Met Office

Developments in the Met Office InTEM volcanic ash source estimation system Part 1: Concepts

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Contents

Abstract

The Met Office's volcanic ash inversion system uses satellite observations of volcanic ash clouds and results from the NAME dispersion model to estimate volcanic ash source characteristics. This report describes a number of changes made to the system. The main changes are in the method of coarse-graining the satellite data, in the algorithm used to find the optimal source characteristics, and in the *a priori* emission model. This report focuses on describing the changes, with examples of the results presented in a companion report (Webster H. N., D. J. Thomson and M. C. Cooke, Developments in the Met Office InTEM volcanic ash source estimation system Part 2: Results. *Forecasting Research Technical Report* 618, Met Office, UK). The change to the coarse-graining of the satellite data concerns the way pixels assessed as containing ash and clear sky pixels are combined onto a coarser grid for input to the inversion computation; the changes in the solution algorithm involve expressing the cost function in a form which is cheaper to evaluate and also replacing the simulated annealing approach with an 'active set' method; and the change in the *a priori* emission model involves introducing a stochastic model for the emissions with uncertainties in the plume rise height, in the total emission rate, and in the vertical profile of the emissions all represented separately. Some possible further developments are also discussed.

1 Introduction

An inversion method for volcanic ash source estimation was implemented operationally in January 2015 to assist the Met Office and the London Volcanic Ash Advisory Centre in providing guidance (Pelley et al. [12]). The approach uses the atmospheric dispersion model "NAME" (Numerical Atmospheric-Dispersion Modelling Environment) together with observations of the rise height of the volcanic plume and satellite retrievals of ash column load, and adjusts the emissions in the atmospheric dispersion model to obtain the best (in some sense) agreement with the available data. The inversion method used to adjust the emissions is implemented in the "InTEM" system (Inversion Technique for Emissions Modelling).

This note and a companion note (Webster et al. [18]) describe the development of a number of revisions to the inversion method, with this note focusing on the concepts and the companion note describing the results. There are three key revisions concerning:

- The method of coarse-graining the satellite data
- The algorithm for the solution of the optimisation problem
- The *a priori* emission model.

The revised approach was adopted operationally in December 2015.

2 Outline of approach and notation

The general approach of Pelley et al. [12] is retained. In particular our approach is Bayesian and seeks to estimate a single 'best' value by finding the peak of a Gaussian pdf (or minimum of a quadratic cost function) over the quadrant of non-negative emissions, with the emissions used as the primary variables rather than, e.g., considering the logarithm of the emissions as a way of avoiding the problem of negatives. Although this choice implies a potentially significant lack of consistency arising from truncation of negative values, this approach allows us to retain the advantages arising from the linearity of the dispersion model and allows the use of efficient solution methods. We note that, for a Gaussian pdf (or quadratic cost function) there is a unique local peak (or local minimum) in any closed convex set and, in particular, in the non-negative quadrant, so that there is no problem arising from multiple local peaks (or minima).

The use of a Bayesian approach, and in particular the use of a prior distribution, reduces the risk of over-fitting to the satellite observations and enables knowledge of the general behaviour of volcanic eruptions to be used to constrain the results. The main aspect of general volcano behaviour used here is the typical relationship between the plume rise height and emission rate, and the variability in this. In addition we choose to use near source observations of the rise height of the plume to constrain the prior distribution (as opposed to, e.g., using such observations in the same way as the satellite data to determine the *a posteriori* distribution from the *a priori* distribution).

We (mostly) follow the notation of Pelley et al. [12]. The variation of the emissions with height and time is represented by discretising the source into source elements covering different height and time ranges. The emissions from the various source elements are represented as a vector $\mathbf{e}$ of effective emissions. The emissions are 'effective' because they account for the net effect of a range of near source processes (plume rise etc.). Satellite retrievals of ash column load as a function of horizontal position and time are given by a vector $\mathbf{o}_a$. This vector describes not the raw retrievals but a coarse-grained version with a resolution which matches that chosen for the NAME model output grid. The dispersion resulting from the source elements is represented by the NAME model with the dispersing ash represented as a passive (but sedimenting and depositing) tracer. The NAME model gives model predictions $\mathbf{o}_m$ for ash column loads at the retrieved locations as a linear function of the emissions which we write as $\mathbf{o}_m = \mathbf{M}\mathbf{e}$. The matrix $\mathbf{M}$ is obtained from the NAME model by separately simulating the dispersion from each source element with a unit source strength. We make estimates for (aspects of) the *a priori* distribution of emissions (in the Bayesian sense) using estimates of the plume rise height and various modelling assumptions. The mean emission vector and covariance matrix of the emissions in this *a priori* distribution (which are the aspects that we estimate) are written as $\mathbf{e}_{ap}$ and $\mathbf{B}$. We also use information from the satellite retrievals to make estimates for the covariance matrix $\mathbf{R}$ of the errors in the coarse grained satellite data. There is no explicit accounting for errors in the transport and dispersion (i.e. errors in $\mathbf{M}$). Conceptually one could regard such errors as being wrapped up in $\mathbf{R}$, but the true correlation structure of the transport and dispersion errors is complex and difficult to model.

Using the above notation, the problem is to find the minimum of the cost function

$$J = (\mathbf{Me} - \mathbf{o}_a)^T \mathbf{R}^{-1} (\mathbf{Me} - \mathbf{o}_a) + (\mathbf{e} - \mathbf{e}_{ap})^T \mathbf{B}^{-1} (\mathbf{e} - \mathbf{e}_{ap})$$

subject to the constraint $e_i \geqslant 0 \; \forall i$.

We use $\mathbb{E}$ to denote the expectation of random quantities and $\mathbb{P}$ to denote the probability of events. Also I_A (sometimes written $I[A]$) is the indicator function defined by

$$I_A = \begin{cases} 1 & \text{if event } A \text{ occurs} \\ 0 & \text{otherwise.} \end{cases}$$

3 Coarse-graining of the satellite data

The way in which satellite pixel column load values are combined into lower resolution data for comparison with NAME predictions has been revised. NAME's output for operational volcanic ash inversion currently uses output grid squares representing approximately 40 km $\times$ 40 km horizontal averages and hourly time averages. To produce satellite data with matching resolution, the various pixels available within a particular NAME grid square and one hour period need to be combined. For simplicity in the following we will often just refer to 'a NAME grid square' with the time interval being understood.

Each pixel is classified by the retrieval algorithm as having ash detected ("ash pixels"), as having no significant ash – i.e. no significant ash detected and no significant cloud which could hide ash ("clear sky pixels"), or as falling into neither category ("unclassified pixels"). The original approach for coarse-graining the satellite data is described by Pelley et al. [12]. In the revised approach, the mean ash column load for a NAME grid square is taken as the mean column load of the ash and clear sky pixels within the NAME grid square (with the clear sky pixels taken as having zero load). The standard deviation of column load for the NAME grid square is taken to be the average of the standard deviations of the ash and clear sky pixels within the NAME grid square with the clear sky pixels taken as having a standard deviation of 0.5 g m^{-2}, based on estimates of the minimum detectable column load. (In ideal conditions it is possible to detect column loads of order 0.1 g m^{-2} [19]. However, the retrieval method of Francis et al. [7], as used here, uses a conservative detection method to avoid excessive noise in less than ideal situations and does not often give column loads less than of order 0.5 g m^{-2}.)

Errors in satellite retrievals are likely to be correlated over nearby pixels and averaging the standard deviations represents this pragmatically by assuming in effect perfect correlation of errors between pixels in the same NAME grid square. To justify this we consider n pixels with actual column loads c_i and with column load retrievals (with errors) $y_i = c_i + \epsilon_i$, and we assume $\mathbb{E}[\epsilon_i] = 0$, $\mathbb{E}[\epsilon_i^2] = \sigma_i^2$. Then the error in the mean over the pixels is $\frac{1}{n}\sum_i \epsilon_i$ and the variance of the error is $\frac{1}{n^2}\sum_i\sum_j \mathbb{E}[\epsilon_i\epsilon_j]$. With perfectly correlated errors the standard deviation of the error equals $\sqrt{\frac{1}{n^2}\sum_i\sum_j \sigma_i\sigma_j}$ which equals the average of the standard deviations $\frac{1}{n}\sum_i \sigma_i$. Covariances between NAME grid squares are assumed zero, assuming in effect zero correlation of errors between pixels in different NAME grid squares. Clearly this sharp cut-off is not ideal but represents a convenient pragmatic choice while respecting the idea of correlation decreasing with distance.

Note that although this approach treats retrieval errors it ignores representativity errors. These occur when not all pixels in a NAME grid square are ash or clear sky pixels and the actual ash load varies between pixels. The representativity error will be larger when fewer pixels are classified as ash pixels or clear sky pixels. To partially treat this problem we only use retrievals for the NAME grid squares in which either 50% of pixels are ash pixels or 90% of pixels are either ash or clear sky pixels. The different thresholds reflect the fact that if the classified pixels in a NAME grid square are dominated by clear sky pixels then the amount of ash could be underestimated, possibly significantly so if ash is hiding in the unclassified pixels, and so the mean over the NAME grid square may be biased. Viewed another way we don't want to use grid squares with zero or small estimated column load unless we are reasonably confident that there is not a lot of ash concealed in the unclassified pixels. The different thresholds are also a pragmatic way to limit the number of clear sky grid squares which, at least for some solution methods, may have a significant impact on the computational cost of the inversion. We also ignore errors caused by the assumptions about the ash properties such as the ash refractive index. It seems possible such errors will lead to retrieval errors which are correlated between widely separated pixels.

The NAME grid squares for which column loads have been calculated are then classified into squares containing some ash pixels ('ash grid squares') and squares containing only clear sky and unclassified pixels ('clear sky grid squares'). This allows the differences between using only the ash grid squares and including the clear sky grid squares too to be studied.

Although this approach is similar to before, there are significant differences of detail. For example previously it was possible to classify a grid square as clear sky and assign it a zero column load, even if there were a few pixels with ash within it, provided clear sky pixels dominated.

4 Algorithm for solution of the optimisation problem

The optimisation method implemented operationally in January 2015 used a hybrid simplex plus simulated-annealing method and assumed that the covariance matrices were all diagonal. The approach used the method of Press et al. [13, pp. 443-447] with some modifications to ensure emissions are greater than zero. [Note we do mean greater than zero and not greater than or equal to zero – the method cannot give exactly zero emissions although it can give small values.] The simplex-annealing method was chosen originally because of experience with this method within the Atmospheric Dispersion and Air Quality team and because it does not make strong demands on the cost function having particular properties.

The optimisation method has been revised in two respects.

The first revision is to pre-calculate the sums over satellite observations so that the cost function is expressed as a quadratic function of the emissions with known coefficients, rather than as a quadratic function of both the emissions and the satellite observations. This increases the speed of the code for cases with many satellite observations and many cost function evaluations. In addition, expressing the cost function as a quadratic function of the emissions only is necessary for the second step.

The second revision is to use the more direct "NNLS" (non-negative least squares) solution method from Lawson and Hanson [8, chap. 23, sec. 3]. This is designed for finding the $\mathbf{x}$ which minimizes $|\mathbf{Lx}-\mathbf{f}|^2$ subject to the constraints $x_i \geqslant 0$, but is easily adapted to more general quadratic cost functions $\mathbf{x}^T\mathbf{Gx} + \mathbf{d}^T\mathbf{x}$ with positive-semi-definite $\mathbf{G}$ (by, e.g., using Cholesky decomposition of $\mathbf{G}$ to find values of $\mathbf{L}$ and $\mathbf{f}$ which make the first problem equivalent to the second). It is an "active-set method" (see Nocedal and Wright [11]) that iterates over possible choices for the set of the x_i which are equal to zero, i.e. for which the non-negative constraint is active. The method is guaranteed to converge to the true minimum in a finite time. Also each iteration improves the solution, so that stopping before complete convergence normally gives a reasonable approximation to the true solution. A negative aspect of this choice is that it offers no flexibility for altering the optimisation problem to anything that isn't a non-negative quadratic optimisation problem. However any development of our inversion modelling beyond quadratic cost functions might well involve other radical changes, such as the use of Monte Carlo Markov Chain methods. The NNLS algorithm has been previously used in atmospheric dispersion source determinations (see Boichu et al. [2], [3]).

