

Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Contents

Manual Status	16
1 An Overview Of The Bayesian Analysis Software	19
1.1 The Server Software	19
1.2 The Client Interface	22
1.2.1 The Global Pull Down Menus	24
1.2.2 The Package Interface	24
1.2.3 The Viewers	27
2 Installing the Software	29
3 the Client Interface	33
3.1 The Global Pull Down Menus	35
3.1.1 the Files menu	35
3.1.2 the Packages menu	40
3.1.3 the WorkDir menu	45
3.1.4 the Settings menu	46
3.1.5 the Utilities menu	50
3.1.6 the Help menu	50
3.2 The Submit Job To Server area	51
3.3 The Server area	52
3.4 Interface Viewers	52
3.4.1 the Ascii Data Viewer	53
3.4.2 the fid Data Viewer	53
3.4.3 Image Viewer	59
3.4.3.1 the Image List area	59
3.4.3.2 the Set Image area	62
3.4.3.3 the Image Viewing area	62
3.4.3.4 the Grayscale area on the bottom	63
3.4.3.5 the Pixel Info area	63
3.4.3.6 the Image Statistics area	64
3.4.4 Prior Viewer	65
3.4.5 Fid Model Viewer	68
3.4.5.1 The fid Model Format	70

3.4.5.2	The Fid Model Reports	71
3.4.6	Plot Results Viewer	71
3.4.7	Text Results Viewer	74
3.4.8	Files Viewer	80
3.5	Common Interface Plots	80
3.5.1	Data, Model And Residual Plot	81
3.5.2	Posterior Probability For A Parameter	82
3.5.3	Maximum Entropy Histograms	83
3.5.4	Markov Monte Carlo Samples	83
3.5.5	Probability Vs Parameter Samples plot	86
3.5.6	Expected Log Likelihood Plot	88
3.5.7	Scatter Plots	88
3.5.8	Logarithm of the Posterior Probability Plot	91
3.5.9	Fortran/C Code Viewer	91
3.5.9.1	Fortran/C Model Viewer Popup Editor	94
4	An Introduction to Bayesian Probability Theory	99
4.1	The Rules of Probability Theory	99
4.2	Assigning Probabilities	102
4.3	Example: Parameter Estimation	109
4.3.1	Define The Problem	110
4.3.1.1	The Discrete Fourier Transform	110
4.3.1.2	Aliases	113
4.3.2	State The Model—Single-Frequency Estimation	114
4.3.3	Apply Probability Theory	115
4.3.4	Assign The Probabilities	118
4.3.5	Evaluate The Sums and Integrals	120
4.3.6	How Probability Generalizes The Discrete Fourier Transform	123
4.3.7	Aliasing	126
4.3.8	Parameter Estimates	132
4.4	Summary and Conclusions	136
5	Given Exponential Model	137
5.1	The Bayesian Calculation	139
5.2	Outputs From The Given Exponential Package	141
6	Unknown Number of Exponentials	143
6.1	The Bayesian Calculations	145
6.2	Outputs From The Unknown Number of Exponentials Package	148
7	Inversion Recovery	151
7.1	The Bayesian Calculation	153
7.2	Outputs From The Inversion Recovery Package	154

