

Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Chapter 15

Magnetization Transfer Kinetics

The Magnetization Transfer Kinetics Package analyzes two site magnetization exchange data as a function of temperature. To accomplish this the equations governing two site exchange are supplemented with the Eyring equation. This equation gives the exchange rate constants as a function of temperature in terms of four more fundamental quantities. These four quantities are the entropies and enthalpies of activation, ΔH_{ab} , ΔH_{ba} , ΔS_{ab} , ΔS_{ba} respectively. The primary purpose of this package is to infer these four quantities. For more on these calculations and for a better description of the thermodynamics used in this chapter see [21, 22, 26]. The interface to this package is shown in Fig. 15.1. Note this interface has four package specific widgets: a widget used to set the temperature of each sample, a widget to set the uncertainty in the temperature, a widget to load a viscosity table, and one to display the current viscosity table. To use this package you must:

Select the Magnetization Transfer Kinetic Package from the Package menu.

Load one or more three column Ascii data sets using either the “Files/Load Ascii/File” menu. Data can also be loaded by loading an Fid and selecting the two exchanging resonances using a double cursor and hitting the “Get Peak” button, or Bayes Analyze amplitude estimates can be loaded using the “Files/Load Ascii/Bayes Analyze” menu. When a data set is successfully loaded the data is plotted in the Ascii Data viewer, see Fig. 14.2 for an example of such data.

Using the “Set” entry box, enter the temperature for each set as you load it. Alternatively, you can display each data set in the Ascii File viewer and then enter a temperature for it. Note, this package will not run until a temperatures has been set for each data set.

Using the “Uncertainty” widgets set the uncertainty in the temperature measurement. It is assumed that all of the data were acquired on the same sample and that the signal-to-noise ratio is not changing as a function of temperature. Consequently, it is assumed that there is a single uncertainty and it is applied to all temperatures.

Load a viscosity table if the solvent is not water. The format of the viscosity table is shown in Fig. 15.3 and is discussed later.

Review the prior probabilities for parameters would normally go here, but the Magnetization Transfer Kinetics Package sets its priors internally. So there are no prior probabilities to review.