For our problem the NNLS method is essentially the same as Algorithm 16.1 of Nocedal and Wright [11] and the "Fast-NNLS" method of Bro and De Jong [4]. The key difference is that these algorithms work directly with $\mathbf{G}$ rather than with $\mathbf{L}$. This is potentially a large advantage if working with an $\mathbf{L}$ where the number of rows is much greater than the number of columns; converting from $\mathbf{L}$ to $\mathbf{G}$ amounts in effect to performing the sum over observations which we have discussed above. However for our problem we are calculating $\mathbf{L}$ from $\mathbf{G}$ and would naturally choose to make $\mathbf{L}$ a square matrix; in this situation there is unlikely to be a large performance gain from these alternative approaches. Some gain may be possible from the avoidance of the need to pre-calculate $\mathbf{L}$ from $\mathbf{G}$ (and to recalculate $\mathbf{G}$ from $\mathbf{L}$ within the algorithm itself, depending on exactly what method is used for the unconstrained optimisations needed within the algorithms). Other differences between the algorithms include the question of what happens when an iteration step leads to more than one previously non-zero variable being set equal to zero and the range of options for initialising the algorithm. The former question seems of little significance in that such events are expected to be rare and, while the difference will lead to different routes to the solution, it seems unlikely to have much systematic impact on the computational cost. However the options for initialising the algorithm may be of value to us in a "rolling framework" context (see Pelley et al. [12]) where, instead of having a single optimisation problem, the optimisation problem needs to be repeated as new observations become available. Here it seems likely that making use of the previous solution as a starting point could reduce the cost significantly. This is similar conceptually to the situations considered by Bro and De Jong [4]. We don't consider these possibilities further here, but they could be considered in due course as possible further improvements.

The optimisation method implemented operationally in January 2015 used a sparse matrix representation for aspects of the cost function in cases where this was likely to be beneficial. The matrix $\mathbf{G}$ occurring in the cost function will have non-zero off-diagonal components only for components corresponding to two source elements for which either of the following conditions hold:

- the two source elements can both contribute to the model prediction of column load at a common location for which there is a satellite retrieval of column load;
- the *a priori* emissions are conditionally correlated, i.e. the *a priori* emissions for the two sources are correlated when conditioned on the values of the other emissions (this amounts to the relevant off-diagonal component of $\mathbf{B}^{-1}$ being non-zero – see Rue and Held [14, p. 22]).

This means that although the matrix $\mathbf{G}$ is fairly sparse when the source elements are uncorrelated *a priori*, the introduction of correlations between the source elements (which is discussed in the next section) will reduce the sparseness of $\mathbf{G}$. Hence we have not attempted to make use of sparse representations in the revised approach.

5 *A priori* emission model

5.1 Motivation

The aim is to introduce a more probabilistically consistent model for the *a priori* distribution of emissions. Conceptually we aim to achieve this by a stochastic model which can generate an ensemble of emission scenarios, with the emission statistics being computed by averaging over the ensemble. However, for our stochastic model, it turns out to be possible to calculate the required statistics by numerically evaluating some integrals, without the need to actually generate the ensemble of emissions. The 'consistency' arises because all the statistics emerge from a single conceptual model. For example variations in rise height within the ensemble give rise to a complicated behaviour of the mean and variance of emissions near the mean rise height. This is because the ensemble includes cases where the emissions are zero at a particular height because the plume does not rise high enough, and also cases where the emissions are large because the plume rises above the height in question and because the total emissions increase strongly with rise height. Also the correlations between the emissions from the various source elements can be calculated from the stochastic model and can take account of, for example, the fact that variations in rise height can affect emissions at all heights. These aspects were treated differently previously and, in particular, no *a priori* correlation was assumed between the emissions from the various source elements.

The ability to include correlations is one of the main benefits of the approach. With no correlations the *a priori* description allows for a lot of small scale variability but the implied large scale variability, e.g. variability in the total emissions integrated over all heights and over some time period, will be too small. Hence the *a priori* distribution will overly constrain the integrated emissions and/or allow too much small scale 'noise' (allowing over-fitting to the satellite data on the small scales). In contrast, if we assumed high a priori correlations, the implied small scale variability in emissions will be too small; the 'shape' of the height-time profile of emissions will be over constrained and/or the integrated emissions will be under constrained. Including correlations will also reduce the sensitivity of results to the way the emissions are discretised into source elements in time and height. The inclusion of correlations in time also means that the inversion estimates for the very latest emissions (which are generally unconstrained directly by satellite observations) do not simply revert to the *a priori* mean. Including correlations can be regarded as seeking a midway position between the previous approach of assuming independence and the approach of describing the source through a small number of parameters with many aspects of the source assumed perfectly correlated at the outset (see Denlinger et al. [5] and Zidikheri and Potts [20]).

In our stochastic model we want to include correlations induced by variations in plume rise height H or variations in the total mass release rate M for given H. These variations will affect releases at all heights and so should induce correlations in the vertical. However, conditional on H and M, we want to allow for quite a lot of variability in the shape of the profile. This variability in profile shape should be specified separately from the uncertainties in H and M as there is no physical reason why they should be related. [Previously the variability in profile shape came about as a result of allowing the emission for each source element to vary in a way which reflects the uncertainties in H and M with no correlation between the source elements – if there was no variability in H and M then there would have been no shape variability.]

In the absence of an inversion calculation our operational configuration assumes a uniform emission profile from the volcano summit to the best estimate, H_b, of the plume rise height made from local observations (Webster et al. [17]). The emission is based on a power law relationship between emissions and plume rise height of the type proposed by Sparks et al. [15, section 5.2] and Mastin et al. [9]. We want the *a priori* mean to agree with what we would use operationally in the absence of an inversion calculation, in order to ensure that the inversion result will be the usual operational emission choice for the special case of no satellite data (at least for the bulk of the source profile – it's not possible near the top of the plume if we are to account properly for uncertainties in plume rise height which are ignored in the usual operational emission choice). This precludes calculating the mean of the emission rate per unit height M/H by (i) taking the mean of M conditional on the rise height H to follow the power law (which has $\mathbb{E}[M|H] \propto H^\alpha$ with α close to 4), (ii) dividing by H to get the conditional mean of the emissions per unit height, $\mathbb{E}\left[\frac{M}{H}|H\right]$, and (iii) integrating over the probability distribution of H. This is because the non-linearity of $H \to \mathbb{E}\left[\frac{M}{H}|H\right]$ will alter the mean. As a result we linearise the power law (expressed in the form of emission rate per unit height as a function of rise height) about H_b.

Because we are going to solve a (constrained) Gaussian optimisation problem we want a stochastic emission model for which the emission means and covariances (but not necessarily higher order statistics) are calculable reasonably easily. The higher order statistics in the stochastic emission model needn't be Gaussian, but these higher order aspects of the model will be ignored and Gaussian assumptions made in the optimisation problem.

We note that in principle the inclusion of correlations in time will allow us to make estimates of future emissions within the inversion calculation by including them in the optimisation process. However this either would require an assumption that H_b remains constant in the future perhaps with an increased variability of H about H_b or would require an additional model for the stochastic evolution of H_b.

5.2 Model description

Here we describe our *a priori* emission model in detail. The model is based on the ideas and requirements discussed above.

We consider a model for H with H being uniformly distributed in $[H_b - \delta H, H_b + \delta H]$ where δH is an error estimate. $(H - H_b)/\delta H$ is assumed to be exponentially correlated in time with time scale T_H, with $(H - H_b)/\delta H$ remaining constant between jumps to independently chosen values with exponentially distributed waiting times. We did consider an alternative model in which H is a Gaussian process with mean H_b, with standard deviation σ_H, and with $(H - H_b)/\sigma_H$ exponentially correlated in time with time scale T_H. However this model cannot completely exclude the possibility of H going negative and, more significantly, cannot prevent H going below the (positive) threshold at which the linearised version of the power law formula (Sparks et al. [15], Mastin et al. [9]) gives negative emissions. More complex models are possible which would ensure the H fluctuations are suitably bounded and also ensure H, $(H - H_b)/\delta H$, or $(H - H_b)/\sigma_H$ vary continuously. However because the input H_b will normally not vary continuously and because the additional complexity does not seem justified, we do not consider this further.

The (conditional on H) mean $\mathbb{E}\left[\frac{M}{H}\middle|H\right]$ of the emission rate per unit height is determined by linearising the power law estimate $c_M H^{\alpha_3}$ about H_b to get

$$c_M\left(H_b^{\alpha_3} + \alpha_3 H_b^{\alpha_2}(H - H_b)\right) = c_M H_b^{\alpha_3}\left(\alpha_3 \frac{H}{H_b} - \alpha_2\right).$$

Here $\alpha_3 \equiv \alpha - 1$ and $\alpha_2 \equiv \alpha - 2$. This notation is intended to reflect the fact that $\alpha \simeq 4$ and so $\alpha_3 \simeq 3$ and $\alpha_2 \simeq 2$. Note also that $\alpha_3 - \alpha_2$ equals 1. We need $\frac{H}{H_b} \geqslant \frac{\alpha_2}{\alpha_3}$, and hence $\frac{\delta H}{H_b} \leqslant \frac{1}{\alpha_3}$, to avoid negative emissions.

We note that, although we have chosen the models for H and $\mathbb{E}\left[\frac{M}{H}\middle|H\right]$ to avoid the possibility of negative emissions, negative emissions may not matter as only the 1st and 2nd order moments of the emissions will be used. However we will see below that negative emissions can have some unsatisfactory consequences which supports the choices we have made here.

We then take $\frac{M}{H} = \mathbb{E}\left[\frac{M}{H}\middle| H\right](1+r)$ where r is a random function of time t, independent of H, with mean zero and covariance function $\sigma_r^2 \mathrm{e}^{-\frac{|t_2-t_1|}{T_r}}$. Here r represents the fractional variability in the total emission rate for a given plume rise height.

The emission rate per unit height at height $z(\geqslant 0)$ above the summit and at time t, $e(z,t)$, is then assumed to be given by

$$e(z,t) = \frac{M}{H}(1+s)I_{z\leqslant H}$$

where s is a random function of z and t representing the variability in the shape of the vertical emission profile. While we could model s as a random function of height and time, perhaps with exponentially decaying correlations, this would alter the total mass emission rate M. This may not be a problem and could be compensated for by reducing the variability in r. However it is clearer to keep the variability in the shape completely separate from the variability in the total mass emission. We do this by modelling s as $q - \frac{1}{H}\int_0^H q\,dz$ where q is modelled as a random function of z and t with exponentially decaying correlations. More specifically we model q, conditional on H, as a random function of z and t, independent of r, with mean zero and with covariance function

$$\sigma_q^2 \mathrm{e}^{-\frac{|t_2-t_1|}{T_q}} \mathrm{e}^{-\frac{|\eta_2-\eta_1|}{L_q}} I_{\text{not } J(t_1,t_2)}.$$

Here $\eta = z/H$ and $J(t_1,t_2)$ is the event that $(H-H_b)/\delta H$ jumps between time t_1 and time t_2. We have introduced a factor $I_{\text{not } J}$ so that q is uncorrelated either side of a jump in H. The inclusion of the factor $I_{\text{not } J}$ seems qualitatively plausible and also turns out to have advantages in the analysis. The covariance function of s is derived in appendix A together with a discussion of some other possible ways of ensuring that s does not alter the total mass emission.

Combining the above yields

$$e(z,t) = \mathbb{E}\left[\frac{M}{H}\middle| H\right](1+r)(1+s)I_{z\leqslant H} = c_M H_b^{\alpha_3}\left(\alpha_3\frac{H(t)}{H_b} - \alpha_2\right)(1+r)(1+s)I_{z\leqslant H}.$$

The factor r represents the randomness in the total mass release rate while the factor s represents the randomness in the shape of the emission profile.

We note that the 1st and 2nd order moments of the emissions depend on r and s only through the 1st and 2nd order moments of r and s conditional on H. As a result we do not need to make any assumptions about the higher order moments of r and s. Generally we have chosen correlation functions to be exponential decays rather than e.g. Gaussian functions. This is because exponential decays (unlike Gaussians) correspond to broad spectra and so allow variability on scales much less than the decay scale. This should also make the inversion more robust to numerical errors as, by avoiding having correlations very close to 1, there is less danger of, e.g., a supposedly positive definite matrix failing to be positive definite due to numerical errors.

