Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Chapter 13

Big Magnetization Transfer

The Big magnetization transfer package analyzes data where two sites are exchanging magnetization under the assumption that one of the sites is essentially infinite compared to the other. Consequently, the big site is essentially unchanging and the solution for the other site simplifies, Eq. (13.1) below. The interface to this package is shown in Fig. 13.1. To use this package, you must do the following:

Select the Big Magnetization Transfer package from the Package menu.

Load one or more Ascii data sets using the Files menu. When the data have been successfully loaded, the data are displayed in the Ascii Data viewer.

Check the Analysis Options/Find Outliers box if you suspect outliers are present in the data.

Review the prior probabilities for the K_d, R_d and R_w parameters using the Prior Viewer.

Select the server that is to process the analysis.

Check the status of the selected server to determine if the server is busy, change to another server if the selected server is busy.

Run the the analysis on the selected server by activating the Run button.

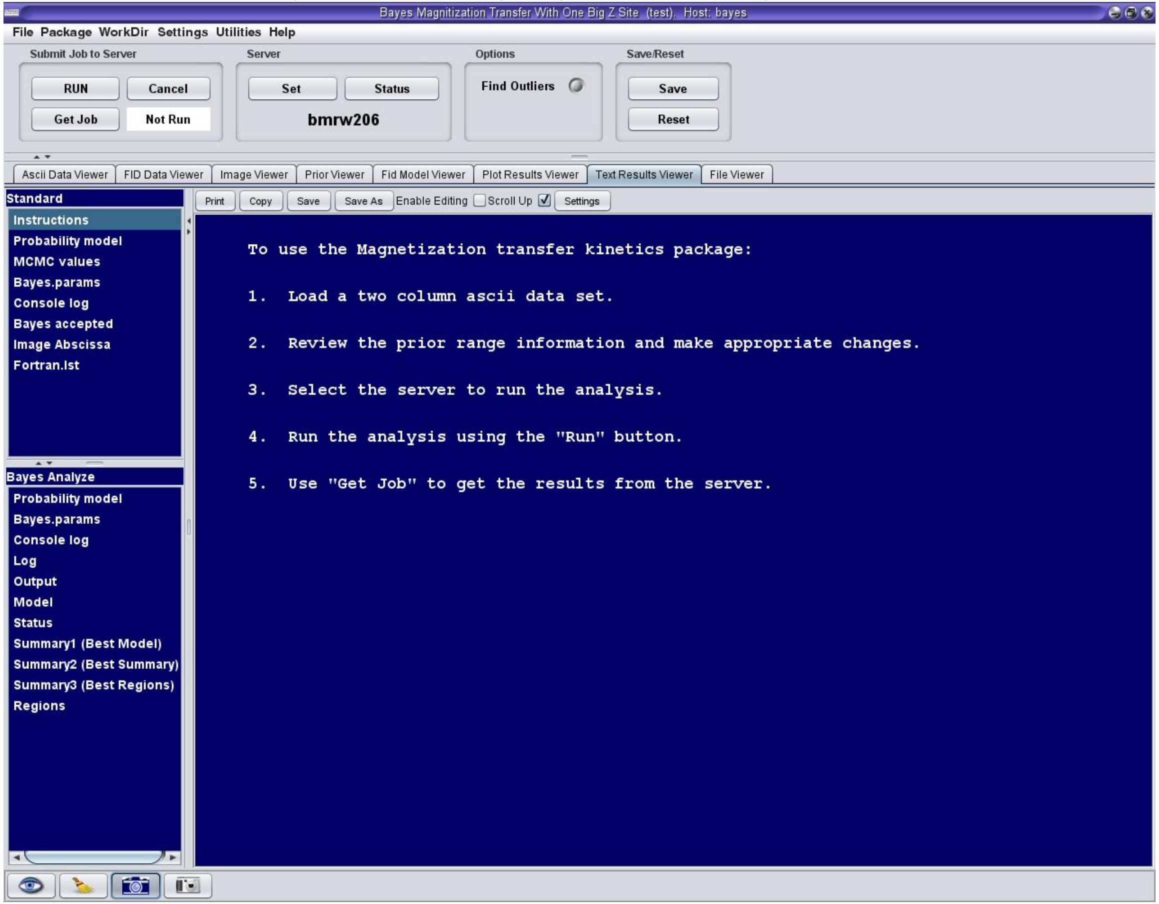
Get the the results of the analysis by activating the Get Job button. If the analysis is running, this button will return the Accepted report containing the status of the current run. Otherwise, it will fetch and display the results from the current analysis.