8	Bayes Analyze	155
8.1	Bayes Model	159
8.2	The Bayes Analyze Model Equation	161
8.3	The Bayesian Calculations	167
8.4	Levenberg-Marquardt And Newton-Raphson	171
8.5	Outputs From The Bayes Analyze Package	176
8.5.1	The “bayes.params.nnnn” Files	177
8.5.1.1	The Bayes Analyze File Header	178
8.5.1.2	The Global Parameters	182
8.5.1.3	The Model Components	184
8.5.2	The “bayes.model.nnnn” Files	185
8.5.3	The “bayes.output.nnnn” File	186
8.5.4	The “bayes.probabilities.nnnn” File	190
8.5.5	The “bayes.log.nnnn” File	193
8.5.6	The “bayes.status.nnnn” and “bayes.accepted.nnnn” Files	196
8.5.7	The “bayes.model.nnnn” File	197
8.5.8	The “bayes.summary1.nnnn” File	198
8.5.9	The “bayes.summary2.nnnn” File	199
8.5.10	The “bayes.summary3.nnnn” File	200
8.6	Bayes Analyze Error Messages	200
9	Big Peak/Little Peak	207
9.1	The Bayesian Calculation	209
9.2	Outputs From The Big Peak/Little Peak Package	216
10	Metabolic Analysis	219
10.1	The Metabolic Model	223
10.2	The Bayesian Calculation	225
10.3	The Metabolite Models	228
10.3.1	The IPGD_D2O Metabolite	228
10.3.2	The Glutamate.2.0 Metabolite	232
10.3.3	The Glutamate.3.0 Metabolite	235
10.4	The Example Metabolite	236
10.5	Outputs From The Bayes Metabolite Package	238
11	Find Resonances	239
11.1	The Bayesian Calculations	241
11.2	Outputs From The Bayes Find Resonances Package	246
12	Diffusion Tensor Analysis	247
12.1	The Bayesian Calculation	249
12.2	Using The Package	254
13	Big Magnetization Transfer	259
13.1	The Bayesian Calculation	259
13.2	Outputs From The Big Magnetization Transfer Package	262

14 Magnetization Transfer	265
14.1 The Bayesian Calculation	267
14.2 Using The Package	271
15 Magnetization Transfer Kinetics	275
15.1 The Bayesian Calculation	277
15.2 Using The Package	281
16 Given Polynomial Order	285
16.1 The Bayesian Calculation	287
16.1.1 Gram-Schmidt	287
16.1.2 The Bayesian Calculation	288
16.2 Outputs From the Given Polynomial Order Package	290
17 Unknown Polynomial Order	293
17.1 Bayesian Calculations	295
17.1.1 Assigning Priors	296
17.1.2 Assigning The Joint Posterior Probability	297
17.2 Outputs From the Unknown Polynomial Order Package	299
18 Errors In Variables	303
18.1 The Bayesian Calculation	305
18.2 Outputs From The Errors In Variables Package	308
19 Behrens-Fisher	311
19.1 Bayesian Calculation	311
19.1.1 The Four Model Selection Probabilities	314
19.1.1.1 The Means And Variances Are The Same	315
19.1.1.2 The Mean Are The Same And The Variances Differ	317
19.1.1.3 The Means Differ And The Variances Are The Same	318
19.1.1.4 The Means And Variances Differ	319
19.1.2 The Derived Probabilities	320
19.1.3 Parameter Estimation	321
19.2 Outputs From Behrens-Fisher Package	322
20 Enter Ascii Model	329
20.1 The Bayesian Calculation	331
20.1.1 The Bayesian Calculations Using Eq. (20.1)	331
20.1.2 The Bayesian Calculations Using Eq. (20.2)	332
20.2 Outputs Form The Enter Ascii Model Package	335
21 Enter Ascii Model Selection	337
21.1 The Bayesian Calculations	339
21.1.1 The Direct Probability With No Amplitude Marginalization	340
21.1.2 The Direct Probability With Amplitude Marginalization	342
21.1.2.1 Marginalizing the Amplitudes	343
21.1.2.2 Marginalizing The Noise Standard Deviation	348

