User Guide to the Aldworth-Jackson Fitting Tool version 1.0 (beta)

Introduction

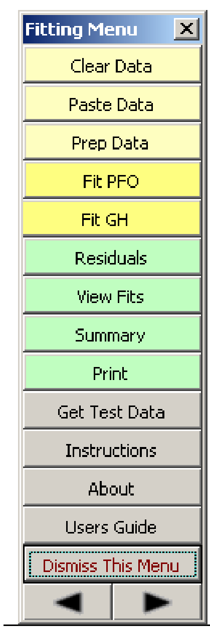
The paper published in Pesticide Management Science by Jeremy Aldworth and Scott Jackson (*Pest Manag Sci* **64**:536–543 (2008)) proposes a method to obtain more accurate estimates of dissipation times when statistically analyzing environmental fate dissipation data. This Excel based tool uses the methods illustrated in that paper and provides an easy-to-use system for analyzing such data.

The tool is designed to be mostly self-explanatory. This user guide shows the recommended work-flow, provides a little more detail on the inner-workings of the spreadsheet, and discusses briefly the analysis of the included test data.

Using the tool – the essentials.

To use the tool to analyze your data there are four straightforward steps that must be performed in order. First load the spreadsheet. Excel macros MUST be enabled (you may see a security warning depending on your settings).

STEP 1



Prepare a clean worksheet ready to receive your data. Press the '**Clear Data**' button on the Fitting Menu.

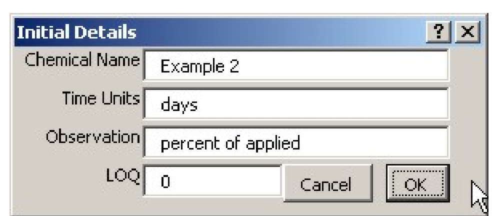
STEP 2

Find your data – either in another spreadsheet or from a plain text file. Data must be in two columns, time and value. Replicates should be on separate lines. Do not average the data prior to analysis if you have replicates.

Click the '**Paste Data**' button.

STEP 3

Prepare the data. Press the '**Prep Data**' button. This step ensures that all the calculations are ready to be performed. You may also specify treatment of zero values – enter the LOQ value (or a substitute value eg ½ LOQ) if you believe it is appropriate. Enter the name of the chemical, the time units and the residue units. Then click '**OK**'



STEP 4

Fit the two alternate models: click the '**Fit PFO**' and '**Fit GH**' buttons. If fits are achieved this is indicated in the spreadsheet.

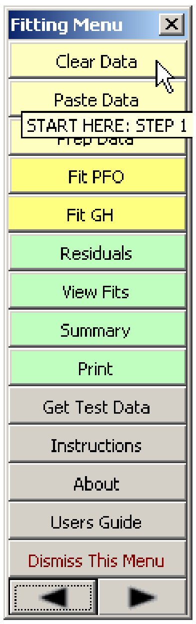
This is ALL that is absolutely required to generate fits. However you should *examine the residuals*, *view the summary*, and *look at the visual fit*. Use the green buttons to do this. Use the arrow buttons to page back and forth between the tabs. Once you are satisfied that the fits are acceptable use the '**Print**' button to generate your output as a record of the results.

An illustrated example

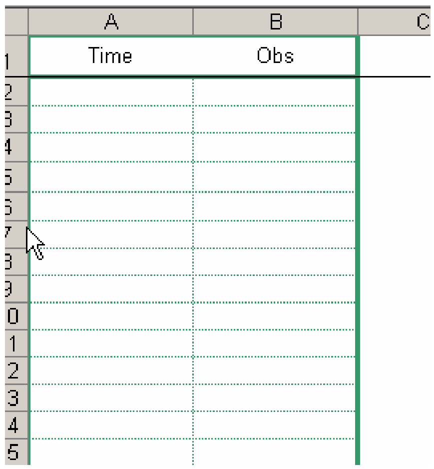
Four example data sets are included with this fitting tool to enable users to get a feel for what the tool does, and how you might interpret the results. One example (no. 2) is illustrated here.

Following the five step procedure show above this example will be worked through, with explanation.

Step 1 – clear out old data

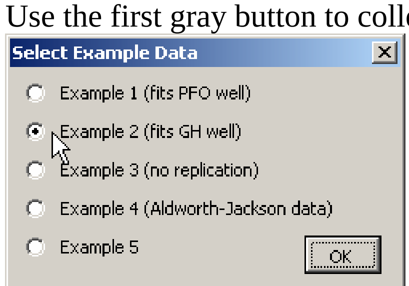


Click the clear data button on the Fitting Menu. You should see the front page like this:



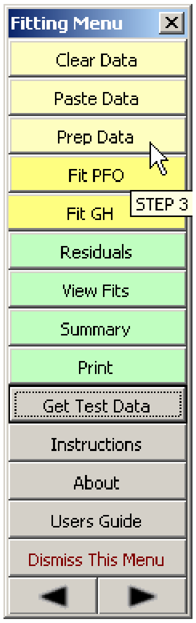
Step 2 – get some new data

Use the first gray button to collect some test data to work with. We'll use Example 2.

