretches or contracts the
 203 vertical range of spatial correlation relative to the horizontal range. The model still
 204 requires us to assume that the sills are identical in the horizontal and vertical
 205 dimensions, however.

206 More flexible three-dimensional covariance functions have been devised to
 207 represent the spatial and temporal variation of properties. These functions are
 208 reviewed by De Cesare et al. (2001) and Kyriakidis and Journel (1999). The simplest
 209 space–time models are said to be separable. The spatial correlation is independent of
 210 the temporal correlation. Separable functions can be formed from the sum or product
 211 of a spatial and a temporal covariance function. Rouhani and Myers (1990) pointed
 212 out that the sum sometimes leads to singular kriging equations, and the assumption
 213 of independent spatial and temporal correlation functions is rather limiting.
 214 Therefore several non-separable models have been proposed. Two of the most widely
 215 used (written in terms of horizontal and vertical rather than spatial and temporal
 216 lags) are the sum metric model:

$$C(h, v) = C_H(h) + C_V(v) + C_{HV}(\sqrt{h^2 + \alpha v^2}) . \quad (6)$$

217 and the product sum model:

$$C(h, v) = C_H(h) + C_V(v) + kC_H(h)C_V(v) , \quad (7)$$

218 where $k > 0$ is a parameter. Both of these models permit different sills and distance
 219 parameters in the horizontal and vertical dimensions, and they account for the
 220 dependence between the spatial correlations in each dimension.

221 All of the models described so far require the assumption that the random effects
 222 are stationary. This means that the covariances are functions of the lags between
 223 pairs of points and only of the lags; they do not depend on the specific locations of
 224 the points. A further complication in our study is that not only is there a trend of
 225 increasing EC_a down the profile but also an increase in the variance—see Fig. 2. This
 226 increasing variance can be accommodated if the covariance matrix is scaled on both
 227 sides by a diagonal matrix \mathbf{S} . Thus the covariance matrix becomes \mathbf{SCS} where the
 228 elements of the main diagonal of \mathbf{S} are a function of location. We refer to this
 229 function as a scaling function, $S(d)$. Our chosen scaling functions are linear,
 230 quadratic and cubic polynomials of $\ln(d)$ and a discontinuous function where a

231 different scaling value is estimated for each depth. We used polynomials of $\ln(d)$
232 rather than polynomials of d because $\ln(d)$ had a stronger linear correlation with the
233 standard deviation. We thus have LMMs comprising random and fixed effects.

234 The AIC, Equation (2), is based on maximum likelihood (ML) estimates of the
235 parameters. There is a small bias, however, in ML estimates of variance parameters in
236 the presence of fixed effects. So, once we have determined the most suitable model for
237 the LMM we re-estimate the parameters by REML. Then we use the empirical best
238 linear unbiased predictor (E-BLUP) or universal kriging predictor (Lark et al., 2006)
239 to predict the EC_a on a regular three-dimensional grid. The REML estimator
240 minimizes the bias, but the residual likelihood cannot be used to calculate the AIC.
241 Then we use the empirical best linear unbiased predictor (E-BLUP) or universal
242 kriging predictor (Lark et al., 2006) to predict the EC_a on a regular three-dimensional
243 grid. There is a small bias in ML estimates of variance parameters in the presence of
244 fixed effects. The REML estimator minimizes this bias, but the residual likelihood
245 cannot be used to calculate the AIC, Equation (2).

246 5. Results

247 The summary validation statistics for the model with stationary isotropic random
248 effects might be considered acceptable (Table 1). The mean square deviation ratio,
249 MSDR, is 1.00, and the medSDR is 0.29.

250 Including geometric anisotropy in the models, however, diminishes the AIC
251 substantially. There is a further decrease in the negative log-likelihood when the sum
252 metric covariance function is used. The additional parameters in this model cause the
253 AIC to increase, however. For models with stationary random effects the smallest
254 AIC is obtained when the covariance function is a product sum model. The ML
255 estimated variogram for this model appears to be consistent with the
256 method-of-moments point estimates in all dimensions (Fig. 3). These point estimates,
257 however, do not vary with depth. When the horizontal variograms for the separate
258 depths are plotted individually the ML model appears to over-estimate the variogram

259 near the surface of the soil and to under-estimate it at greater depths. We also see
260 that the MSDR is considerably less than 1 near the surface and considerably greater
261 than 1 for great depths (Fig. 5).