While the model is conceptually fairly simple, it is quite complex to calculate with. However it is not clear that a simpler model could be devised with the desired properties. Many aspects of the approach use simple pragmatic assumptions which are not robustly established and the model has quite a lot of constants which need to be specified but are not well known. However including a poorly known correlation is likely to be better than neglecting the correlation completely and should ensure that the inversion is better behaved. In addition the inclusion of the poorly known parameters helps to make explicit what it is that we don't know. This contrasts with e.g. determining the uncertainty in the shape of the emission profile implicitly from the uncertainty in H and M and the assumption of uncorrelated emissions in different height ranges as was done previously. While the previous approach reduces the number of explicit assumptions it really hides the implicit assumptions about profile shape uncertainty. The various constants provide scope for adjustment (either empirically or based on volcano theory/models/observations or on expert judgement/elicitation). Automatic tuning of the parameters (through giving them a distribution and optimising the values within the Bayesian framework) is also a possibility but is not considered here.

It is likely that the results will not be overly sensitive to the details of the model. One reason for this is that we are only using the model to fix the 1st and 2nd order moments of the *a priori* emissions. Another reason is that, with enough observed data for the inversion, the observed data should provide a stronger constraint on the emissions than the *a priori* model. However the assumptions still need to be plausible. For example a complete lack of correlations with a finely resolved source distribution in space and time – i.e. many source elements with each having a small height-time extent – is likely to constrain the total emissions integrated over space and time much too much unless the individual source elements have a very large variance.

5.3 Choice of parameters

The values assumed for the various parameters are as follows.

$$\alpha = 1/0.241 = 4.15, \quad c_M = 0.05 \times 140.84 \text{ kg s}^{-1} \text{ km}^{-4.15},$$

$$T_H = 12 \text{ h}, \quad \sigma_r = 1, \quad T_r = 12 \text{ h}, \quad \sigma_q = 1, \quad T_q = 3 \text{ h}, \quad L_q = 0.3.$$

δH is not included here because, like H_b, it is treated as an input parameter which can be input as a time series rather than as a single value. However we note that for all the examples shown in the companion report, Webster et al. [18], δH is chosen to be the estimate of rise height error given by Pelley et al. [12] for the Eyjafjallajökull 2010 and Grímsvötn 2011 eruptions, namely $\delta H = 2000$ m. This value is broadly consistent with the size of the discrete steps in the estimated rise height time series for those eruptions (see Pelley et al. [12] and Webster et al. [18]) and with the tendency of the raw radar estimates of rise height for those eruptions to cluster around certain values which reflects the discrete scanning elevation angles available (see Arason et al. [1]).

α and c_M are derived from Mastin et al.'s [9] relationship between emissions and rise height, assuming a magma density of 2500 kg m^{-3} to convert from volume to mass emission rate, and with an additional factor of 0.05 (the 'distal fine ash fraction') which is an estimate of the fraction of ash which forms the far field effective source due to it being finer than 100 μm in diameter and not depositing rapidly due to aggregation (see Webster et al. [17]). T_H is based on experience of the rate of change of observations of plume height during Eyjafjallajökull with the assumption that the errors evolve on a similar time scale to the plume height itself. T_r is chosen to reflect the idea that the mass emission is likely to evolve on a similar time scale to the plume height (due to large scale changes in the volcano state) and/or on a time scale related to changes in meteorology (which will influence the relationship between M and H). σ_q, T_q and L_q are chosen to allow considerable variations in the profile shape on a time scale which is somewhat faster than T_H and T_r.

Before discussing σ_r we note that the assumed errors in H induce uncertainty in the total mass released. With a rise height of 10 km and the default δH giving a rise height range of 8 to 12 km, the uncertainty in the total mass released induced by the uncertainty in H ranges between 0.4 and 2.1 times the central estimate based on a 10 km rise height. Now Mastin et al. [9] estimate the errors in their M-H formulae as giving a 50% chance of errors greater than a factor of 4. However Mastin et al.'s height estimates, which often involve single values for a whole eruption, are likely to have errors at least as large as, and probably significantly larger than, the 2000 m estimated for well-monitored Icelandic volcanoes. Hence part of the scatter in the M-H relationship seen by Mastin et al. is likely to be due to height errors which we allow for through δH. Hence their error estimate should be compared with the total error induced by δH and σ_r. As a result $\sigma_r = 1$ seems a reasonable choice. It allows a reasonable chance of having a total emission rate which is several times the Mastin et al. value calculated from $H_b + \delta H$ and also a reasonable chance of having a very small total emission rate. With our Gaussian assumptions we cannot reflect the symmetry of Mastin et al.'s estimates for the error in the log of the emissions (i.e. a factor of 4 up or down). We probably underestimate the error on the upside, especially if we also consider that the errors in the distal fine ash fraction should be included in σ_r, and overestimate the error on the downside. However, once the error in the rise height is accounted for, the error on the upside will not be grossly underestimated. Also larger values of σ_r would increase the inconsistencies caused by imposing the non-negative constraint.

In part 2 (Webster et al. [18]) a number of tests of the sensitivity of the inversion calculations to some of these parameters is presented.

We noted above that we need $\frac{\delta H}{H_b} \leqslant \frac{1}{\alpha_3}$ to avoid negative emissions in the model but that this might not matter because we only use the 1st and 2nd order moments from the model together with a Gaussian assumption and a non-negative constraint. Here we show that violating this inequality does have some unsatisfactory consequences and we describe how we adjust the parameters to avoid this. From equation (2) in appendix B we note that

$$\frac{d}{d\hat{z}}\mathbb{E}[e(z,t)] = \begin{cases} c_M H_b^{\alpha_3}\left(-\frac{1}{2} - \alpha_3 \frac{\delta H}{H_b}\frac{\hat{z}}{2}\right) & \text{if } \hat{z} \in [-1,1] \\ 0 & \text{otherwise} \end{cases}$$

where $\hat{z}$ is $\frac{z-H_b}{\delta H}$. This should be less than or equal to zero because, conditional on H, the mean emissions are uniform with height between the summit and H, and so, as z increases, $\mathbb{E}[e(z,t)]$ should stay the same or decrease because the probability of the emissions reaching the height z will stay the same or decrease. However $\frac{d}{d\hat{z}}\mathbb{E}[e(z,t)]$ can be greater than zero if $\frac{\delta H}{H_b} > \frac{1}{\alpha_3}$. This is because, if $\frac{\delta H}{H_b} > \frac{1}{\alpha_3}$, then we have the possibility of negative values of $\mathbb{E}\left[\left.\frac{M}{H}\right| H\right]$. Increasing $\hat{z}$ (i.e. increasing z) eliminates contributions from values of H with $\mathbb{E}\left[\left.\frac{M}{H}\right| H\right] < 0$ which allows $\mathbb{E}[e(z,t)]$ to increase. This is probably undesirable and certainly against the spirit of the model, and so it is probably best to ensure $\frac{\delta H}{H_b} \leqslant \frac{1}{\alpha_3}$. If δH is larger than this allows, then we can either reduce δH or reduce the sensitivity of $\mathbb{E}\left[\left.\frac{M}{H}\right| H\right]$ to fluctuations in H around H_b, by reducing α_3 in its multiplicative role in $\mathbb{E}\left[\left.\frac{M}{H}\right| H\right] = c_M H_b^{\alpha_3}\left(\alpha_3\frac{H}{H_b} - \alpha_2\right)$ while retaining its value in the exponent (and maintaining the relationship $\alpha_2 = \alpha_3 - 1$ between the constants in their multiplicative roles). We choose to do the latter, but only for the duration of the period with $\frac{\delta H}{H_b} > \frac{1}{\alpha_3}$. More precisely we put $\alpha_{3\times} = \min(\alpha_3, H_b/\delta H)$, $\alpha_{2\times} = \alpha_{3\times} - 1$, and $\mathbb{E}\left[\left.\frac{M}{H}\right| H\right] = c_M H_b^{\alpha_3}\left(\alpha_{3\times}\frac{H}{H_b} - \alpha_{2\times}\right)$. This is not ideal, but reflects the need to balance competing requirements within the framework adopted here. We have not accounted for this modification in the analysis presented in appendix B; however the modifications required are straightforward.

5.4 Evaluating the first and second order moments

The 1st and 2nd order moments have been evaluated in two ways. The first involves obtaining closed form expressions for the moments as described in appendix B. To evaluate the expressions for the 2nd order moments, some numerical integrations need to be performed. The second approach involves simulating many random realisations of $e(z,t)$ and computing the moments from these realisations. Both approaches have been programmed and satisfactory agreement between the two approaches has been obtained, with results agreeing to the extent expected given the sampling noise arising from the use of a finite number of realisations and the numerical errors arising from the numerical integration. This provides a reasonable degree of assurance that the analysis in appendix B and the computer code are both correct. The use of the closed form expressions from appendix B avoids the sampling error issue and is quicker (assuming the number of realisations in the second approach is chosen to ensure that the sampling error is not too big). Hence we have adopted the appendix B approach. A potential drawback of this is that the appendix B results are only valid for this specific form of model and could not be easily adapted to models that have more than minor differences in form.

6 Possible further developments

Here we discuss a range of possible improvements, from relatively straightforward adjustments to extensive developments requiring significant effort. We focus mainly on possible developments in the inversion technique itself and do not give much consideration to the improvements that will come about from advances in the quality of the meteorological data, satellite data, dispersion modelling, model resolution etc., except where these have the potential to interact with the inversion technique.

As discussed by Pelley et al. [12], the satellite retrievals only detect ash particles with diameters between about 1 μm and 30 μm. This is treated by releasing the normal default particle size distribution with sizes up to 100 μm and by scaling down the NAME predicted column loads by 5%. This 5% factor is sufficiently small in comparison to the other uncertainties that it should not make much difference. However the treatment method is not correct in general. For example the particles with diameters larger than 30 μm may have mostly fallen out in NAME before reaching the location of interest and, in this situation, the column load should not be reduced by as much because it has already been reduced by the sedimentation processes in NAME. A better approach would be to only release particles in the relevant size range or to produce output just from particles in this size range.

Altering the starting point for the iterations in the NNLS solver, as discussed in section 4, may reduce the computational cost further when the inversion is carried out repeatedly as more data becomes available. It is also possible that the solver could be altered to work directly with $\mathbf{G}$ without the need to calculate $\mathbf{L}$ first, as discussed in section 4.

An obvious possible improvement is to increase the resolution of the satellite data and the NAME model output. For example, the 'representativity errors' (in the sense discussed in section 3) in the satellite data could be reduced by reducing the amount of resolution degradation caused by coarse graining. However this may require developments in the treatment of satellite error correlations. This is because the assumption that the satellite retrieval errors are uncorrelated between NAME grid squares may become poorer at higher resolution. In addition, higher resolution may mean that the model plume, or certain small scale features within the plume, will, due to errors in modelling the plume position, not match the satellite data as well. Methods of addressing these are discussed below and may be necessary to fully realise the benefits of increased resolution.

Including meteorological uncertainty and potentially altering the model ash cloud state to better match the observations (as well as adjusting the emissions) is a possible direction of development. Using meteorological ensembles is relatively straightforward conceptually although computationally expensive. One would assign the ensemble members equal *a priori* probabilities, but would calculate different *a posteriori* probabilities. This would require time-coherent ensembles of meteorological analyses which are in principle available in some approaches to ensemble generation and ensemble data assimilation. One could also use the rather crude approaches of either enhancing the model diffusion so that the model better reflects an ensemble average over the meteorological uncertainties and/or considering a range of plume displacements/distortions as a substitute for an ensemble of meteorology. Alternatively, these techniques could possibly be used in addition to using an ensemble of meteorology, in order to better sample the variability which is not fully captured by an ensemble with a small number of members. One could either select a best choice member of the meteorological ensemble and/or best choice displacement/distortion using the *a posteriori* probabilities, or one could obtain an ensemble of such choices with various probabilities. Of course the meteorology interacts strongly with the emission estimation process and the use of ensembles could in principle improve cases where the inversion is poor because the model plume is displaced from the actual plume. This may be more significant when clear sky satellite data is used; the results presented in the companion report by Webster et al. [18] suggest that sometimes the clear sky data can remove too much ash due to a displacement of the model plume.

