

The AW_PHILOW_MF and AW_PHILUP_MF folders contain the modflow files for the two the optimised models described in Hemmings et al. (2018).

AW_PHILUP_MF provided an acceptable replication of observation data overall and a stable numerical solution, but had a higher phi value than the AW_PHILOW_MF realisation. See Section 4.4 of Hemmings et al (2018) for details (text pasted below). Note that the AW_PHILUP_MF is referred to as the The Acceptable-Limit Model in Hemmings

The modflow files for the 165 modflow files retained after the EMMA-based rejection sampling of the >4,000 null space monte carlo realisations are not provided here

The .ftl file output from the modflow simulations links the flow solution to mt3d

The run_files contains the mt3d files for the median nitrate concentration load layer

4.4 The Acceptable-Limit Model

The calibrated model described above minimises the weighted misfit (residual) between model outputs and observations. However, the calibrated parameter set caused some model instability in subsequent tests and scenario runs. This instability means that the calibrated parameter set is not suitable for calculating the sensitivity matrix that relates parameter values to model outputs, for use in subsequent uncertainty analysis (Hemmings et al. 2018). The parameters associated with the previous iteration of the calibration (prior to application of the final parameter upgrades), demonstrate greater stability during subsequent model tests and can be used to calculate the sensitivity matrix required in the uncertainty analysis. Although this model has a higher misfit than the calibrated model described above (i.e. a greater objective function or Φ value), the model-to-measurement misfit (presented in Appendix A2.2) was deemed “acceptable” by ECan. The model-to-measurement misfit produced by this “acceptable-limit” model also provides the upper limit of acceptability in the subsequent uncertainty analysis Hemmings et al. 2018.

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