Figure 15.1: Magnetization Transfer Kinetics Package Interface

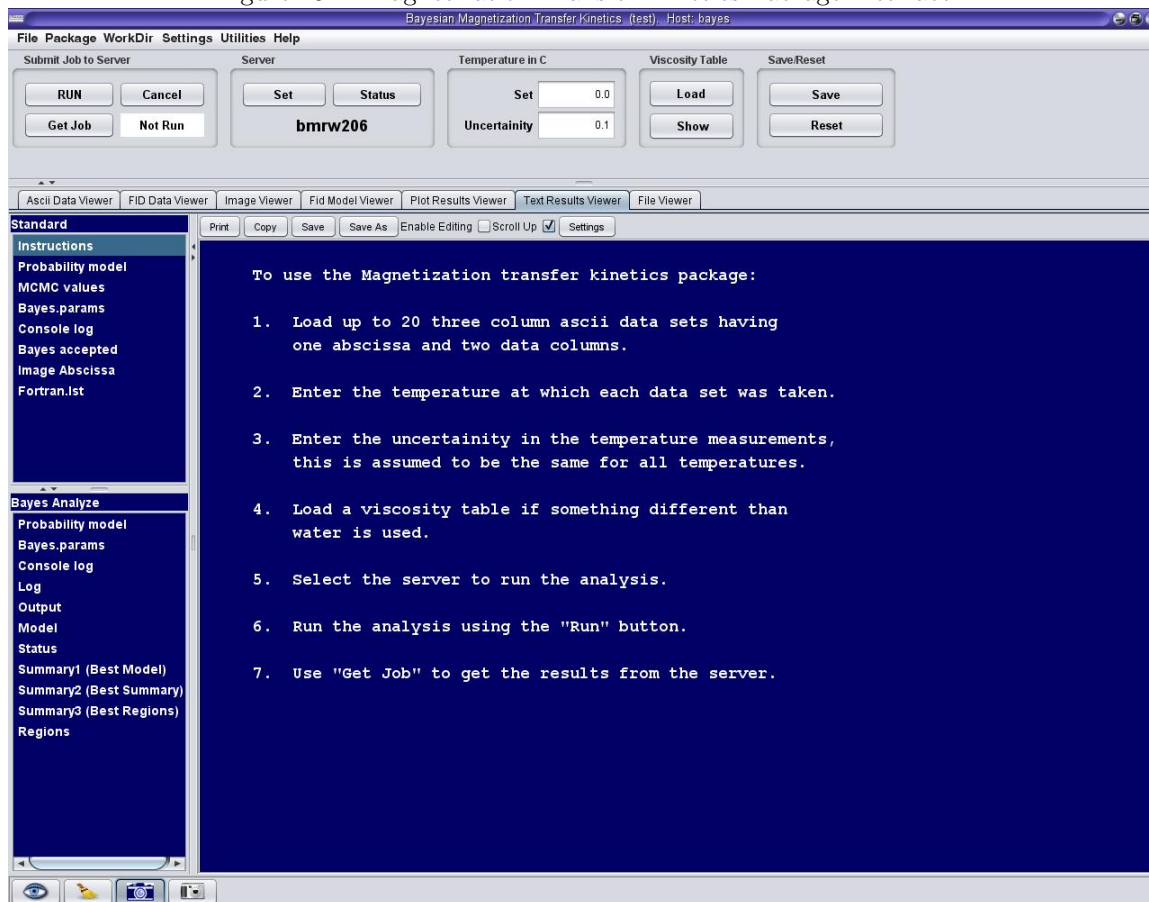


Figure 15.1: The magnetization transfer Kinetics Packages analyzes up to 20 data set having no more than 100 data values using the equations governing two site magnetization exchange with the Eyring equation to predict the exchange rates. The inferred parameters are the Entropy and Enthalpy of activation. For more on the actual calculations and the widgets see the text.

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.

15.1 The Bayesian Calculation

The Magnetization Transfer Kinetics Package analyzes problems involving magnetization transfer. The differential equations governing this exchange are the McConnell modification of the Bloch equations, Eq. (14.3,14.4). For a fixed temperature, τ_j , the “a” and “b” site magnetizations must satisfy these equations. These magnetizations, Eq. (14.5 and 14.6), are related to the data by

$$d_a(t_i, \tau_j) = M_a(t_i, \tau_j) + \text{error} \quad (15.1)$$

and

$$d_b(t_i, \tau_j) = M_b(t_i, \tau_j) + \text{error} \quad (15.2)$$

where $d_a(t_i, \tau_j)$ is the “a” site data gathered at time t_i at temperature τ_j . Similarly, $d_b(t_i, \tau_j)$ are the “b” site data. The functions, $M_a(t_i, \tau_j)$ and $M_b(t_i, \tau_j)$, are given by Eqs. (14.5 and 14.6) respectively and “error” represents the misfit between the data and the model. The functions $M_a(t_i, \tau_j)$ and $M_b(t_i, \tau_j)$ are functions of the exchange rates K_{ab} and K_{ba} as well as the relaxation rates R_{1a} and R_{1b} . The exchange rates $K_{ab}(\tau_j)$ and $K_{ba}(\tau_j)$ are calculated from the Eyring equations,

$$K_{ab}(\tau_j) = \kappa \left(\frac{k\tau_j}{\hbar} \right) \exp \left\{ \frac{\Delta S_{ab}}{R} - \frac{\Delta H_{ab}}{R\tau_j} \right\}, \quad (15.3)$$

and

$$K_{ba}(\tau_j) = \kappa \left(\frac{k\tau_j}{\hbar} \right) \exp \left\{ \frac{\Delta S_{ba}}{R} - \frac{\Delta H_{ba}}{R\tau_j} \right\} \quad (15.4)$$

respectively where κ is a transmission coefficient, here set equal to one, k is Boltzmann’s constant, \hbar is Plank’s constant and R the universal gas constant. Over the temperature range that most experiments can be performed the relaxation times, T_{1a} and T_{1b} , can be expanded as a linear function of temperature:

$$\frac{1}{R_{1a}} = T_{1a} = T_{1a\infty} + \Delta T_{1a\infty} \frac{v(\tau_j)}{\tau_j} \quad (15.5)$$

and

$$\frac{1}{R_{1b}} = T_{1b} = T_{1b\infty} + \Delta T_{1b\infty} \frac{v(\tau_j)}{\tau_j} \quad (15.6)$$

where $T_{1a\infty}$ is the relaxation time at infinite temperature, $\Delta T_{1a\infty}$ is the slope of this line, and $v(\tau_j)$ is the viscosity at temperature τ_j . Similar definitions hold for the “b” site.