More use could be made of other information available from satellite. A measure of ash cloud height and effective particle diameter is obtained in our retrieval method (Francis et al. [7]) and could be included in the cost function. One could also consider extending the range of parameters which are estimated by the inversion model if there is a reasonable prospect of the available data constraining these parameters. Examples might include the effective source's particle size distribution or possibly the ash refractive index. Optimising over possible values for the refractive index might require closer integration with the satellite retrieval calculations, but might allow an extra source of uncertainty to be properly accounted for. It also seems likely that there is quite a lot of information in the satellite data which is not currently used. This includes low grade information, especially in the large regions which are currently not assessed as either containing ash or as being clear of ash, and also qualitative information from visible pictures and estimates of cloud top height at the volcano. It would be interesting to explore whether some of this information could be used effectively by integrating even more closely with the satellite retrieval calculations, e.g. by estimating the radiances implied by the model (as in Millington et al. [10]) and performing the optimisation on the raw radiances rather than the retrieved column loads etc.

The correlation scale of errors in the satellite data deserves more attention. Currently this is treated simply by assuming correlated errors within a NAME output grid square and ignoring longer range correlations. Improvements in the treatment of this may be beneficial, especially with higher spatial resolution satellite data. The adoption of a correlation function with more than one characteristic scale (e.g. reflecting errors due to the ash plume structure, the meteorology, and the refractive index errors) might be worth consideration.

Currently our main source of satellite data is the SEVIRI instrument on the geostationary MSG2 satellite. There is a lot of scope for making use of other instruments and platforms such as hyperspectral resolution instruments, active instruments such as lidars, other geostationary satellites, low earth orbiters, limb sounders etc. However it is not possible to do justice to this topic here; the topic really deserves a separate discussion.

Ground and aircraft based instruments such as lidars are a further source of data. This will often be in the form of ash concentrations rather than column loads. There are challenges in making use of such data as a result of small scale variability in the concentration field and the possibility of vertically thin plumes combined with errors in the modelled plume height.

The use of deposition data is also a possibility, although it is likely to be more useful for post event analysis than for emergency response. Deposition processes also interact in a complex way with near source aggregation. This is a barrier to the straightforward use of deposition data in estimating the distal airborne plume, but including such data in the inversion could be an effective tool for diagnosing aggregation.

With the use of a wider range of observation data types, there is probably little reason to maintain the current approach of regarding the near source observations of rise height as part of the *a priori* description; instead they could be regarded as just more observations. The *a priori* description would then of course need to include a wide range of possible volcano behaviours, e.g. a wide range of possible rise heights.

The *a priori* model could be developed in various ways. For example the effect of meteorology on the plume rise versus mass emission rate relationship could be included by linking to plume rise models (Devenish [6]). The *a priori* model could also move away from the assumption of, on average, having a uniform emission with height. A more top heavy profile is likely to be more probable, but it would be important to include the possibility of significant releases at all heights. Avoiding the linearisation of the relationship between the emission per unit height and the variation of rise height within it's uncertainty range could also be beneficial, either by using the Mastin et al. formula [9] directly without linearisation, or by running a plume rise model for a range of possible emissions and/or rise heights. Similarly the sharp edged top-hat distribution for H could be improved or the correlation decay shapes refined (e.g. it may be beneficial for the correlation of r to not decay completely, reflecting variability from volcano to volcano or from eruption to eruption and allowing more freedom on the total mass emitted for a long eruption). It is also possible that some of the parameters in the *a priori* model (e.g. T_H, σ_r etc. for the model described in this note) could be further tuned, either by hand or by giving them uncertainty probability distributions and optimising them in a Bayesian fashion. Assessing the values by hand could include looking at the extent to which the probabilistic assumptions and the data are consistent, along the lines of the work presented in section 6 of the companion report (Webster et al. [18]).

Avoiding the assumption of Gaussian distributions may be beneficial, although this is likely to require more expensive solution algorithms. The large variability seen in eruptions means that there can be substantial negative-emission tails to the Gaussian distributions, and the need to truncate these negative values is a significant inconsistency. It would be better to impose the non-negative emission constraint directly through the *a priori* assumptions rather than through the solution method. Simply switching to log-normal distributions is unlikely to be a good solution to this as the model should allow a significant probability for a source to be exactly zero. In any case, the use of a log-normal distribution removes some of the computational advantages of the Gaussian assumptions because the relationship between emissions and the log of concentration or the log of column load is non-linear, and so there is little reason not to consider more general approaches. Non-Gaussian distributions would probably also be beneficial or necessary in connection with some of the other possible developments considered above (e.g. assuming distributions for T_H, σ_r etc.). If a single best-fit description of the emissions is needed then, with non-Gaussian distributions, some care is needed in choosing this as the mode, mean and median will all be different. When combined with the desire to quantify uncertainty better, this leads naturally to considering more sophisticated solution methods such as using Monte Carlo Markov Chain (MCMC) approaches to compute an ensemble of volcano emissions and of ash cloud states. This would involve a significant increase in the computational cost, but the benefits may well make this worthwhile. We note that an advantage of such an approach would be that, with intermediate variables like H, r and q included in the model of the volcano state, it would not be necessary to carry out the type of calculation described in appendix B; this calculation is already rather complex and it is unlikely that it would be cost effective to carry it out for significantly more complex models. Hybrid approaches which mix Gaussian and non-Gaussian elements and/or which mix NNLS or direct solvers with MCMC methods are also possible.

It is currently rather unclear which of this large choice of options is likely to lead to the most benefit for the effort expended and, even after some of the ideas have been implemented, it will be a significant effort to assess the benefits. Currently most of the effort on inversion has been limited to the Eyjafjallajökull 2010 and Grímsvötn 2011 eruptions and it would be worthwhile using data from a larger set of eruptions to avoid making conclusions that are too strongly biased to these two eruptions. Extending the approach to the inversion of volcanic SO_2 sources and potentially to other dispersion problems will provide a wider range of case studies for assessing the various approaches.

7 Conclusions

We have described a number of developments that have been implemented in our volcanic ash source inversion system. In part 2 (Webster et al. [18]) we will present a range of tests of the system.

Appendices

A Methods of ensuring s does not alter M

To ensure s does not alter M we need to impose the constraint $\int_0^H s(z,t)\,dz = 0$. In this appendix we discuss various possible ways to achieve this.

As in the main text we write $\eta = z/H$ and we will regard s and q as functions of η and t. It is convenient to work in terms of η because the covariance function assumed for q is expressed in terms of η. However, everything in this appendix is conditional on H, and so there is no essential difference between working with z or η.

The constraint can be imposed by considering $q(\eta,t)$ which is generated without the constraint and then defining $s(\eta,t) = q(\eta,t) - a(\eta,t)\int_0^h q(\eta',t)\,d\eta'$ with $\int_0^h a(\eta',t)\,d\eta' = 1$ to ensure that $\int_0^h s(\eta',t)\,d\eta' = 0$. Here h, the upper limit of η, is 1 but is written as h to enable dimensional-analysis checking – it is a spatial coordinate value and if we define $\eta = z/(H$ in metres) then η and h have dimensions. We will write the vertical covariance functions of q and s as $\sigma_q^2 Q_z(\eta'-\eta)$ and $\sigma_q^2 S_z(\eta',\eta)$ (note we use the same σ_q^2 in both cases which is the variance of q not s and so $S_z(\eta,\eta) \neq 1$). The temporal correlation functions of q and s will be written as $Q_t(t',t)$ and $S_t(t',t)$.

Using the shorthand $q_{\eta t} \equiv q(\eta,t)$ etc., $\int_\eta \equiv \int d\eta$ and an overbar for $\mathbb{E}$, we have

$$\overline{s_{\eta t}s_{\eta' t'}} = \overline{q_{\eta t}q_{\eta' t'}} - a_{\eta' t'}\,\overline{q_{\eta t}\int_{\eta''} q_{\eta'' t'}} - a_{\eta t}\,\overline{q_{\eta' t'}\int_{\eta''} q_{\eta'' t}} + a_{\eta t}a_{\eta' t'}\,\overline{\left(\int_{\eta''} q_{\eta'' t}\right)\left(\int_{\eta''} q_{\eta'' t'}\right)}.$$

With $\overline{q_{\eta t}q_{\eta' t'}} = \sigma_q^2 Q_z(\eta'-\eta)Q_t(t',t)$ and a (as a function of η) independent of t, this gives

$$\overline{s_{\eta t}s_{\eta' t'}} = \overline{s_{\eta t}s_{\eta' t}}Q_t(t',t),$$

which shows $S_t = Q_t$, as well as

$$\overline{s_{\eta t}s_{\eta' t}} = \overline{q_{\eta t}q_{\eta' t}} - a_{\eta'}\,\overline{q_{\eta t}\int_{\eta''} q_{\eta'' t}} - a_\eta\,\overline{q_{\eta' t}\int_{\eta''} q_{\eta'' t}} + a_\eta a_{\eta'}\,\overline{\left(\int_{\eta''} q_{\eta'' t}\right)^2}$$

and

$$\overline{s_{\eta t}^2} = \overline{q_{\eta t}^2} - 2a_\eta\,\overline{q_{\eta t}\int_{\eta''} q_{\eta'' t}} + a_\eta^2\,\overline{\left(\int_{\eta''} q_{\eta'' t}\right)^2}.$$

For our choice $Q_z(\eta'-\eta) = \mathrm{e}^{\frac{|\eta'-\eta|}{L_q}}$ we have

$$\overline{q_{\eta t}\int_{\eta''} q_{\eta'' t}} = \sigma_q^2\int_0^h \mathrm{e}^{-\frac{|\eta-\eta'|}{L_q}}\,d\eta' = \sigma_q^2 L_q\left(2 - \mathrm{e}^{-\frac{\eta}{L_q}} - \mathrm{e}^{-\frac{h-\eta}{L_q}}\right)$$

and

$$\overline{\left(\int_{\eta''} q_{\eta'' t}\right)^2} = \sigma_q^2\int_0^h\int_0^h \mathrm{e}^{-\frac{|\eta'-\eta''|}{L_q}}\,d\eta'\,d\eta'' = 2\sigma_q^2 L_q^2\left(\frac{h}{L_q} - 1 + \mathrm{e}^{-\frac{h}{L_q}}\right).$$

(For those familiar with Taylor's (1922) turbulent dispersion result [16], we note the analogy between that and the last result above.)

There are clearly many possible methods of choosing $a(\eta,t)$. The simplest is $a = 1/h$ (as adopted in the main text) leading to

$$S_z = Q_z - \frac{L_q}{h}\left(4 - \mathrm{e}^{-\frac{\eta}{L_q}} - \mathrm{e}^{-\frac{h-\eta}{L_q}} - \mathrm{e}^{-\frac{\eta'}{L_q}} - \mathrm{e}^{-\frac{h-\eta'}{L_q}}\right) + 2\frac{L_q^2}{h^2}\left(\frac{h}{L_q} - 1 + \mathrm{e}^{-\frac{h}{L_q}}\right). \tag{1}$$

As a check, we note that $S_z \to 0$ for $L_q/h \to \infty$ and $S_z \to Q_z$ for $L_q/h \to 0$. We also note that, for L_q much smaller than h and away from the top and bottom of the emission, the variance of s is reduced from that of q by $\sim 2\sigma_q^2 L_q/h$.