262 We could overcome some of these shortcomings by using non-stationary
263 covariance matrices—see models 5–8 in the appendix. This adaptation led to further
264 decreases in the AIC. The smallest AIC was achieved for the model with a unique
265 scaling value for each depth, and the cubic polynomial led to the smallest AIC for a
266 continuous scaling function. In Figs 4 and 5 we see that the cubic (red) and
267 discontinuous (green) scaling functions lead to better fitted horizontal variograms
268 across the several depths and that the MSDR for the different depths do not deviate
269 so far from 1.0.

270 We favour the non-stationary model with a cubic scaling function since this can
271 be used to predict EC_a and hence soil salinity at any depth, whereas the model with
272 discontinuous scaling function is limited to the depths at which soil salinity was
273 measured. Figure 6 shows the kriged predictions from this model at several different
274 depths. The quadratic horizontal trend and linearly increasing trend in salinity with
275 depth are clearly evident.

276 6. Discussion

277 In many respects the procedures for estimating geostatistical models in
278 three-dimensions are the same as those in two-dimensions. The observed
279 measurements can be treated as a realization of an LMM. These models can be
280 estimated by ML and the suitability of different fixed and random effects structures in
281 the model can be compared via the AIC. Also, one can validate these models by
282 calculating the MSDR.

283 The primary difference in the three-dimensional case is the potential for more
284 complex patterns of variation and hence the existence of more ways in which the
285 observed data can deviate from the assumed model. When we decide on the structure
286 of the LMM we need to look for trends in expected values and variances both

287 horizontally and vertically. We have seen that calculation of the MSDR averaged over
288 the entire set of data is insufficient to validate these models. This summary statistic
289 can disguise large deviations from the assumed model. Instead it is important that
290 we understand the assumptions that our models imply and devise tests of the
291 appropriateness of these assumptions. For example, we tested the assumption that
292 the random effects were independent of depth by looking individually at the MSDR
293 for each depth and we established that this assumption should be relaxed.

294 We could identify the best fitting model from our list of candidate models.
295 However, the fit was by no means perfect. The medSPE was rather less than 0.45 and
296 there were still some depths where the MSDR deviated from 1. This indicates that
297 further generalizations of the geostatistical model might be required.

298 In Fig 6, the quadratic horizontal trend and linearly increasing trend in salinity
299 with depth are clearly evident in the field studied. The predictions vary smoothly in
300 both the horizontal and vertical directions. This contrasts with the corresponding
301 graphs in Li et al. (2013) where there were discontinuities in the predictions down the
302 profile. Those discontinuities resulted from measurements from the different soil
303 depths being treated as different variables.

304 However, the true value in our statistical model is that we have increased
305 confidence that the uncertainty of our predictions has been reliably quantified.
306 Therefore farmers can account for this uncertainty when they decide whether or not
307 to grow rice. For example, rather than considering the expected EC_a it might be
308 relevant to explore the risk or probability that the soil salinity exceeds a critical
309 threshold at each location. The FAO (1976) suggests that soil salinity equivalent to
310 an EC_a of 123 mS m^{-1} is likely to lead to a 25 % reduction in rice yield compared
311 with non-saline soil. Since the kriging predictor yields both a prediction of EC_a and
312 an estimate of the prediction interval at each point in the field we can easily
313 determine the probability that this threshold is exceeded (Fig 7). Thus we see that in
314 the majority of the field and particularly at depth it is very likely that salinity will

315 lead to loss of yield.

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325 **References**

- 326 Abramowitz, M., Stegun, I.A., 1972. Handbook of Mathematical Functions with
327 Formulas, Graphs, and Mathematical Tables. Wiley-Interscience, New York.
- 328 Akaike, H., 1973. Information theory and an extension of the maximum likelihood
329 principle. In: Second International Symposium on Information Theory (eds
330 B.N. Petrov and F. Csáki), pp 267–281. Akadémiai Kiadó, Budapest.
- 331 Borchers, B., Uram, T., Hendrickx, J.M.H., 1997. Tikhonov regularization of
332 electrical conductivity depth profiles in field soils. Soil Science Society of
333 America Journal 61, 1004–1009.
- 334 De Cesare, L., Myers, D.E., Posa, D., 2001. Estimating and modelling space-time
335 correlation structures. Statistics & Probability Letters 51, 9–14.
- 336 FAO, 1976. Prognosis of salinity and alkalinity. Soils Bulletin No 31, FAO, Rome.
- 337 Kyriakidis, P.K., Journel, A.G., 1999. Geostatistical space-time models: A review.
338 Mathematical Geology 31, 651–684.