21.2	Outputs Form The Enter Ascii Model Package	349
26	Phasing An Image	395
26.1	The Bayesian Calculation	396
26.2	Using The Package	402
27	Phasing An Image Using Non-Linear Phases	405
27.1	The Model Equation	405
27.2	The Bayesian Calculations	407
27.3	The Interfaces To The Nonlinear Phasing Routine	409
28	Analyze Image Pixel	411
28.1	Modification History	413
29	The Image Model Selection Package	415
29.1	The Bayesian Calculations	417
29.2	Outputs Form The Image Model Selection Package	418
A	Ascii Data File Formats	423
A.1	Ascii Input Data Files	423
A.2	Ascii Image File Formats	424
A.3	The Abscissa File Format	425
B	Markov chain Monte Carlo With Simulated Annealing	439
B.1	Metropolis-Hastings Algorithm	440
B.2	Multiple Simulations	441
B.3	Simulated Annealing	442
B.4	The Annealing Schedule	442
B.5	Killing Simulations	443
B.6	the Proposal	444
C	Thermodynamic Integration	445
D	McMC Values Report	449
E	Writing Fortran/C Models	455
E.1	Model Subroutines, No Marginalization	455
E.2	The Parameter File	458
E.3	The Subroutine Interface	460
E.4	The Subroutine Declarations	462
E.5	The Subroutine Body	463
E.6	Model Subroutines With Marginalization	464
F	the Bayes Directory Organization	469
G	4dfp Overview	471

H Outlier Detection

Bibliography

List of Figures

1.1	The Start Up Window	23
1.2	Example Package Exponential Interface	25
2.1	Installation Kit For The Bayesian Analysis Software	31
3.1	The Start Up Window	34
3.2	The Files Menu	35
3.3	The Files/Load Image Submenu	37
3.4	The Packages Menu	41
3.5	The Working Directory Menu	46
3.6	The Working Directory Information Popup	47
3.7	The Settings Pull Down Menu	47
3.8	The McMC Parameters Popup	48
3.9	The Edit Server Popup	49
3.10	The Submit Job Widgets	51
3.11	The Server Widgets Group	52
3.12	The Ascii Data Viewer	54
3.13	The Fid Data Viewer	55
3.14	Fid Data Display Type	56
3.15	Fid Data Options Menu	58
3.16	The Image Viewer	60
3.17	The Image Viewer Right Mouse Popup Menu	61
3.18	The Prior Probability Viewer	66
3.19	The Fid Model Viewer	69
3.20	The Plot Results Viewer	72
3.21	Plot Information Popup	73
3.22	The Text Results Viewer	75
3.23	The Bayes Condensed File	78
3.24	Data, Model, And Resid Plot	81
3.25	The Parameter Posterior Probabilities	82
3.26	The Maximum Entropy Histograms	84
3.27	The Parameter Samples Plot	85
3.28	Posterior Probability Vs Parameter Value	86
3.29	Posterior Probability Vs Parameter Value, A Skewed Example	87
3.30	The Expected Value Of The Logarithm Of The Likelihood	89

3.31	The Scatter Plots	90
3.32	The Logarithm Of The Posterior Probability By Repeat Plot	92
3.33	The Fortran/C Model Viewer	93
3.34	The Fortran/C Code Editor	95
4.1	Frequency Estimation Using The DFT	112
4.2	Aliases	113
4.3	Nonuniformly Nonsimultaneously Sampled Sinusoid	127
4.4	Alias Spacing	128
4.5	Which Is The Critical Time	130
4.6	Example, Frequency Estimation	131
4.7	Estimating The Sinusoids Parameters	133
5.1	The Given And Unknown Number Of Exponential Package Interface	138
6.1	The Unknown Exponential Interface	144
6.2	The Distribution Of Models	149
6.3	The Posterior Probability For Exponential Model	150
7.1	The Inversion Recovery Interface	152
8.1	Bayes Analyze Interface	156
8.2	Bayes Analyze Fid Model Viewer	160
8.3	The Bayes Analyze File Header	179
8.4	The bayes.noise File	180
8.5	Bayes Analyze Global Parameters	183
8.6	The Third Section Of The Parameter File	184
8.7	Example Of An Initial Model In The Output File	187
8.8	Base 10 Logarithm Of The Odds	187
8.9	A Small Sample Of The Output Report	188
8.10	Bayes Analyze Uncorrelated Output	189
8.11	The bayes.proBABILITIES.nnnn File	191
8.12	The bayes.log.nnnn File	193
8.13	The bayes.status.nnnn File	196
8.14	The bayes.model.nnnn File	197
8.15	The bayes.model.nnnn File Uncorrelated Resonances	198
8.16	Bayes Analyze Summary Header	198
8.17	The Summary2 (Best Summary)	199
8.18	The Summary3 Report	201
9.1	The Big Peak/Little Peak Interface	208
9.2	The Time Dependent Parameters	218
10.1	The Bayes Metabolite Interface	220
10.2	The Bayes Metabolite Viewer	222
10.3	Bayes Metabolite Parameters And Probabilities List	227
10.4	The IPGD_D20 Metabolite	229