A second possibility is to consider a conditioned Gaussian process. We consider this first in the abstract and then apply it to our problem. If we have correlated Gaussian random variables x_i with mean zero then we can consider the distribution of the x_i conditional on a number of linear constraints of the form $A_j^\alpha x_j = 0$ being satisfied. Here α ranges over the number of constraints and the summation convention for repeated indices applies. We will also consider how to generate samples of x_i conditional on $A_j^\alpha x_j = 0$. Consider the distribution of $y_i = x_i - a_i^\alpha A_j^\alpha x_j$ where the a_i^α are chosen to ensure there is no correlation between y_i and the $A_j^\alpha x_j$. This is always possible and, if the constraints are non-degenerate, possible uniquely (e.g. could choose uncorrelated linear combinations of the $A_j^\alpha x_j$ and decorrelate the x_i from each in turn). Then we have that $\mathbb{E}[A_j^\alpha y_j A_k^\alpha y_k] = A_j^\alpha A_k^\alpha \mathbb{E}[y_j(x_k - a_k^\beta A_m^\beta x_m)] = A_j^\alpha \mathbb{E}[y_j A_k^\alpha x_k] - A_j^\alpha A_k^\alpha a_k^\beta \mathbb{E}[y_j A_m^\beta x_m)] = 0$ (using the absence of correlation twice). Hence $A_j^\alpha y_j = 0$. Also the distribution of the x_i conditional on $A_j^\alpha x_j = 0$ equals that of the y_i conditional on $A_j^\alpha x_j = 0$ (because $x_i = y_i$ if $A_j^\alpha x_j = 0$) which equals the unconditional distribution of the y_i (because the y_i are uncorrelated with, and so independent of, the $A_j^\alpha x_j$). Hence the distribution of the y_i gives us the required distribution and the y_i themselves provide a method of generating samples. The equation which needs to be solved for the a_i^α is $A_k^\beta \mathbb{E}[x_i x_k] = a_i^\alpha A_j^\alpha A_k^\beta \mathbb{E}[x_j x_k]$. We note also that this choice of a_i^α minimises the variance of $x_i - a_i^\alpha A_j^\alpha x_j$. Any other choice of a_i^α amounts to adding a random variable which is uncorrelated with y_i to y_i and so must increase the variance.

For orientation we consider the special case with a single constraint $\sum_i x_i = 0$. Then the equation for the a_i is $\sum_k \mathbb{E}[x_i x_k] = a_i \sum_{jk} \mathbb{E}[x_j x_k]$, $a_i = \sum_k \mathbb{E}[x_i x_k] / \sum_{jk} \mathbb{E}[x_j x_k]$, and $y_i = x_i - \sum_j x_j \sum_k \mathbb{E}[x_i x_k] / \sum_{jk} \mathbb{E}[x_j x_k]$.

Now consider $q(\eta, t) \equiv q_{\eta t}$ with the constraints $\int_0^h q(\eta, t)\, d\eta = 0$. The equation for $a(\eta, t, T) \equiv a_{\eta t}^T$ (there is one constraint for each time T) is

$$A_{\eta' t'}^T \mathbb{E}[q_{\eta t} q_{\eta' t'}] = a_{\eta t}^{T'} A_{\eta' t'}^{T'} A_{\eta'' t''}^T \mathbb{E}[q_{\eta' t'} q_{\eta'' t''}]$$

in discrete form with summations, where $A_{\eta t}^T = 1$ when $t = T$ and is zero otherwise. This translates to the continuous form with integrals given by

$$\int_{\eta'} \mathbb{E}[q_{\eta t} q_{\eta' T}] = \int_{\eta', \eta'', T'} a_{\eta t}^{T'} \mathbb{E}[q_{\eta' T'} q_{\eta'' T}],$$

i.e.

$$\int_0^h \mathbb{E}[q_{\eta t} q_{\eta' t}]\, d\eta' Q_t(t, T) = \int_0^h \int_0^h \mathbb{E}[q_{\eta' T} q_{\eta'' T}]\, d\eta'\, d\eta'' \int_{-\infty}^{\infty} a_{\eta t}^{T'} Q_t(T', T)\, dT'$$

or

$$\int_0^h \mathrm{e}^{-\frac{|\eta - \eta'|}{L_q}}\, d\eta' Q_t(t, T) = \int_0^h \int_0^h \mathrm{e}^{-\frac{|\eta' - \eta''|}{L_q}}\, d\eta'\, d\eta'' \int_{-\infty}^{\infty} a_{\eta t}^{T'} Q_t(T', T)\, dT'.$$

This is satisfied by $a_{\eta t}^{T'} = a(\eta)\delta(t - T')$ where

$$a(\eta) = \frac{\int_0^h \mathrm{e}^{-\frac{|\eta-\eta'|}{L_q}}\,d\eta'}{\int_0^h\int_0^h \mathrm{e}^{-\frac{|\eta'-\eta''|}{L_q}}\,d\eta'\,d\eta''} = \frac{L_q\left(2 - \mathrm{e}^{-\frac{\eta}{L_q}} - \mathrm{e}^{-\frac{h-\eta}{L_q}}\right)}{2L_q^2\left(\frac{h}{L_q} - 1 + \mathrm{e}^{-\frac{h}{L_q}}\right)}.$$

This leads to

$$S_z = Q_z - \frac{\left(2 - \mathrm{e}^{-\frac{\eta}{L_q}} - \mathrm{e}^{-\frac{h-\eta}{L_q}}\right)\left(2 - \mathrm{e}^{-\frac{\eta'}{L_q}} - \mathrm{e}^{-\frac{h-\eta'}{L_q}}\right)}{2\left(\frac{h}{L_q} - 1 + \mathrm{e}^{-\frac{h}{L_q}}\right)}.$$

As before, we check that $S_z \to 0$ for $L_q/h \to \infty$ and $S_z \to Q_z$ for $L_q/h \to 0$. We also note that, for L_q much smaller than h and away from the top and bottom of the emission, $a \sim 1/h$ and, as before, the variance of s is reduced from that of q by $\sim 2\sigma_q^2 L_q/h$.

We will also explore a third option with the aim of making $\overline{s^2}$ constant with height. We have

$$\overline{s_{\eta t}^2} = \overline{q_{\eta t}^2} - 2a\,\overline{q_{\eta t}\int_{\eta'} q_{\eta' t}} + a^2\,\overline{\left(\int_{\eta'} q_{\eta' t}\right)^2}$$

so that, writing the variance reduction $\overline{q_{\eta t}^2} - \overline{s_{\eta t}^2}$ as A, we require

$$a^2\,\overline{\left(\int q\right)^2} - 2a\,\overline{q\int q} + A = 0$$

or

$$a = \frac{\overline{q\int q} \pm \left(\left(\overline{q\int q}\right)^2 - A\overline{\left(\int q\right)^2}\right)^{1/2}}{\overline{\left(\int q\right)^2}}.$$

It isn't possible to satisfy $\int_\eta a_\eta = 1$ with a consistent choice of sign (because $\int_\eta a_\eta > 1$ for the plus sign and $\int_\eta a_\eta < 1$ for the minus sign). It is in fact possible to satisfy $\int_\eta a_\eta = 1$ if we allow the sign choice to vary with η (and it's even possible with no reduction in variance). However this seems unsatisfactory and so we conclude that it is not possible to satisfactorily ensure that the variance of s is constant with height.

There seems no clear physical or mathematical reason to choose between the $a = 1/h$ model and the conditioned Gaussian process value of a (or other approaches). Hence we chose the simpler model $a = 1/h$.

B Closed form expressions for the first and second order moments of the *a priori* emission distribution

In this section we will derive closed form expressions for the 1st and 2nd order moments of the emissions. In doing this we consider slightly more general models than considered in the main text. This is because our initial analysis considered different models and it is useful to record that analysis because (i) it may be useful in the future, (ii) some of these models give moments that do not require numerical integration to evaluate them, and (iii) the similarities and differences between the different approaches help to give confidence that the analysis is correct. The generalisations concern the form of the covariance functions for r and s. Before describing these generalisations, we need to introduce some notation for the covariance functions.

The covariance function of r will be written as $\sigma_r^2 R(t_2 - t_1)$. In the model in the main text we have $R(t_2 - t_1) = \mathrm{e}^{-\frac{|t_2-t_1|}{T_r}}$. The covariance function of s (conditional on H) will be written as $\sigma_q^2 S(z_2, z_1, t_2, t_1) = \sigma_q^2 S_z(z_2, z_1) S_t(t_2, t_1) = \sigma_q^2 S_z(z_2, z_1) S_t^*(t_2, t_1)(I_{\text{not } J(t_1,t_2)} + \lambda I_{J(t_1,t_2)})$. For the model in the main text we have $\lambda = 0$ and $S_t^* = \mathrm{e}^{-\frac{|t_2-t_1|}{T_q}}$. $S_z(z_2, z_1)$ is given by (1) where $Q_z(z_2, z_1)$, the vertical correlation function of q, is equal to $\mathrm{e}^{\frac{|\eta_2-\eta_1|}{L_q}}$ with $\eta = z/H$. This notation is consistent with that used in appendix A, except for the use of z instead of η as the independent variable in the vertical correlation functions. While the use of z is less convenient for the model in the main text (as it implies a hidden dependence on H through η) there is no particular advantage for the generalisations considered here (as hidden dependencies are possible with both z and η). The purpose of introducing λ is so that, by setting $\lambda = 1$, it is possible to remove the factor $I_{\text{not } J(t_1,t_2)}$ (using the fact that $I_{\text{not } J(t_1,t_2)} + I_{J(t_1,t_2)} = 1$).

The main generalisations concern the form of the covariance function for s. Firstly we allow the form of S_z to be different, provided it still depends on $H(t)$, for fixed z_1 and z_2, only through $H_1 \equiv H(t_1)$ and $H_2 \equiv H(t_2)$ (and remains independent of r). One reason why one might want to use a different form is that one might want to alter the way s is calculated from q and hence the way S_z is calculated from the vertical correlation function Q_z for q (see discussion in appendix A). Also one might want to alter the way, for fixed z_1 and z_2, the value of Q_z depends of H_1 and H_2. In the main model it depends on H through $\eta = z/H$ but this could be changed, e.g., to depend instead on $\zeta = z/H_b$ so that, for fixed z_1 and z_2, S_z is independent of H. This change also allows Q_z to be altered from an exponential decay to any desired correlation function shape. Secondly we allow λ to equal either 0 or 1. As noted above setting $\lambda = 1$ removes the factor $I_{\text{not } J}$ from S_t. Finally (and trivially) we allow S_t^* and R to be altered from exponential decays to any desired correlation function shapes. We note that the analysis in appendix A remains valid except in the case of some possible generalisations to S_z.

Moments conditional on H

We start by evaluating moments conditional on H. The mean emission rate per unit height at height z (conditional on H) is given by

$$\mathbb{E}[e(z,t)|H] = \mathbb{E}\left[\mathbb{E}\left[\frac{M}{H}\middle| H\right](1+r)(1+s)I\middle| H\right] = \mathbb{E}\left[\frac{M}{H}\middle| H\right] I = c_M H_b^{\alpha_3}\left(\alpha_3 \frac{H}{H_b} - \alpha_2\right) I$$

where $I = I_{H \geqslant z}$. Similarly, with $e_1 \equiv e(z_1, t_1)$ etc., we have

$$\mathbb{E}[e_1 e_2 | H_1, H_2] = \mathbb{E}\left[\mathbb{E}\left[\frac{M_1}{H_1} \middle| H_1 \right] \mathbb{E}\left[\frac{M_2}{H_2} \middle| H_2 \right] (1+r_1)(1+r_2)(1+s_1)(1+s_2) I_1 I_2 \middle| H_1, H_2 \right]$$

$$= \mathbb{E}\left[\frac{M_1}{H_1} \middle| H_1 \right] \mathbb{E}\left[\frac{M_2}{H_2} \middle| H_2 \right] (1+\sigma_r^2 R)(1+\sigma_q^2 S) I_1 I_2$$

$$= c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3} \left(\alpha_3 \frac{H_1}{H_{b1}} - \alpha_2 \right) \left(\alpha_3 \frac{H_2}{H_{b2}} - \alpha_2 \right) (1+\sigma_r^2 R)(1+\sigma_q^2 S) I_1 I_2.$$

Integration over H

We can now take the expectation over H to give

$$\mathbb{E}[e] = \mathbb{E}[\mathbb{E}(e(z,t)|H)] = c_M H_b^{\alpha_3} \mathbb{E}\left[\left(\alpha_3 \frac{H}{H_b} - \alpha_2 \right) I \right]$$

and

$$\mathbb{E}[e_1 e_2] = \mathbb{E}[\mathbb{E}(e_1 e_2 | H_1, H_2)]$$
$$= c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3} (1+\sigma_r^2 R) \mathbb{E}\left[\left(\alpha_3 \frac{H_1}{H_{b1}} - \alpha_2 \right) I_1 \left(\alpha_3 \frac{H_2}{H_{b2}} - \alpha_2 \right) I_2 (1+\sigma_q^2 S) \right].$$