- 339 Lark, R.M., Cullis, B.R., Welham, S.J., 2006. On spatial prediction of soil
340 properties in the presence of a spatial trend: the empirical best linear unbiased
341 predictor (E-BLUP) with REML. *European Journal of Soil Science* 57, 787–799.
- 342 Li, H.Y., Shi, Z., Webster, R., Triantifilis, J., 2013. Mapping the three-dimensional
343 variation of soil salinity in a rice-paddy soil. *Geoderma* 195–196, 31–41.
- 344 Li, H.Y., Webster, R., Shi, Z., 2015. Mapping soil salinity in the Yangtze delta:
345 REML and universal kriging (E-BLUP) revisited. *Geoderma* 237–238, 71–77.
- 346 Marchant, B.P., Lark, R.M. 2007. The Matérn variogram model: Implications for
347 uncertainty propagation and sampling in geostatistical surveys. *Geoderma* 140,
348 337–345.
- 349 Matérn, B., 1960. *Meddelanden från Statens Skogsforskningsinstitut* 49, 1-144.
- 350 McNeill, J.D., 1980. *Electromagnetic Terrain Conductivity Measurement at Low*
351 *Induction Numbers*. Technical Note TN-6. Geonics Limited, Mississauga,
352 Ontario.
- 353 Rouhani, S., Myers, D.E., 1990. Problems in space-time kriging of geohydrological
354 data. *Mathematical Geology* 22, 611–623.
- 355 Webster, R., Oliver, M.A., 2007. *Geostatistics for Environmental Scientists*, 2nd
356 Edition. John Wiley and Sons, Chichester.

357 Appendix

358 Below, we list the parametric functions for the specific forms of the LMM,
359 Equation (1), considered in the paper. For all of these models the columns of the
360 design matrix for the fixed effects, \mathbf{M} , are 1s, x , y , d , x^2 , y^2 and xy . All covariance
361 functions are Matérn functions, Equation (4).

362 *Model 1, isotropic*

$$363 \quad S(d) = \alpha_0,$$

$$364 \quad C(h, v) = C_{\text{HV}}(\sqrt{h^2 + v^2}).$$

365 *Model 2, geometric anisotropic*

$$366 \quad S(d) = \alpha_0,$$

$$367 \quad C(h, v) = C_{\text{HV}}(\sqrt{h^2 + \alpha v^2}).$$

368 *Model 3, Sum metric*

$$369 \quad S(d) = \alpha_0,$$

$$370 \quad C(h, v) = C_{\text{H}}(h) + C_{\text{V}}(v) + C_{\text{HV}}(\sqrt{h^2 + \alpha v^2}).$$

371 *Model 4, Product sum*

$$372 \quad S(d) = \alpha_0,$$

$$373 \quad C(h, v) = C_{\text{H}}(h) + C_{\text{V}}(v) + kC_{\text{H}}(h)C_{\text{V}}(v).$$

374 *Model 5, Product sum*

$$375 \quad S(d) = \alpha_0 + \alpha_1 \ln(d),$$

$$376 \quad C(h, v) = C_{\text{H}}(h) + C_{\text{V}}(v) + kC_{\text{H}}(h)C_{\text{V}}(v).$$

377 *Model 6, Product sum*

$$378 \quad S(d) = \alpha_0 + \alpha_1 \ln(d) + \alpha_2 \{\ln(d)\}^2,$$

$$379 \quad C(h, v) = C_{\text{H}}(h) + C_{\text{V}}(v) + kC_{\text{H}}(h)C_{\text{V}}(v).$$

380 *Model 7, Product sum*

381 $S(d) = \alpha_0 + \alpha_1 \ln(d) + \alpha_2 \{\ln(d)\}^2 + \alpha_3 \{\ln(d)\}^3,$

382 $C(h, v) = C_H(h) + C_V(v) + kC_H(h)C_V(v).$

383 *Model 8, Product sum*

384 $S(d) = \alpha_i$ if $d = d_i,$

385 $C(h, v) = C_H(h) + C_V(v) + kC_H(h)C_V(v).$

386 The d_i for $i = 1, 2, \dots, 10$ are the depths at which EC_a was observed, and the α_i are

387 parameters.