These equations along with the solution to the Block-McConnell given enough structure to the problem to be able to solve this problem using Bayesian probability theory and we will do that shortly. However, before doing that we want to note one problem. The prefactor multiplying the exponential in the Eyring equations is on the order of $6 \times 10^{12} \text{ s}^{-1}$. So any attempt to modify ΔH_{ab} or ΔS_{ab} must be done carefully because a tiny change in the exponential will result in a huge change in the exchange rate, K_{ab} . Consequently, the program that implements this calculation uses a type of sum and difference variables that change both H_{ab} and S_{ab} simultaneously in a way that avoids this problem.

The parameters of interest are the entropy, and enthalpy of activation, ΔH_{ab} , ΔH_{ba} , ΔS_{ab} , ΔS_{ba} , and to a lesser degree the parameters used in the linear expansion of the relaxation time, $T_{1a\infty}$, $\Delta T_{1a\infty}$ and $T_{1b\infty}$, $\Delta T_{1b\infty}$. In addition, we have designated the true temperature as τ_j and it should be clear that these quantities are unknown parameters about which we have to make inferences. We do have a measured value, τ'_j , that is related to τ_j by

$$\tau'_j = \tau_j + \text{error} \quad (15.7)$$

where “error” represents the error in the temperature measurement. In the course of this calculation, we will eventually have to assign a prior probability for this temperature error and when we do that we will assign a Gaussian prior centered on the measurement and the Gaussian will have a standard deviation σ_{τ_j} which we will assume is known. So when the program runs it tries to vary these temperatures, consistent with what is known about the temperature uncertainty.

The Bayesian posterior probability for the entropies and enthalpies given the exchange data has much in common with the calculation presented in Chapter 14 and if you have not reviewed that material it would be advisable to do so now. In what follows we will use much of the same notation introduced in that Chapter. For example the three amplitudes of the j th inversion will be designated as M_{j1} , M_{j2} and M_{j3} . Similarly, the standard deviation of the noise prior probability used to assign the likelihood of the j th data set will be represented by σ_j . If we designate the set of interesting parameters as Θ ,

$$\Theta \equiv \{\Delta H_{ab}, \Delta H_{ba}, \Delta S_{ab}, \Delta S_{ba}, T_{1a\infty}, \Delta T_{1a\infty}, T_{1b\infty}, \Delta T_{1b\infty}, \tau_1, \dots, \tau_m\}, \quad (15.8)$$

the set of amplitudes as M , and the set of standard deviations as σ then the posterior probability for the interesting parameters given all the data D is given by

$$P(\Theta|DI) = \int P(\Theta M \sigma | DI) dM d\sigma \quad (15.9)$$

where the marginalization integrals are over all of the amplitudes and standard deviations. Applying Bayes' theorem to the right-hand side of this equation one obtains

$$P(\Theta|DI) \propto \int P(\Theta M \sigma | I) P(D | \Theta M \sigma I) dM d\sigma. \quad (15.10)$$

If we now factor the prior probability for all of the parameters as

$$P(\Theta M \sigma | I) = P(\Theta | I) \prod_{j=1}^m [P(M_{j1} | I) P(M_{j2} | I) P(M_{j3} | I) P(\sigma_j | I)] \quad (15.11)$$

where for the time being we have left the prior probability for the interesting parameters unfactored. Similarly, the probability for the data, $P(D|\Theta M\sigma I)$, may be factored into a product of likelihoods given by

$$P(D|\Theta M\sigma I) = \prod_{j=1}^m P(D_j|\Theta M_{j1}M_{j2}M_{j3}\sigma_j I) \quad (15.12)$$

where $P(D_j|\Theta M_{j1}M_{j2}M_{j3}\sigma_j I)$ is the likelihood used in Chapter 14. If we now substitute the likelihood Eq. (15.12) and the prior Eq.(15.11) into the joint posterior probability of the interesting parameters, Eq. (15.10), one obtains

$$P(\Theta|DI) \propto P(\Theta|I) \prod_{j=1}^m \left[\int P(M_{j1}|I)P(M_{j2}|I)P(M_{j3}|I)P(\sigma_j|I) \right. \\ \left. \times P(D_j|\Theta M_{j1}M_{j2}M_{j3}\sigma_j I) dM_{j1}dM_{j2}dM_{j3}d\sigma_j \right] \quad (15.13)$$