13.1 The Bayesian Calculation

The Big magnetization transfer problem is one in which a very large spin reservoir is exchanging magnetization with a much smaller spin reservoir. We will call the larger reservoir the Solvent, and the other the Small reservoir or resonance. When one reservoir is much greater than the other, the Solvent is unaffected by the the transfer of magnetization to or from Small reservoir. Consequently, the solution to magnetization exchange equations simplify, one obtains

$$M_d(t) = M_{z0}\left(1 - \frac{2K_d}{R_w - K_d - R_d}\left[\mathrm{e}^{-(R_d+K_d)t_i} - \mathrm{e}^{-R_w t_i}\right]\right) \tag{13.1}$$

Figure 13.1: The Big Magnetization Package Interface



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To use the Magnetization transfer kinetics package:

1.  Load a two column ascii data set.

2.  Review the prior range information and make appropriate changes.

3.  Select the server to run the analysis.

4.  Run the analysis using the "Run" button.

5.  Use "Get Job" to get the results from the server.
```

Figure 13.1: The interface to the Big Magnetization Transfer Package is shown here. The Big magnetization transfer interface allows you to analyze magnetization transfer data where one of the two sites may be considered as infinite compared to the other, see text for details.

where M_{z0} is the initial Small reservoir magnetization, K_d is the rate at which the Small reservoir is exchanging magnetization to the Solvent, R_w is the inverse of the T_2 time for Solvent reservoir, R_d is the R_2 relaxation rate of the Small reservoir and this equation implicitly assumes that the magnetization is fully inverted.

Markov chain Monte Carlo is used to draw samples from the joint posterior probability for all of the parameters. Form these samples, the marginal posterior probability for each parameter is computed. For example the posterior probability for the exchange rate K_d is computed as

$$P(K_d|DI) = \int P(K_d M_{z0} R_w R_d \sigma|DI) dM_{z0} dR_w dR_d d\sigma \tag{13.2}$$

where all of the parameters except the parameter of interest have been removed by marginalization. The joint posterior probability for the parameters, the integrand of this equation, is factored using Bayes' theorem and the product rule to become

$$P(K_d M_{z0} R_w R_d \sigma|DI) \propto P(K_d M_{z0} R_w R_d \sigma|I) P(D|K_d M_{z0} R_w R_d \sigma I) \tag{13.3}$$

where $P(K_d M_{z0} R_w R_d \sigma|I)$ is the joint prior probability for the parameters and $P(D|K_d M_{z0} R_w R_d \sigma I)$ is the likelihood. The joint prior probability or the parameters is factored into independent prior probabilities for each of the parameters separately

$$P(K_d M_{z0} R_w R_d \sigma|I) = P(K_d|I) P(M_{z0}|I) P(R_w|I) P(R_d|I) P(\sigma|I). \tag{13.4}$$