10.5	Bayes Metabolite IPGD_D20 Spectrum	230
10.6	Bayes Metabolite, The Fraction of Glucose	231
10.7	Glutamate Example Spectrum	233
10.8	Estimating The F_{c0} , y and F_{a0} Parameters	236
10.9	Bayes Metabolite, The Ethyl Ether Example	237
11.1	The Find Resonances Interface With The Ethyl Ether Spectrum	240
12.1	The Diffusion Tensor Package Interface	248
12.2	Diffusion Tensor Parameter Estimates	256
12.3	Diffusion Tensor Posterior Probability For The Model	257
13.1	The Big Magnetization Package Interface	260
13.2	Big Magnetization Transfer Example Fid	262
13.3	Big Magnetization Transfer Expansion	263
13.4	Big Magnetization Transfer Peak Pick	264
14.1	The Magnetization Transfer Package Interface	266
14.2	Magnetization Transfer Package Peak Picking	272
14.3	Magnetization Transfer Example Data	273
14.4	Magnetization Transfer Example Spectrum	274
15.1	Magnetization Transfer Kinetics Package Interface	276
15.2	Magnetization Transfer Kinetics Package Arrhenius Plot	282
15.3	Magnetization Transfer Kinetics Water Viscosity Table	283
16.1	Given Polynomial Order Package Interface	286
16.2	Given Polynomial Order Scatter Plot	291
17.1	Unknown Polynomial Order Package Interface	294
17.2	The Distribution of Models On The Console Log	298
17.3	The Posterior Probability For The Polynomial Order	300
18.1	The Errors In Variables Package Interface	304
18.2	The McMC Values File Produced By The Errors In Variables Package	310
19.1	The Behrens-Fisher Interface	312
19.2	Behrens-Fisher Hypotheses Tested	313
19.3	Behrens-Fisher Console Log	323
19.4	Behrens-Fisher Status Listing	324
19.5	Behrens-Fisher McMC Values File, The Preamble	325
19.6	Behrens-Fisher McMC Values File, The Middle	326
19.7	Behrens-Fisher McMC Values File, The End	327
20.1	Enter Ascii Model Package Interface	330
21.1	The Enter Ascii Model Selection Package Interface	338

26.1	Absorption Model Images	396
26.2	The Interface To The Image Phasing Package	397
26.3	Linear Phasing Package The Console Log	403
27.1	Nonlinear Phasing Example	406
27.2	The Interface To The Nonlinear Phasing Package	410
28.1	The Interface To The Analyze Image Pixels Package	412
29.1	The Interface To The Image Model Selection Package	416
29.2	Single Exponential Example Image	419
29.3	Single Exponential Example Data	420
29.4	Posterior Probability For The ExpOneNoConst Model	421
A.1	Ascii Data File Format	424
D.1	The McMC Values Report Header	450
D.2	McMC Values Report, The Middle	451
D.3	The McMC Values Report, The End	452
E.1	Writing Models A Fortran Example	456
E.2	Writing Models A C Example	457
E.3	Writing Models, The Parameter File	459
E.4	Writing Models Fortran Declarations	463
E.5	Writing Models Fortran Example	466
E.6	Writing Models The Parameter File	467
G.1	Example FDF File Header	473
H.1	The Posterior Probability For The Number of Outliers	476
H.2	The Data, Model and Residual Plot With Outliers	478