We now need to evaluate the various expectations which occur in these expressions starting with the expectations needed for the 1st order moments. We have

$$\mathbb{E}[I] = \mathbb{P}[H \geqslant z] = \begin{cases} 1 & \text{if } 0 \leqslant z \leqslant H_b - \delta H \\ \frac{H_b + \delta H - z}{2\delta H} & \text{if } H_b - \delta H \leqslant z \leqslant H_b + \delta H \\ 0 & \text{otherwise} \end{cases}$$

and

$$\mathbb{E}[HI] = \mathbb{E}[HI | H \geqslant z] \mathbb{P}[H \geqslant z] = \begin{cases} H_b & \text{if } 0 \leqslant z \leqslant H_b - \delta H \\ \frac{H_b + \delta H + z}{2} \frac{H_b + \delta H - z}{2\delta H} & \text{if } H_b - \delta H \leqslant z \leqslant H_b + \delta H \\ 0 & \text{otherwise} \end{cases}$$

$$= H_b \begin{cases} 1 & \text{if } 0 \leqslant z \leqslant H_b - \delta H \\ \frac{(H_b + \delta H)^2 - z^2}{4 H_b \delta H} & \text{if } H_b - \delta H \leqslant z \leqslant H_b + \delta H \\ 0 & \text{otherwise.} \end{cases}$$

Before considering the other expectations required for the 2nd order moments, we re-evaluate $\mathbb{E}[I]$ and $\mathbb{E}[HI]$ in a slightly different way. This is for consistency with the way we will treat some of the other expectations and also serves as a check on the calculations. Let us define $\hat{H} \equiv (H - H_b)/\delta H$. Then

$$H = H_b + \delta H \hat{H} \quad \text{and} \quad I = I\left[\hat{H} \geqslant \frac{z - H_b}{\delta H} \right].$$

If we put $\hat{z} \equiv \frac{z-H_b}{\delta H}$ then $I = I_{\hat{H} \geqslant \hat{z}}$. To avoid to many 'if's in the following we also use $\hat{y}$ to denote a version of $\hat{z}$ which is limited to lie in $[-1, 1]$, i.e. $\hat{y} \equiv (\hat{z} \wedge 1) \vee -1$ where $\wedge$ denotes $\min$ and $\vee$ denotes $\max$. Now, because $\hat{H}$ is uniformly distributed in $[-1, 1]$, we can deduce that

$$\mathbb{E}[I] = \mathbb{P}[\hat{H} \geqslant \hat{z}] = \frac{1-\hat{y}}{2}$$

and

$$\mathbb{E}\left[\left(\frac{H}{H_b} - 1\right) I\right] = \mathbb{E}\left[\frac{\delta H}{H_b}\hat{H}\middle|\, \hat{H} \geqslant \hat{z}\right]\mathbb{P}[\hat{H} \geqslant \hat{z}] = \left(\frac{\delta H}{H_b}\frac{1+\hat{y}}{2}\right)\frac{1-\hat{y}}{2} = \frac{\delta H}{H_b}\frac{1-\hat{y}^2}{4}.$$

using the fact that the mean of a random variable which is uniformly distributed in $[\hat{y}, 1]$ is $\frac{1+\hat{y}}{2}$. It is easily checked that this agrees with the previous calculation.

We now consider the expectations needed for the 2nd order moments. These terms involve values of H (and I which depends on H) at two times, both directly and through the value of S. We consider the two events corresponding to whether or not a jump occurs in $\hat{H} \equiv (H - H_b)/\delta H$ between t_1 and t_2. If J denotes that a jump occurs, then we have

$$\mathbb{E}[\cdots] = \mathbb{E}[\cdots|J]\mathbb{P}[J] + \mathbb{E}[\cdots|\text{not } J]\mathbb{P}[\text{not } J] = \mathbb{E}[\cdots|J]\left(1 - \mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}\right) + \mathbb{E}[\cdots|\text{not } J]\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}.$$

If a jump occurs, H_1 and H_2 are independent and we can write $H_i = H_{bi} + \delta H_i \hat{H}_i$ etc. If a jump doesn't occur then $\hat{H}_1 = \hat{H}_2$ and, with the common value denoted by $\hat{H}$, we have

$$H_i = H_{bi} + \delta H_i \hat{H} \quad \text{and} \quad I_i = I\left[\hat{H} \geqslant \frac{z_i - H_{bi}}{\delta H_i}\right].$$

If we put $\hat{z}_i = \frac{z_i - H_{bi}}{\delta H_i}$ and $\hat{z}_m = \hat{z}_1 \vee \hat{z}_2$ then $I_i = I_{\hat{H} \geqslant \hat{z}_i}$ and $I_1 I_2 = I_{\hat{H} \geqslant \hat{z}_1 \vee \hat{z}_2} = I_{\hat{H} \geqslant \hat{z}_m}$. Like before, we also use $\hat{y}_i$ and $\hat{y}_m$ to denote versions of $\hat{z}_i$ and $\hat{z}_m$ which are limited to lie in $[-1, 1]$.

We now consider the required expectations conditional on J and not J. These can be expressed in terms of integrals as

$$\mathbb{E}[\cdots I_1 I_2|J] = \frac{1}{4}\int_{\hat{y}_1}^{1}\int_{\hat{y}_2}^{1} \cdots \, d\hat{H}_2 \, d\hat{H}_1,$$

$$\mathbb{E}[\cdots I_1 I_2|\text{not } J] = \frac{1}{2}\int_{\hat{y}_m}^{1} \cdots \, d\hat{H},$$

$$\mathbb{E}[\cdots I_1 I_2 S|J] = \lambda S_t^* \mathbb{E}[\cdots I_1 I_2 S_z|J] = \lambda S_t^* \frac{1}{4}\int_{\hat{y}_1}^{1}\int_{\hat{y}_2}^{1} \cdots S_z \, d\hat{H}_2 \, d\hat{H}_1$$

and

$$\mathbb{E}[\cdots I_1 I_2 S|\text{not } J] = S_t^* \mathbb{E}[\cdots I_1 I_2 S_z|\text{not } J] = S_t^* \frac{1}{2}\int_{\hat{y}_m}^{1} \cdots S_z \, d\hat{H}$$

for "$\cdots$" equal to $H_1 H_2$, H_1, H_2 and 1. In the integral over $\hat{H}_1$ and $\hat{H}_2$, it is implied that H_1 and H_2 within the integral are to be expressed in terms of $\hat{H}_1$ and $\hat{H}_2$, including for any dependency of the value of S_z for fixed z_1 and z_2 on H_1 and H_2. Similarly, in the integral over $\hat{H}$, it is implied that H_1

and H_2 within the integral are to be expressed in terms of $\hat{H} = \hat{H}_1 = \hat{H}_2$ (which is valid for the not-J case). The factors of $1/4$ and $1/2$ arise from the pdfs of $(\hat{H}_1, \hat{H}_2)$ (for the J case) and $\hat{H}$ (for the not-J case) which are uniformly distributed over $[-1,1] \times [-1,1]$ and $[-1,1]$ respectively. The two expectations involving S are not easily evaluated analytically (except where S_z is independent of H or, for the first expectation, where $\lambda = 0$) and are best treated by numerical integration. However the quantities not involving S can be expressed more simply. Because H_1 and H_2 are conditionally independent given J, the expectations of $H_1 H_2 I_1 I_2$, $H_1 I_1 I_2$, $H_2 I_1 I_2$ and $I_1 I_2$ given J are straightforward to express using the already evaluated $\mathbb{E}[HI]$ and $\mathbb{E}[I]$. Also, because $\hat{H}$ is uniformly distributed in $[-1,1]$, we can deduce that

$$\mathbb{E}[I_1 I_2 | \text{not } J] = \mathbb{P}[\hat{H} \geqslant \hat{z}_m] = \frac{1 - \hat{y}_m}{2},$$

$$\mathbb{E}\left[\left(\frac{H_i}{H_{bi}} - 1\right) I_1 I_2 \middle| \text{not } J\right] = \mathbb{E}\left[\frac{\delta H_i}{H_{bi}} \hat{H} \middle| \hat{H} \geqslant \hat{z}_m\right] \mathbb{P}[\hat{H} \geqslant \hat{z}_m]$$

$$= \left(\frac{\delta H_i}{H_{bi}} \frac{1 + \hat{y}_m}{2}\right) \frac{1 - \hat{y}_m}{2} = \frac{\delta H_i}{H_{bi}} \frac{1 - \hat{y}_m^2}{4}$$

and

$$\mathbb{E}\left[\left(\frac{H_1}{H_{b1}} - 1\right)\left(\frac{H_2}{H_{b2}} - 1\right) I_1 I_2 \middle| \text{not } J\right] = \mathbb{E}\left[\frac{\delta H_1 \delta H_2}{H_{b1} H_{b2}} \hat{H}^2 \middle| \hat{H} \geqslant \hat{z}_m\right] \mathbb{P}[\hat{H} \geqslant \hat{z}_m]$$

$$= \frac{\delta H_1 \delta H_2}{H_{b1} H_{b2}} \left[\left(\frac{1 + \hat{y}_m}{2}\right)^2 + \frac{(1 - \hat{y}_m)^2}{12}\right] \frac{1 - \hat{y}_m}{2} = \frac{\delta H_1 \delta H_2}{H_{b1} H_{b2}} \frac{1 - \hat{y}_m^3}{6}$$

using the fact that the mean and variance of a random variable which is uniformly distributed in $[\hat{y}_m, 1]$ are $\frac{1+\hat{y}_m}{2}$ and $\frac{(1-\hat{y}_m)^2}{12}$.

We can now give expressions for $\mathbb{E}[e]$ and $\mathbb{E}[e_1 e_2]$. In doing this it is often convenient to use the equality $\alpha_3 \frac{H}{H_b} - \alpha_2 = \alpha_3 \left(\frac{H}{H_b} - 1\right) + 1 = \alpha_3 \frac{\delta H}{H_b} \hat{H} + 1$ etc. For the mean we have

$$\mathbb{E}[e] = c_M H_b^{\alpha_3} \mathbb{E}\left[\left(\alpha_3 \frac{\delta H}{H_b} \hat{H} + 1\right) I\right] = c_M H_b^{\alpha_3} \left(\frac{1 - \hat{y}}{2} + \alpha_3 \frac{\delta H}{H_b} \frac{1 - \hat{y}^2}{4}\right). \tag{2}$$

For the 2nd order moments we have

$$\mathbb{E}[e_1 e_2] = c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3} (1 + \sigma_r^2 R)$$

$$\times \left\{ \left(1 - \mathrm{e}^{-\frac{|t_2 - t_1|}{T_H}}\right) \mathbb{E}\left[\left(\alpha_3 \frac{\delta H_1}{H_{b1}} \hat{H}_1 + 1\right) I_1 \left(\alpha_3 \frac{\delta H_2}{H_{b2}} \hat{H}_2 + 1\right) I_2 (1 + \sigma_q^2 S) \middle| J\right]\right.$$

$$\left. + \mathrm{e}^{-\frac{|t_2 - t_1|}{T_H}} \mathbb{E}\left[\left(\alpha_3 \frac{\delta H_1}{H_{b1}} \hat{H} + 1\right) I_1 \left(\alpha_3 \frac{\delta H_2}{H_{b2}} \hat{H} + 1\right) I_2 (1 + \sigma_q^2 S) \middle| \text{not } J\right]\right\}.$$