as the posterior probability for the interesting parameters. If you examine the quantity in the big square brackets, except for a little notational differences, you will discover that this calculation is exactly the same calculation that occurred when we did the Magnetization Transfer calculation in Chapter 14. The notation difference relates to the fact that in the Magnetization Transfer calculation we were trying to infer the exchange rates, while here its the entropy and enthalpy of activation that is being inferred. If we now substitute the posterior probability computed in Chapter 14 into Eq. (15.13), one obtains

$$P(\Theta|DI) \propto P(\Theta|I) \prod_{j=1}^m |g_{lk}|^{-\frac{1}{2}} \left[2N_j(\bar{d}^2)_j - (\bar{h}^2)_j \right]^{\frac{3-N_j}{2}} \quad (15.14)$$

as the posterior probability for the interesting parameters. If we now use the product rule to factor the prior probability for the interesting parameters, Eq. (15.14) becomes

$$P(\Theta|DI) \propto P(\Delta H_{ab}|I)P(\Delta H_{ba}|I)P(\Delta S_{ab}|I)P(\Delta S_{ba}|I) \\ \times P(T_{1a\infty}|I)P(T_{1b\infty}|I)P(\Delta T_{1a\infty}|I)P(\Delta T_{1b\infty}|I) \\ \times \prod_{j=1}^m P(\tau_j|\tau'_j I) |g_{lk}|^{-\frac{1}{2}} \left[2N_j(\bar{d}^2)_j - (\bar{h}^2)_j \right]^{\frac{3-N_j}{2}} \quad (15.15)$$

which is the posterior probability for the interesting parameters.

The probability for the temperature, τ_j , given the measured value of the temperature, τ'_j , will be assigned a Gaussian of the form:

$$P(\tau_j|\tau'_j I) \propto \exp \left\{ -\frac{(\tau'_j - \tau_j)^2}{2\sigma_{\tau_j}^2} \right\} \quad (15.16)$$

where the uncertainty in the temperature, σ_{τ_j} , is input from the interface.

Finally, if we assign a uniform prior probability for $P(\Delta H_{ab}|I)$, $P(\Delta H_{ba}|I)$, $P(\Delta S_{ab}|I)$, $P(\Delta S_{ba}|I)$, $P(T_{1a\infty}|I)$, $P(T_{1b\infty}|I)$, $P(\Delta T_{1a\infty}|I)$, and $P(\Delta T_{1b\infty}|I)$ the final posterior probability for the interesting parameters becomes

$$P(\Theta|DI) \propto \prod_{j=1}^m \exp \left\{ -\frac{(\tau'_j - \tau_j)^2}{2\sigma_{\tau_j}^2} \right\} |g_{lk}|^{-\frac{1}{2}} \left[2N_j(\overline{d^2})_j - (\overline{h^2})_j \right]^{\frac{3-N_j}{2}}. \quad (15.17)$$

It is this posterior probability that is implemented in the Markov chain Monte Carlo simulations.

In addition to the Θ parameters the analysis also outputs samples of a number of derived parameters. That is to say the program uses the samples of the interesting parameters to compute some other quantities of interest that can be computed from the interesting parameters, these include: K_{ab} , K_{ba} , τ , T_{1a} , T_{1b} , R_{1a} , R_{1b} ,

$$K_{eq} \equiv \frac{K_{ab}}{K_{ba}}, \quad P_a = \frac{K_{ba}}{K_{ab} + K_{ba}}, \quad P_b = \frac{K_{ab}}{K_{ab} + K_{ba}}, \quad \tau_{ab} \equiv \frac{1}{K_{ab}} \quad \text{and} \quad \tau_{ba} \equiv \frac{1}{K_{ab}}. \quad (15.18)$$

Note that each of these quantities is temperature dependent, and the outputs include a posterior probability for these parameters at each temperature.

We mentioned earlier that the large prefactor multiplying the exponential in the Eyring equation introduces substantial correlations in the values of the entropy and enthalpy. This problem is so severe, that the program that does this calculation uses a set of sum and difference variables that automatically change ΔH_{ab} , ΔH_{ba} , ΔS_{ab} , and ΔS_{ba} in a way that keeps Eqs. (15.3 and 15.4) greater than zero and finite. The real problem is that if you make a change to ΔS , either “ ab ” or “ ba ,” and do not make an appropriate change to ΔH , the exponential could change by many orders of magnitude. Indeed changing ΔS by even one and not changing ΔH could change the exchange rates 10^{10} ! The way the program prevents this is to introduce a type of sum and difference variables:

$$U_x = \frac{\Delta S_x}{R} - \frac{\Delta H_x}{RT^*} \quad (15.19)$$

and

$$V_x = \frac{\Delta S_x}{R} + \frac{\Delta H_x}{RT^*} \quad (15.20)$$

where x means either the “ ab ” or the “ ba ” sites and T^* is the average input temperature at which the various inversion recovery data sets were acquired. If you look at Eq. (15.3) you will find that U_x is just the exponent of this equation evaluated at the average temperature. Similarly, V_x is the exponent but with a plus sign, again evaluated at the average temperature. When running the analysis small changes, on the order of 0.01, can be made to U_x while changes on the order of one or two can be made to V_x . These changes translate into substantial changes in the exchange rates. However, the problem remains of how to pick a set of U_x and V_x that can be used to initialize the Markov chain Monte Carlo simulations. The program does this by generating set of enthalpies distributed random around zero with a standard deviation of 10,000:

$$\Delta S_x = \pm \sigma_{10,000}. \quad (15.21)$$

Next the program generates an entropy

$$\Delta H_x = \left[\Delta S_x + R \log \left(\frac{KT^*}{\hbar} \right) \right] T^* \pm \sigma_3 \quad (15.22)$$

where by $\pm\sigma_3$ we mean that the program add a Gaussian distributed random number of standard deviation 3 to this quantity. If you now look at Eq. (15.3) and plug in these numbers you will find that

$$K_x = \exp\{\pm\sigma_3\}. \quad (15.23)$$

So generating the entropies and enthalpies in this way allows the program to initialize the entropies and enthalpies in such a way that they cover all reasonable values of these quantities. Finally, the program computes these sum and difference variables from the generated entropies and enthalpies, and using these sum and difference variables the program can then thoroughly explore the parameter space.

15.2 Using The Package

The Text outputs files from the Magnetization Transfer Kinetics Package consist of: “Bayes.prob.model,” “BayesMtZKinetics.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 for each data set, there are probability density functions for each parameter appearing in the model, as well as probability density functions for the derived parameters mentioned earlier. Because some of the parameters are temperature dependent, the number of probability density functions can be fairly large, one the order of a hundred.

In addition to the standard plots, the Magnetization Transfer Kinetics Package outputs several additional scatter plots. These plots are thermodynamics plots and are intended to show you how uncertain you are of the thermodynamics. An example of these plots is shown in Fig. 15.2. This figure contains four panels: Panels (A) and (B) contain an Arrhenius and van’t Hoff plot. The Arrhenius plot is for the K_{ab} exchange rate. The simulations also produce an Arrhenius plot for the K_{ba} exchange rate, although we did not show it here. Panel (C) contains a plot of the Gibbs free energy for the “a” site going to the transition state, and there to the b site. Again the simulations also produces a plot of the Gibbs free energy for the b site going to the transition state and then onto the “a” site. Finally, panel (D) is a plot of the relaxation time, T_{1a} , for the “a” site. The plot for the b site is not shown.

The expansion of the relaxation times requires the viscosity of the solvent in the expansion. The program uses the viscosity of water, but allows the user to supply alternative viscosity tables. An example of the viscosity table is shown in Table 15.3. This table contains the first few lines of the viscosity table located in “/vnmr/bayes/Bayes.test.data”. The file name is “WaterViscosityTable”. The table must be uniformly sampled. The first two lines in the table are the low and high temperature covered by the table in Kelvin. The third line is the number of entries in the table, in this case 101. Finally the viscosity entries are in units of “cp”. You can change the viscosity table using the interface by activating the “Load” button under the Viscosity Table label. The maximum number of entries in this table is 501, and the minimum is 2, although using this minimum is probably not very desirable. When the package is running the viscosity is needed as a continuous parameter and to do this from a discrete table the program uses linear interpolation. Linear interpolation requires a reasonably good digitization of the viscosity table to ensure the interpolated values are accurate. In the water viscosity table there are 101 total entries, one at each degree Kelvin, and this is more