List of Tables

8.1	Multiplet Relative Amplitudes	165
8.2	Bayes Analyze Models	181
8.3	Bayes Analyze Short Descriptions	195

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

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

Figure 13.1: The Big Magnetization Package Interface

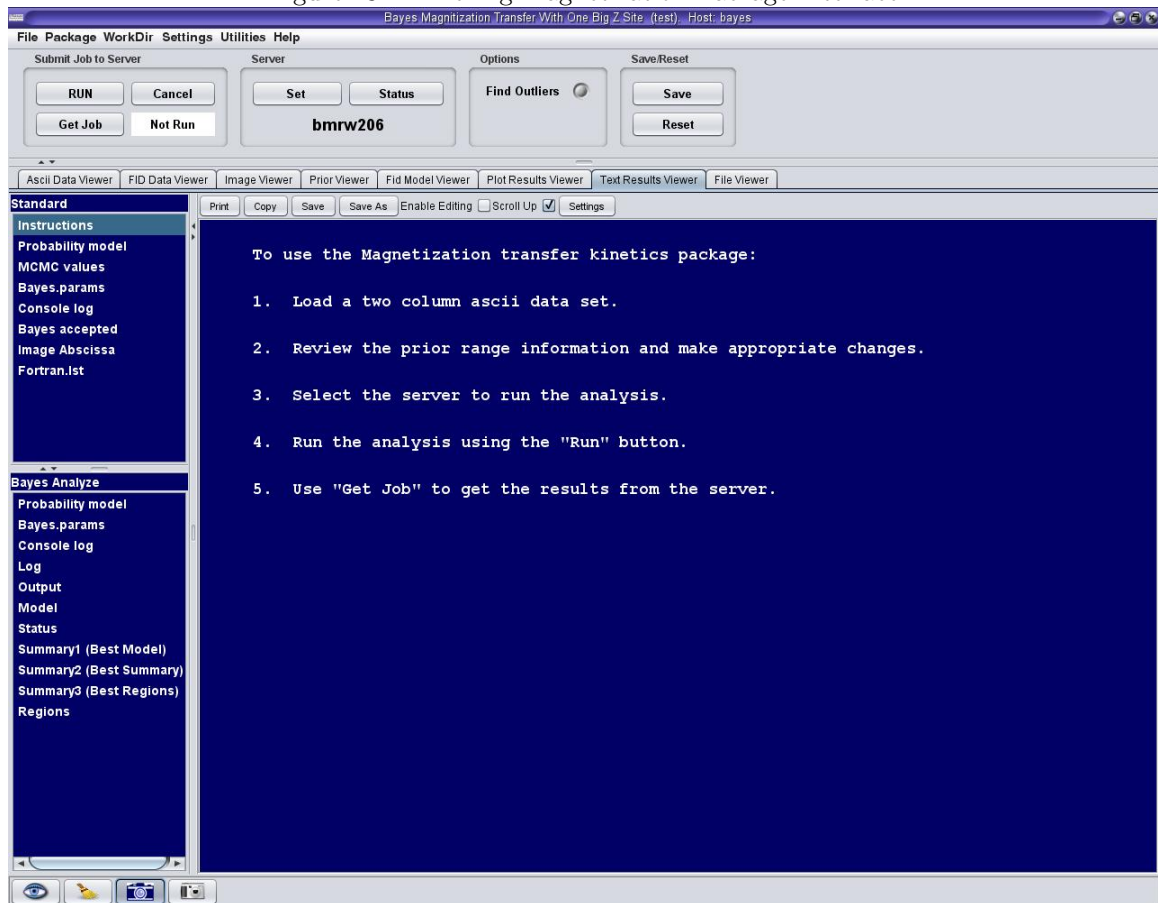


Figure 13.1: The interface to the Big Magnetization Transfer Package is shown here. The Big magnetization transfer interface allows you to analyze magnetization transfer data where one of the two sites may be considered as infinite compared to the other, see text for details.