While this could be simplified without making further assumptions, the expression will be quite complex. Hence we now restrict attention to the cases where either λ is zero or S_z is independent of H. This includes the model described in the main text ($\lambda = 0$) and the case where the result can be evaluated without numerical integration (S_z independent of H) but excludes cases involving double integrals. With this restriction we have

$$\mathbb{E}[e_1e_2] = c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3}(1+\sigma_r^2 R)\left\{(1+\lambda\sigma_q^2 S_z S_t^*)\left(1-\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}\right)\right.$$

$$\times\mathbb{E}\left[\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H}_1+1\right)I_1\right]\mathbb{E}\left[\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H}_2+1\right)I_2\right]$$

$$\left.+\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}\mathbb{E}\left[\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H}+1\right)I_1\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H}+1\right)I_2(1+\sigma_q^2 S_z S_t^*)\middle|\text{not } J\right]\right\}$$

$$=(1+\sigma_r^2 R)\left\{(1+\lambda\sigma_q^2 S_z S_t^*)\left(1-\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}\right)\mathbb{E}[e_1]\mathbb{E}[e_2]\right.$$

$$\left.+\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}c_M^2 H_{b1}^{\alpha_3}H_{b2}^{\alpha_3}\mathbb{E}\left[\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H}+1\right)I_1\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H}+1\right)I_2(1+\sigma_q^2 S_z S_t^*)\middle|\text{not } J\right]\right\}$$

$$=(1+\sigma_r^2 R)\left\{(1+\lambda\sigma_q^2 S_z S_t^*)\left(1-\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}\right)\mathbb{E}[e_1]\mathbb{E}[e_2]\right.$$

$$\left.+\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}c_M^2 H_{b1}^{\alpha_3}H_{b2}^{\alpha_3}\frac{1}{2}\int_{\hat{y}_m}^{1}\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H}+1\right)\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H}+1\right)(1+\sigma_q^2 S_z S_t^*)\,d\hat{H}\right\}.$$

For the special case where S_z (for fixed z_1 and z_2) is independent of H we have

$$\mathbb{E}[e_1e_2]=(1+\sigma_r^2 R)\left\{(1+\lambda\sigma_q^2 S_z S_t^*)\left(1-\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}\right)\mathbb{E}[e_1]\mathbb{E}[e_2]\right.$$

$$\left.+(1+\sigma_q^2 S_z S_t^*)\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}c_M^2 H_{b1}^{\alpha_3}H_{b2}^{\alpha_3}\mathbb{E}\left[\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H}+1\right)I_1\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H}+1\right)I_2\middle|\text{not } J\right]\right\}$$

$$=(1+\sigma_r^2 R)\left\{(1+\lambda\sigma_q^2 S_z S_t^*)\mathbb{E}[e_1]\mathbb{E}[e_2]\right.$$

$$+\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}c_M^2 H_{b1}^{\alpha_3}H_{b2}^{\alpha_3}\left[(1+\sigma_q^2 S_z S_t^*)\left(\tfrac{1-\hat{y}_m}{2}+\alpha_3\left(\tfrac{\delta H_1}{H_{b1}}+\tfrac{\delta H_2}{H_{b2}}\right)\tfrac{1-\hat{y}_m^2}{4}+\alpha_3^2\tfrac{\delta H_1\delta H_2}{H_{b1}H_{b2}}\tfrac{1-\hat{y}_m^3}{6}\right)\right.$$

$$\left.\left.-(1+\lambda\sigma_q^2 S_z S_t^*)\left(\tfrac{(1-\hat{y}_1)(1-\hat{y}_2)}{4}+\alpha_3\tfrac{\delta H_1}{H_{b1}}\tfrac{(1-\hat{y}_1^2)(1-\hat{y}_2)}{8}+\alpha_3\tfrac{\delta H_2}{H_{b2}}\tfrac{(1-\hat{y}_2^2)(1-\hat{y}_1)}{8}+\alpha_3^2\tfrac{\delta H_1\delta H_2}{H_{b1}H_{b2}}\tfrac{(1-\hat{y}_1^2)(1-\hat{y}_2^2)}{16}\right)\right]\right\}$$

$$=(1+\sigma_r^2 R)\left\{(1+\lambda\sigma_q^2 S_z S_t^*)\mathbb{E}[e_1]\mathbb{E}[e_2]\right.$$

$$+\mathrm{e}^{-\frac{|t_2-t_1|}{T_H}}c_M^2 H_{b1}^{\alpha_3}H_{b2}^{\alpha_3}\left[(1+\sigma_q^2 S_z S_t^*)\tfrac{1-\hat{y}_m}{2}\left(1+\alpha_3\left(\tfrac{\delta H_1}{H_{b1}}+\tfrac{\delta H_2}{H_{b2}}\right)\tfrac{1+\hat{y}_m}{2}+\alpha_3^2\tfrac{\delta H_1\delta H_2}{H_{b1}H_{b2}}\tfrac{1+\hat{y}_m+\hat{y}_m^2}{3}\right)\right.$$

$$\left.\left.-(1+\lambda\sigma_q^2 S_z S_t^*)\tfrac{(1-\hat{y}_1)(1-\hat{y}_2)}{4}\left(1+\alpha_3\tfrac{\delta H_1}{H_{b1}}\tfrac{1+\hat{y}_1}{2}+\alpha_3\tfrac{\delta H_2}{H_{b2}}\tfrac{1+\hat{y}_2}{2}+\alpha_3^2\tfrac{\delta H_1\delta H_2}{H_{b1}H_{b2}}\tfrac{(1+\hat{y}_1)(1+\hat{y}_2)}{4}\right)\right]\right\}.$$

We note (as a check) that $\mathbb{E}[e_1e_2]\geqslant\mathbb{E}[e_1]\mathbb{E}[e_2]$ because

$$\frac{(1-\hat{y}_1)(1-\hat{y}_2)}{4}\leqslant\frac{1-\hat{y}_m}{2},\quad 1+\hat{y}_i\leqslant 1+\hat{y}_m,$$

and

$$\frac{(1+\hat{y}_1)(1+\hat{y}_2)}{4}\leqslant\frac{(1+\hat{y}_m)^2}{4}\leqslant\frac{(1+\hat{y}_m)^2}{4}+\frac{(1-\hat{y}_m)^2}{12}=\frac{1+\hat{y}_m+\hat{y}_m^2}{3}$$

with the last inequality having a nice probabilistic interpretation in terms of the 1st and 2nd order moments of uniform distributions on $[\hat{y}_1, 1]$, $[\hat{y}_2, 1]$ and $[\hat{y}_m, 1]$. Of course $\mathbb{E}[e_1 e_2] \geqslant \mathbb{E}[e_1]\mathbb{E}[e_2]$ is not required probabilistically, but the model design seems likely to ensure all correlations are $\geqslant 0$.

If $e' \equiv e - \mathbb{E}[e]$ denotes the departure from the mean, then, with the restriction that either λ is zero or S_z is independent of H, we have

$$\mathbb{E}[e_1' e_2'] = (\sigma_r^2 R + \lambda\sigma_q^2 S_z S_t^* + \lambda\sigma_r^2 R \sigma_q^2 S_z S_t^*)\mathbb{E}[e_1]\mathbb{E}[e_2] + (1+\sigma_r^2 R)\mathrm{e}^{-\frac{|t_2 - t_1|}{T_H}} \Bigg[c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3}$$

$$\times \frac{1}{2}\int_{\hat{y}_m}^1 \left(\alpha_3 \frac{\delta H_1}{H_{b1}}\hat{H} + 1\right)\left(\alpha_3 \frac{\delta H_2}{H_{b2}}\hat{H} + 1\right)(1+\sigma_q^2 S_z S_t^*)\, d\hat{H} - (1 + \lambda\sigma_q^2 S_z S_t^*)\mathbb{E}[e_1]\mathbb{E}[e_2]\Bigg].$$

For the model in the main text, this becomes

$$\mathbb{E}[e_1' e_2'] = \sigma_r^2 R \mathbb{E}[e_1]\mathbb{E}[e_2] + (1+\sigma_r^2 R)\mathrm{e}^{-\frac{|t_2 - t_1|}{T_H}} \Bigg[c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3}$$

$$\times \frac{1}{2}\int_{\hat{y}_m}^1 \left(\alpha_3 \frac{\delta H_1}{H_{b1}}\hat{H} + 1\right)\left(\alpha_3 \frac{\delta H_2}{H_{b2}}\hat{H} + 1\right)\left(1+\sigma_q^2 S_z S_t^*\right)\, d\hat{H} - \mathbb{E}[e_1]\mathbb{E}[e_2]\Bigg].$$

Moments of discrete source elements

The above moments are for point emission values. However we require moments for the discretised source elements which cover rectangular regions in the z-t plane. Hence the formulae need to be integrated over the source regions. If the source regions are small compared to the scales on which $e(z,t)$ varies, it may be acceptable to just consider a single point within each source element. A better approximation is to sum over a number of points, in effect doing a numerical integration, although we note that for each pair of points a numerical integration over $\hat{H}$ is needed to calculate $\mathbb{E}[e_1 e_2]$ which will make the approach expensive if used with a large number of points. Here we integrate $\mathbb{E}[e]$ over the source regions analytically and, for $\mathbb{E}[e_1 e_2]$, switch the order of integrations so as to do the integration over the source regions analytically and then do the integration over $\hat{H}$ numerically.

For a source element occupying $[\underline{z}, \overline{z}] \times [\underline{t}, \overline{t}]$ (with $\underline{z} \leqslant \overline{z}$, $\underline{t} \leqslant \overline{t}$) the source strength is $E \equiv \int_{\underline{z}}^{\overline{z}} \int_{\underline{t}}^{\overline{t}} e(z,t)\, dt\, dz$. In calculating the moments of the E's, we consider only the model described in the main text and ignore the various generalisations discussed near the start of this appendix. In addition we assume that H_b and δH change only in discrete jumps. The analysis which follows also assumes that these jumps don't occur within a source element; when a jump does in fact occur within one or more source elements, these source elements are divided and the results for the subdivisions are combined to obtain the moments for the original choice of source elements.

To calculate the moments of the E's, we need to integrate the moments of $e(z,t)$ over the regions occupied by the source elements. In doing this it's convenient, in considering the 2nd order moments, to replace $\int_{\hat{y}_m}^1 \cdots d\hat{H}$ by the equivalent expression $\int_{-1}^1 \cdots I_{\hat{H} \geqslant \hat{z}_m}\, d\hat{H}$ which can also be written as $\int_{-1}^1 \cdots I_{\hat{H} \geqslant \hat{z}_1} I_{\hat{H} \geqslant \hat{z}_2}\, d\hat{H}$. The latter form is easier to use here because the varying bounds of the $\hat{H}$ integral can be exchanged for varying bounds in the z integrals.

For the 1st order moments we have

$$\mathbb{E}[E] = \int_{\underline{z}}^{\overline{z}} \int_{\underline{t}}^{\overline{t}} \mathbb{E}[e(z,t)]\, dt\, dz = \int_{\underline{z}}^{\overline{z}} \int_{\underline{t}}^{\overline{t}} c_M H_b^{\alpha_3} \left(\frac{1-\hat{y}}{2} + \alpha_3 \frac{\delta H}{H_b} \frac{1-\hat{y}^2}{4} \right) dt\, dz$$

$$= c_M H_b^{\alpha_3} (\overline{t} - \underline{t}) \left(\int_{[\underline{z},\overline{z}]\cap[0,H_b-\delta H]} + \int_{[\underline{z},\overline{z}]\cap[H_b-\delta H, H_b+\delta H]} \right) \left(\frac{1-\hat{y}}{2} + \alpha_3 \frac{\delta H}{H_b} \frac{1-\hat{y}^2}{4} \right) dz$$

$$= c_M H_b^{\alpha_3} (\overline{t} - \underline{t}) \left[(z \wedge (H_b - \delta H)) \Big|_{z=\underline{z}}^{z=\overline{z}} + \delta H \int_{\underline{\hat{y}}}^{\overline{\hat{y}}} \left(\frac{1-\hat{y}}{2} + \alpha_3 \frac{\delta H}{H_b} \frac{1-\hat{y}^2}{4} \right) d\hat{y} \right]$$

$$= c_M H_b^{\alpha_3} (\overline{t} - \underline{t}) \left[(z \wedge (H_b - \delta H)) \Big|_{z=\underline{z}}^{z=\overline{z}} + \delta H \left(\frac{\hat{y}}{2} - \frac{\hat{y}^2}{4} \right) \Big|_{\hat{y}=\underline{\hat{y}}}^{\hat{y}=\overline{\hat{y}}} + \alpha_3 \frac{(\delta H)^2}{H_b} \left(\frac{\hat{y}}{4} - \frac{\hat{y}^3}{12} \right) \Big|_{\hat{y}=\underline{\hat{y}}}^{\hat{y}=\overline{\hat{y}}} \right].$$