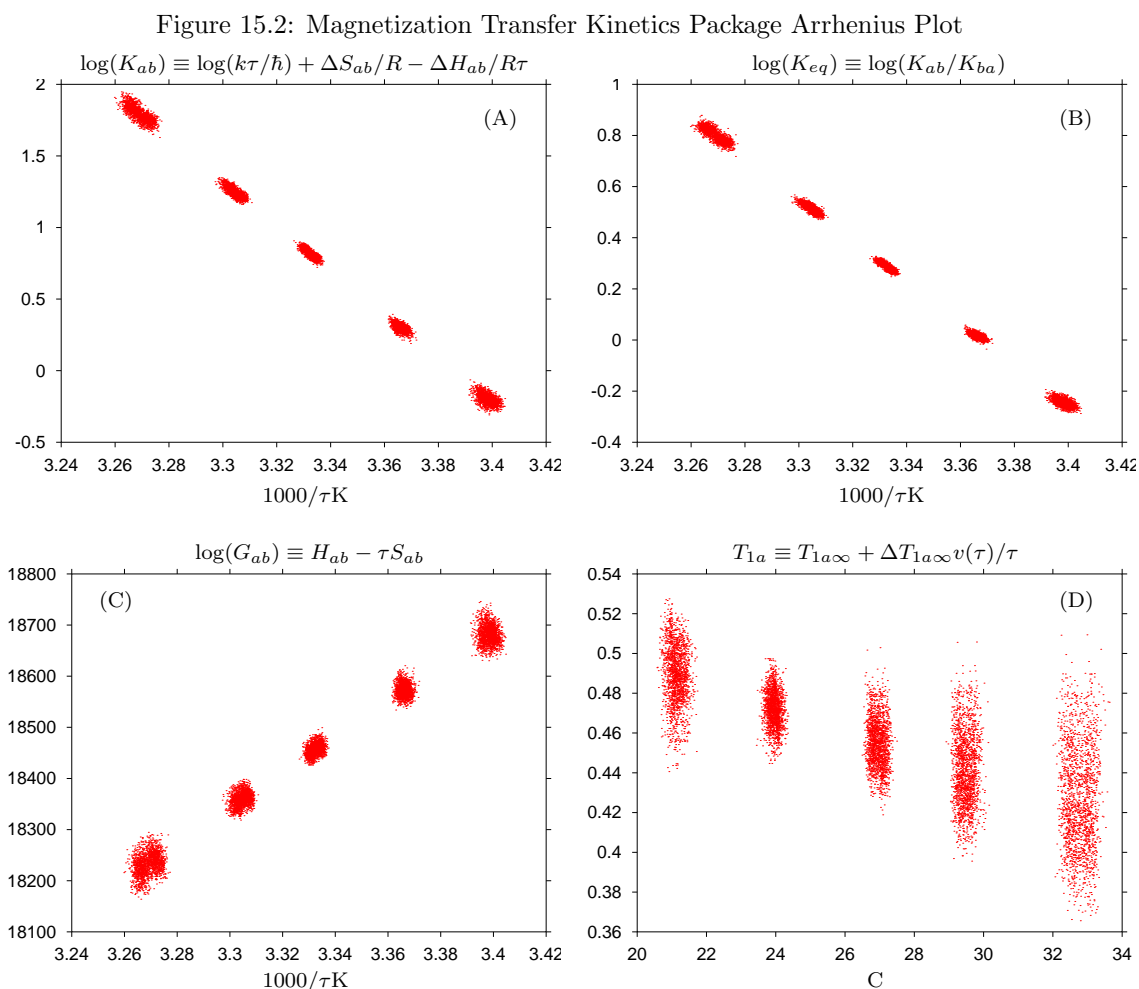


Figure 15.2: Panel (A) Arrhenius plot of the exchange rate. Panel (B) van't Hoff plot of the equilibrium constant. Panel (C) is the natural logarithm of the Gibbs free energy. Panel (D) is a plot of the T_{1a} relaxation time as a function of temperature in Centigrade. Similar, plots are made for the both sites, although we have shown only one here.

Figure 15.3: Magnetization Transfer Kinetics Water Viscosity Table

273.15	The low temperature in Kelvin
373.15	The high temperature in Kelvin
101	The number of entries in the table
1.787	Water viscosity at 273.15K
1.728	Water viscosity at 274.15K
1.671	Etc.
1.618	
1.567	
1.519	
1.472	
1.428	
1.386	
1.346	

Figure 15.3: This table contains the first few lines out of the water viscosity table used in the simulation. The table is a single column ASCII file. The comments in the above table are for explanation only. The viscosity table is strictly the first column.

than enough entries for water. I would recommend you do the same. As far as what temperature range to cover, you must cover all temperatures the program is likely to explore. For example if you data span a temperature range of 30C starting at 10C and ending at 40C and you are uncertain of the temperature to 1 degree, then you will probably need to supply viscosity's from about 5C up to 45C where I have made the assumption that the simulations are very unlikely to explore a five standard deviation temperature variation.

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