where M_{z_0} 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

$$P(K_d|DI) = \int P(K_d M_{z_0} R_w R_d \sigma | DI) dM_{z_0} dR_w dR_d d\sigma \quad (13.2)$$

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

$$P(K_d M_{z_0} R_w R_d \sigma | DI) \propto P(K_d M_{z_0} R_w R_d \sigma | I) P(D | K_d M_{z_0} R_w R_d \sigma I) \quad (13.3)$$

where $P(K_d M_{z_0} R_w R_d \sigma | I)$ is the joint prior probability for the parameters and $P(D | K_d M_{z_0} R_w R_d \sigma I)$ is the likelihood. The joint prior probability or the parameters is factored into independent prior probabilities for each of the parameters separately

$$P(K_d M_{z_0} R_w R_d \sigma | I) = P(K_d | I) P(M_{z_0} | I) P(R_w | I) P(R_d | I) P(\sigma | I). \quad (13.4)$$

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 $P(M_{z_0} | I)$, 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, $P(D | K_d M_{z_0} R_w R_d \sigma I)$ 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_{z_0} and σ , one obtains:

$$P(K_d M_{z_0} R_w R_d \sigma | DI) \propto P(K_d | I) P(R_w | I) P(R_d | I) \left[N \overline{d^2} - \overline{h^2} \right]^{-\frac{N}{2}} \quad (13.5)$$

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

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

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

$$\overline{h^2} = \frac{T^2}{g} \quad (13.7)$$

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

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

Figure 13.2: Big Magnetization Transfer Example Fid

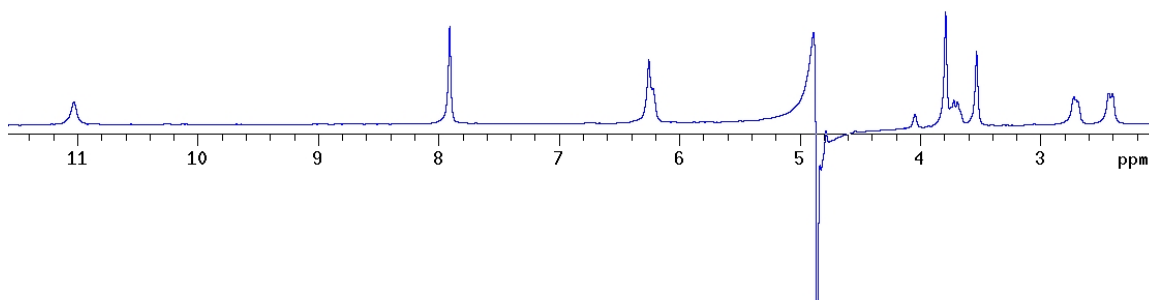


Figure 13.2: The full spectrum of the Fid data used in the big magnetization analysis. Note the water suppression artifact near 5ppm. The peak exchanging magnetization with the water is the small resonance near 11ppm.

and g is the squared length of the model:

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

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

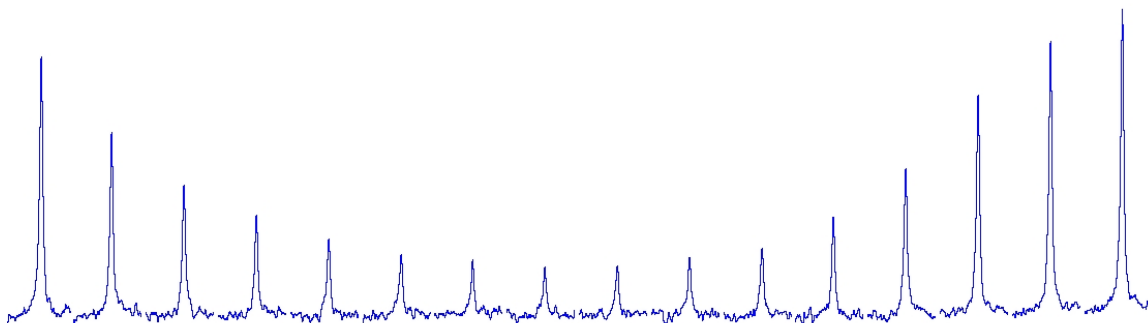


Figure 13.3: The peak exchanging magnetization begins at its equilibrium value. When the Solvent is inverted, negative magnetization flows into the Small reservoir bringing this reservoir down. At different delay times the Solvent is more fully relaxed and the Small resonance begins to recover, until 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 resonance 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

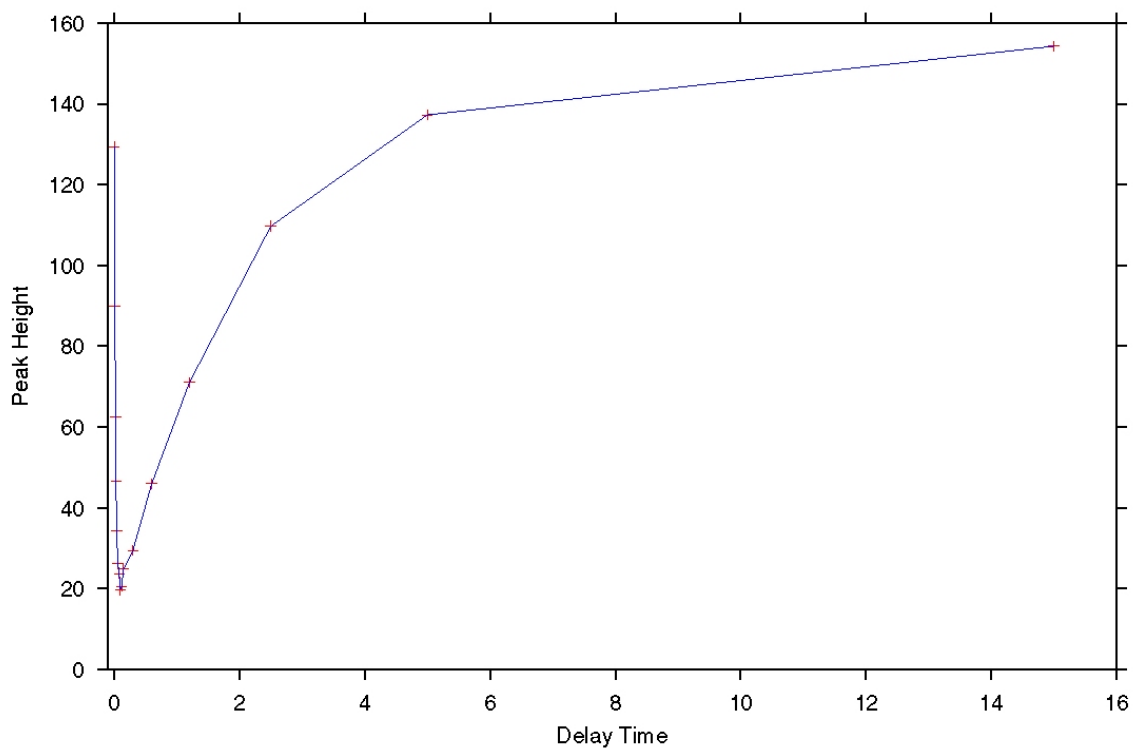


Figure 13.4: The peak heights or amplitudes (as determined by Bayes Analyze) serve as input to the Big magnetization transfer package. Here the peak heights for the spectra shown in Fig. 13.3 were used as input to the analysis. Note the Solvent magnetization starts fully relaxed, then after the Solvent 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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