The prior probability for the standard deviation of the noise prior probability, $P(\sigma|I)$, is assigned a Jeffreys' prior, $P(\sigma|I) \propto 1/\sigma$. The prior probability for the amplitude $P(M_{z0}|I)$, was assigned using a using a very broad unbounded Gaussian of zero mean having a standard deviation of 3×10^5. The remaining three prior probabilities, $P(K_d|I)$, $P(R_w|I)$ and $P(R_d|I)$ all default to a prior positive. However, these priors are under user control and they may changed by the user. The likelihood, $P(D|K_d M_{z0} R_w R_d \sigma I)$ was assigned using a Gaussian prior probability having standard deviation σ. If we now collect all of the priors, assign the likelihood, and evaluate the integrals over both M_{z0} and σ, one obtains:

$$P(K_d M_{z0} R_w R_d \sigma|DI) \propto P(K_d|I) P(R_w|I) P(R_d|I) \left[N\overline{d^2} - \overline{h^2}\right]^{-\frac{N}{2}} \tag{13.5}$$

where $\overline{d^2}$ is the mean-square data value and is given by

$$\overline{d^2} = \frac{1}{N} \sum_{i=1}^{N} d_i^2. \tag{13.6}$$

The sufficient statistic, $\overline{h^2}$, is given by

$$\overline{h^2} = \frac{T^2}{g} \tag{13.7}$$

where T is the projection of the data onto the model and is given by

$$T = \sum_{i=1}^{N} d_i \left(1 - \frac{2K_d}{R_w - K_d - R_d} \left[\mathrm{e}^{-(R_d+K_d)t_i} - \mathrm{e}^{-R_w t_i}\right]\right) \tag{13.8}$$

Figure 13.2: Big Magnetization Transfer Example Fid

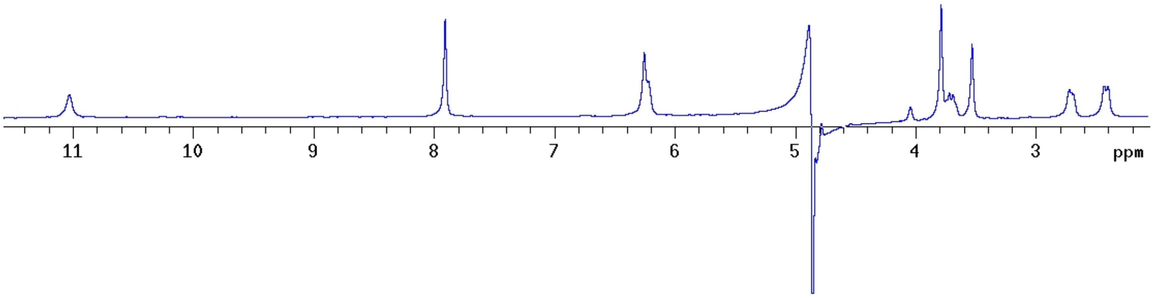

Figure 13.2: The full spectrum of the Fid data used in the big magnetization analysis. Note the water suppression artifact near 5ppm. The peak exchanging magnetization with the water is the small resonance near 11ppm.

and g is the squared length of the model:

$$g = \sum_{i=1}^{N} \left(1 - \frac{2K_d}{R_w - K_d - R_d} \left[\mathrm{e}^{-(R_d+K_d)t_i} - \mathrm{e}^{-R_w t_i} \right] \right)^2 . \tag{13.9}$$

It is Eq. (13.5) that is targeted by the Markov chain Monte Carlo simulations using simulated annealing. Note that this posterior probability does not contain the initial magnetization. However, in the process of computing this quantity the maximum posterior probability estimate of this parameter is computed and output for each value of the exchange and relaxation rates. While not strictly the Bayesian estimate of this parameter, the distribution of these estimates provide good mean and standard deviation estimates of the initial magnetization.

13.2 Outputs From The Big Magnetization Transfer Package

The Big Magnetization Transfer Package is an example of a preloaded Enter Ascii model. Preloaded means that when the Big Magnetization Transfer package is selected, the interface copies an Ascii model, MtZBig.f, from the system directory into the current experiment and starts up the Enter Ascii package. Consequently, the outputs from this package are all Enter Ascii outputs. The Text outputs files from the Big Magnetization Transfer packages consist of: “Bayes.prob.model,” “BayesEnterAscii.mcmc.values,” “Bayes.params,” “Console.log,” “Bayes.accepted” and a “Bayes.Condensed.File.” These output files can be viewed using the