For the 2nd order moments we first consider some integrals of exponentials. We have

$$\int_{\underline{t}}^{\overline{t}} \int_{\underline{t}}^{\overline{t}} \mathrm{e}^{-\frac{|t_2-t_1|}{T}}\, dt_2\, dt_1 = 2T^2 \left(\mathrm{e}^{-\frac{|\overline{t}-\underline{t}|}{T}} - 1 + \frac{|\overline{t}-\underline{t}|}{T} \right) \equiv 2T^2 f\left(\frac{\overline{t}-\underline{t}}{T} \right)$$

with $f(x) = \mathrm{e}^{-|x|} - 1 + |x|$. Also we have

$$\int_{\underline{t}_1}^{\overline{t}_1} \int_{\underline{t}_2}^{\overline{t}_2} \mathrm{e}^{-\frac{|t_2-t_1|}{T}}\, dt_2\, dt_1 = \frac{1}{2} \left(\int_{\underline{t}_1}^{\overline{t}_2} \int_{\underline{t}_1}^{\overline{t}_2} + \int_{\overline{t}_1}^{\underline{t}_2} \int_{\overline{t}_1}^{\underline{t}_2} - \int_{\underline{t}_1}^{\underline{t}_2} \int_{\underline{t}_1}^{\underline{t}_2} - \int_{\overline{t}_1}^{\overline{t}_2} \int_{\overline{t}_1}^{\overline{t}_2} \right) \mathrm{e}^{-\frac{|t_2-t_1|}{T}}\, dt_2\, dt_1$$

$$= T^2 \left[f\left(\frac{\overline{t}_2-\underline{t}_1}{T} \right) + f\left(\frac{\underline{t}_2-\overline{t}_1}{T} \right) - f\left(\frac{\underline{t}_2-\underline{t}_1}{T} \right) - f\left(\frac{\overline{t}_2-\overline{t}_1}{T} \right) \right] \equiv F_{\underline{t}_1,\overline{t}_1,\underline{t}_2,\overline{t}_2}(T)$$

where F is defined by the last equation. One way to derive this is to write the integrals as e.g. $\int_{\underline{t}_1}^{\overline{t}_1} = \int_{t_0}^{\overline{t}_1} - \int_{t_0}^{\underline{t}_1}$ and proceed by analogy with $(\overline{t}_1-\underline{t}_1)(\overline{t}_2-\underline{t}_2) = \frac{1}{2}[(\overline{t}_2-\underline{t}_1)^2+(\underline{t}_2-\overline{t}_1)^2-(\underline{t}_2-\underline{t}_1)^2-(\overline{t}_2-\overline{t}_1)^2]$. For disjoint intervals with $\underline{t}_1, \overline{t}_1 \leqslant \underline{t}_2, \overline{t}_2$ or $\underline{t}_1, \overline{t}_1 \geqslant \underline{t}_2, \overline{t}_2$ we have

$$\int_{\underline{t}_1}^{\overline{t}_1} \int_{\underline{t}_2}^{\overline{t}_2} \mathrm{e}^{-\frac{|t_2-t_1|}{T}}\, dt_2\, dt_1 = T^2 \left[f\left(\frac{\overline{t}_2-\underline{t}_1}{T} \right) + f\left(\frac{\underline{t}_2-\overline{t}_1}{T} \right) - f\left(\frac{\underline{t}_2-\underline{t}_1}{T} \right) - f\left(\frac{\overline{t}_2-\overline{t}_1}{T} \right) \right]$$

$$= T^2 \left(\mathrm{e}^{-\frac{|\overline{t}_2-\underline{t}_1|}{T}} + \mathrm{e}^{-\frac{|\underline{t}_2-\overline{t}_1|}{T}} - \mathrm{e}^{-\frac{|\underline{t}_2-\underline{t}_1|}{T}} - \mathrm{e}^{-\frac{|\overline{t}_2-\overline{t}_1|}{T}} \right)$$

and for identical intervals with $\underline{t}_1 = \underline{t}_2$ and $\overline{t}_1 = \overline{t}_2$ we recover the result for $\int_{\underline{t}}^{\overline{t}} \int_{\underline{t}}^{\overline{t}} \mathrm{e}^{-\frac{|t_2-t_1|}{T}}\, dt_2\, dt_1$ given above. In addition we have

$$\int_{\underline{Y}_1}^{\overline{Y}_1} \left(1 - \mathrm{e}^{-\frac{\eta_1}{L_q}} \right) d\eta_1 = \overline{Y}_1 - \underline{Y}_1 - L_q \left(\mathrm{e}^{-\frac{\underline{Y}_1}{L_q}} - \mathrm{e}^{-\frac{\overline{Y}_1}{L_q}} \right) = L_q \left[f\left(\frac{\overline{Y}_1}{L_q} \right) - f\left(\frac{\underline{Y}_1}{L_q} \right) \right]$$

for $\underline{Y}_1, \overline{Y}_1 \geqslant 0$.

In evaluating $\mathbb{E}[E_1' E_2']$ we will need to calculate the two integrals $\int_{\underline{z}_1}^{\overline{z}_1} \int_{\underline{z}_2}^{\overline{z}_2} I_{\hat{H} \geqslant \hat{z}_1} I_{\hat{H} \geqslant \hat{z}_2}\, dz_2\, dz_1$ and $\int_{\underline{z}_1}^{\overline{z}_1} \int_{\underline{z}_2}^{\overline{z}_2} I_{\hat{H} \geqslant \hat{z}_1} I_{\hat{H} \geqslant \hat{z}_2} S_z\, dz_2\, dz_1$. To do this, we write $\underline{y}_i$ and $\overline{y}_i$ for $\underline{z}_i \wedge H_i$ and $\overline{z}_i \wedge H_i$ and $\underline{Y}_i$ and $\overline{Y}_i$

for $\underline{y}_i/H_i$ and $\overline{y}_i/H_i$. Then we have

$$\int_{\underline{z}_1}^{\overline{z}_1}\int_{\underline{z}_2}^{\overline{z}_2} I_{\hat{H}\geqslant\hat{z}_1} I_{\hat{H}\geqslant\hat{z}_2}\, dz_2\, dz_1 = \int_{\underline{y}_1}^{\overline{y}_1}\int_{\underline{y}_2}^{\overline{y}_2} dz_2\, dz_1 = H_1 H_2(\overline{Y}_1 - \underline{Y}_1)(\overline{Y}_2 - \underline{Y}_2)$$

and

$$\int_{\underline{z}_1}^{\overline{z}_1}\int_{\underline{z}_2}^{\overline{z}_2} I_{\hat{H}\geqslant\hat{z}_1} I_{\hat{H}\geqslant\hat{z}_2} S_z\, dz_2\, dz_1 = \int_{\underline{y}_1}^{\overline{y}_1}\int_{\underline{y}_2}^{\overline{y}_2} S_z\, dz_2\, dz_1 = H_1 H_2 \int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} S_z\, d\eta_2\, d\eta_1.$$

With our form of S_z, namely

$$S_z = \mathrm{e}^{-\frac{|\eta_2-\eta_1|}{L_q}} - L_q\left(4 - \mathrm{e}^{-\frac{\eta_2}{L_q}} - \mathrm{e}^{-\frac{1-\eta_2}{L_q}} - \mathrm{e}^{-\frac{\eta_1}{L_q}} - \mathrm{e}^{-\frac{1-\eta_1}{L_q}}\right) + 2L_q^2\left(\frac{1}{L_q} - 1 + \mathrm{e}^{-\frac{1}{L_q}}\right)$$

(see (1)), we can evaluate the parts of $\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} S_z\, d\eta_2\, d\eta_1$ as follows:

$$\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} \mathrm{e}^{-\frac{|\eta_2-\eta_1|}{L_q}}\, d\eta_2\, d\eta_1 = F_{\underline{Y}_1,\overline{Y}_1,\underline{Y}_2,\overline{Y}_2}(L_q),$$

$$\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} L_q\left(1 - \mathrm{e}^{-\frac{\eta_1}{L_q}}\right) d\eta_2\, d\eta_1 = (\overline{Y}_2 - \underline{Y}_2)L_q^2\left[f\left(\frac{\overline{Y}_1}{L_q}\right) - f\left(\frac{\underline{Y}_1}{L_q}\right)\right]$$

and

$$\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} L_q\left(1 - \mathrm{e}^{-\frac{1-\eta_1}{L_q}}\right) d\eta_2\, d\eta_1 = (\overline{Y}_2 - \underline{Y}_2)L_q^2\left[f\left(\frac{1-\underline{Y}_1}{L_q}\right) - f\left(\frac{1-\overline{Y}_1}{L_q}\right)\right]$$

with similar results when indices 1 and 2 are swapped, and

$$\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} 2L_q^2\left(\frac{1}{L_q} - 1 + \mathrm{e}^{-\frac{1}{L_q}}\right) d\eta_2\, d\eta_1 = (\overline{Y}_1 - \underline{Y}_1)(\overline{Y}_2 - \underline{Y}_2)2L_q^2 f\left(\frac{1}{L_q}\right).$$

It follows that

$$\begin{aligned}
\mathbb{E}[E_1'E_2'] = \frac{\mathbb{E}[E_1]\mathbb{E}[E_2]}{(\bar{t}_1 - \underline{t}_1)(\bar{t}_2 - \underline{t}_2)} &\left[\sigma_r^2 F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}(T_r) - F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}(T_H) - \sigma_r^2 F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}\left(\frac{1}{1/T_H + 1/T_r}\right)\right] \\
&+ \left[F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}(T_H) + \sigma_r^2 F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}\left(\frac{1}{1/T_H + 1/T_r}\right)\right] \\
&\times c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3}\frac{1}{2}\int_{-1}^{1}\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H} + 1\right)\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H} + 1\right) H_1 H_2(\overline{Y}_1 - \underline{Y}_1)(\overline{Y}_2 - \underline{Y}_2)\, d\hat{H} \\
&+ \left[\sigma_q^2 F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}\left(\frac{1}{1/T_H + 1/T_q}\right) + \sigma_r^2\sigma_q^2 F_{\underline{t}_1,\bar{t}_1,\underline{t}_2,\bar{t}_2}\left(\frac{1}{1/T_H + 1/T_r + 1/T_q}\right)\right] \\
&\times c_M^2 H_{b1}^{\alpha_3} H_{b2}^{\alpha_3}\frac{1}{2}\int_{-1}^{1}\left(\alpha_3\frac{\delta H_1}{H_{b1}}\hat{H} + 1\right)\left(\alpha_3\frac{\delta H_2}{H_{b2}}\hat{H} + 1\right) H_1 H_2\left(\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} S_z\, d\eta_2\, d\eta_1\right) d\hat{H}
\end{aligned}$$

with

$$\int_{\underline{Y}_1}^{\overline{Y}_1}\int_{\underline{Y}_2}^{\overline{Y}_2} S_z\, d\eta_2\, d\eta_1 = F_{\underline{Y}_1,\overline{Y}_1,\underline{Y}_2,\overline{Y}_2}(L_q)$$

$$-(\overline{Y}_2-\underline{Y}_2)L_q^2\left[f\left(\frac{\overline{Y}_1}{L_q}\right)-f\left(\frac{\underline{Y}_1}{L_q}\right)\right]-(\overline{Y}_2-\underline{Y}_2)L_q^2\left[f\left(\frac{1-\underline{Y}_1}{L_q}\right)-f\left(\frac{1-\overline{Y}_1}{L_q}\right)\right]$$

$$-(\overline{Y}_1-\underline{Y}_1)L_q^2\left[f\left(\frac{\overline{Y}_2}{L_q}\right)-f\left(\frac{\underline{Y}_2}{L_q}\right)\right]-(\overline{Y}_1-\underline{Y}_1)L_q^2\left[f\left(\frac{1-\underline{Y}_2}{L_q}\right)-f\left(\frac{1-\overline{Y}_2}{L_q}\right)\right]$$

$$+(\overline{Y}_1-\underline{Y}_1)(\overline{Y}_2-\underline{Y}_2)2L_q^2 f\left(\frac{1}{L_q}\right).$$

This leaves two integrals over $\hat{H}$ to evaluate. The second of these integrals in particular is difficult to evaluate exactly and so we have chosen to use numerical methods for both integrals over $\hat{H}$.

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