Text Viewer or they can be viewed using File Viewer by navigating to the current working directory and then selecting the files. The format of the mcmc.values report is discussed in Appendix D and the other reports are discussed in Chapter 3. Additionally, the “Plot Results Viewer” can be used to view the output probability density functions. In addition to the standard data, model and residual plots there are probability density functions for the decay rate constants, decay times, the amplitudes for each data set for each exponential

The full spectrum of data typical of this experiment is shown in Fig. 13.2. Note the presence

Figure 13.3: Big Magnetization Transfer Expansion

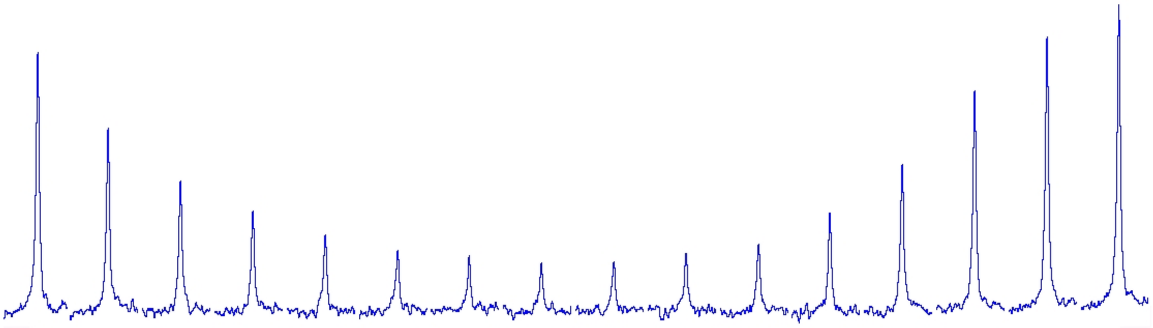

Figure 13.3: The peak exchanging magnetization begins at its equilibrium value. When the Solvent is inverted, negative magnetization flows into the Small reservoir bringing this reservoir down. At different delay times the Solvent is more fully relaxed and the Small resonance begins to recover, until at the longest delay time the Small resonance has returned to equilibrium. It is the amplitudes of the Small resonance that serve as input to this analysis.

of a water suppression artifact near 5ppm. To acquire this data one typically inverts the water, suppresses it, and finally acquires the Fid. The resonance exchanging magnetization with the water is the small resonances located at 11ppm. If we expand this region and then do a horizontal display, one obtains the spectra shown in Fig. 13.3. The Solvent resonance begins at its equilibrium value. When the Solvent resonances is inverted, negative magnetization flows into the Small reservoir bring its value down. At different delay times, different amounts of negative magnetization exchange with the Solvent resonance affecting its intensity in a predictable manner. The peak heights or amplitudes as determined by Bayes Analyze are used as input to the analysis. An example of data using a peak pick is shown in Fig. 13.3. Note that the Solvent resonance was inverted, as the Solvent exchanges negative magnetization with the Small resonance, the Small resonance is eventually pulled down. As the delay time increases the Small resonance has time to relax back toward equilibrium and eventually recovers.

Figure 13.4: Big Magnetization Transfer Peak Pick

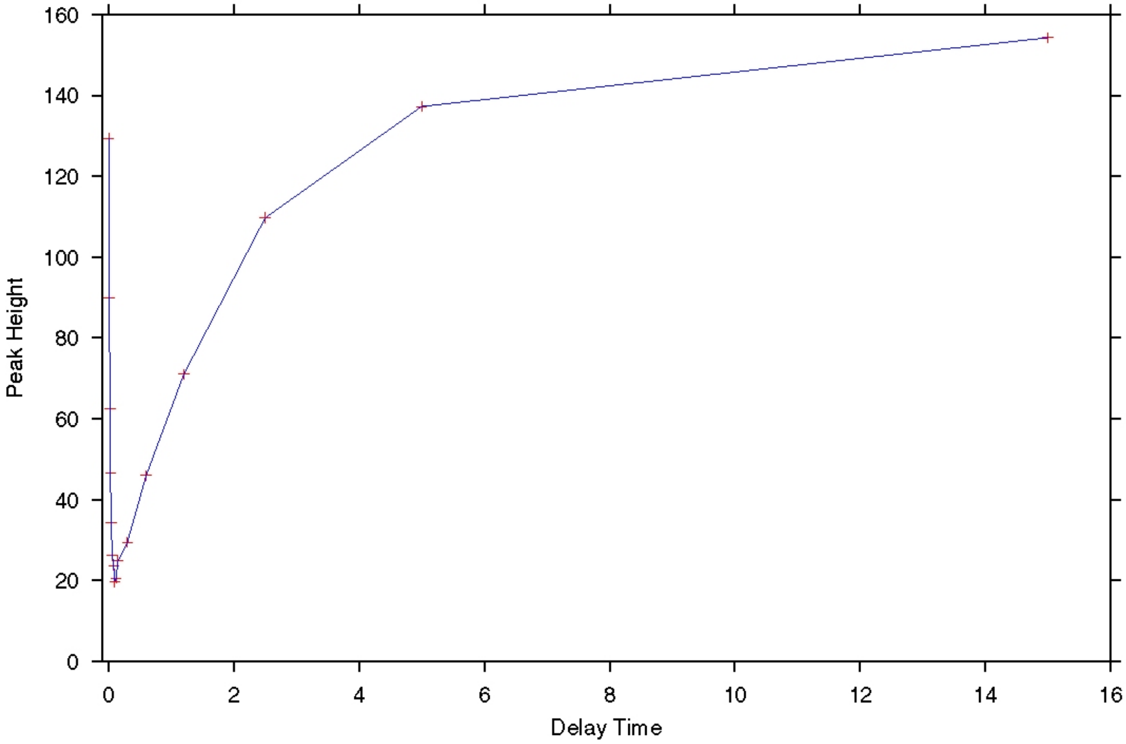

Figure 13.4: The peak heights or amplitudes (as determined by Bayes Analyze) serve as input to the Big magnetization transfer package. Here the peak heights for the spectra shown in Fig. 13.3 were used as input to the analysis. Note the Solvent magnetization starts fully relaxed, then after the Solvent is inverted, the negative Solvent magnetization begins to bring the Small reservoir down. As a function of delay time this continues for a while and then eventually the Small resonance recovers back to equilibrium.

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