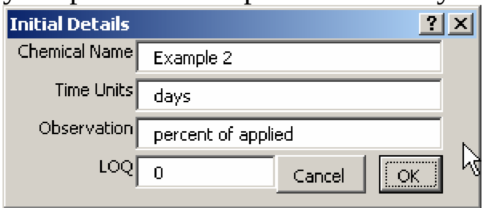


Click the second selection, then choose OK.

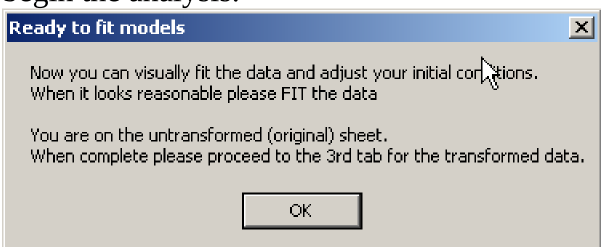
Step 3 – prepare the data for analysis



This is very straightforward – just click the third button. However this is an important step. It makes sure that the data calculation areas are clear (double checks this). It copies all the formulas into the right locations, makes sure you enter the titles and units, and if you wish treats zero values as a value you enter (eg LOQ). In general we would recommend NOT adjusting zero values to any other value for the first analysis. Once your press the 'Prep Data' button you should see the following screen:



Now click 'OK'. You should see the following notice, which indicates you are ready to begin the analysis.

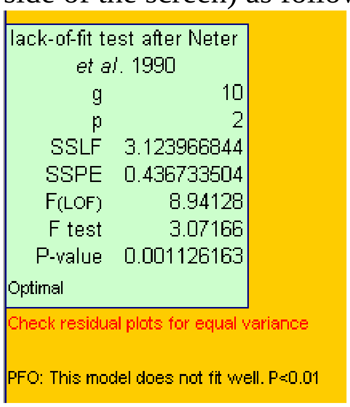


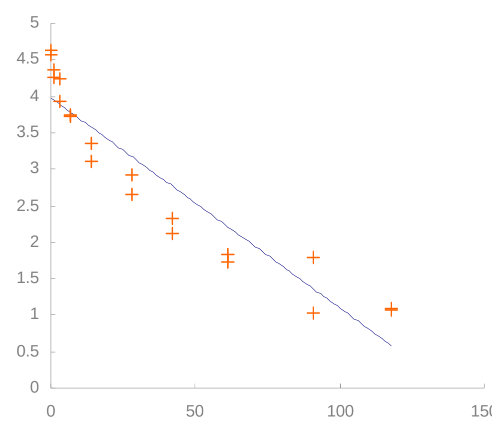
Step 4 – analyze the data

There are two models to test against the data in this fitting tool. The Pseudo-First Order model (PFO) or the Gustafson-Holden model (GH). There are also two scales (transformations) to test. One is the identity transformation (ie untransformed). The other is the log-transformation, which is typically appropriate for this type of data (declining with time towards a measurement threshold). See Aldworth and Jackson's paper for a full discussion.

Click the '**Fit PFO**' button.

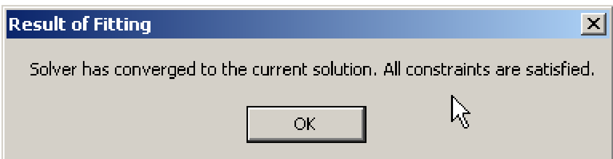
The PFO model (with this example data set) reaches an optimal solution quickly and reports (on the left side of the screen) as follows, with this clearly illustrated in the predicted vs. observed chart. Although the fitted line passes close to the observed data it is clearly not a good fit and the goodness/lack-of fit test shows this – there is significant lack of fit.



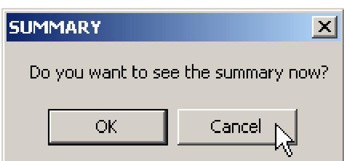


You could of course examine the residuals at this stage to see if the underlying assumption (of equal variance) has been violated but there is no need – the lack of fit is so clear that there is no (immediate) need to do so.

Let's fit the Gustafson-Holden model now. Click the '**Fit GH**' button.
This model doesn't immediately give an optimal fit (some models don't, it depends on the data). However it does converge to a solution and satisfies the constraints placed on the fit. This quite often occurs. If you wish to see whether a better fit can be obtained feel free to try the fit again – sometimes once the initial values have been updated with the first (converged) fit an optimal fit can be obtained. It's worth a try. You will initially see this notice:



And once you click 'OK' you'll be offered a chance to go directly to the summary. For now let's stay here and see if we can obtain a better fit – click cancel on this notice:



Try clicking the '**Fit GH**' button again. You'll see that in this case the solution remains converged (it doesn't indicate 'optimal'). However this is quite often the case, and tells you that you have the best fit that can be obtained with this tool. In fact on the face of it the fit is very good indeed, as indicated by the goodness/lack-of-fit test and by your own visual observation of the predicted and observed results.

First look at the model fits side by side (the GOF tests):

lack-of-fit test after Neter *et al*. 1990	
g	10
p	2
SSLF	3.123966844
SSPE	0.436733504
F(LOF)	8.94128
F test	3.07166
P-value	0.001126163
Optimal	

Check residual plots for equal variance

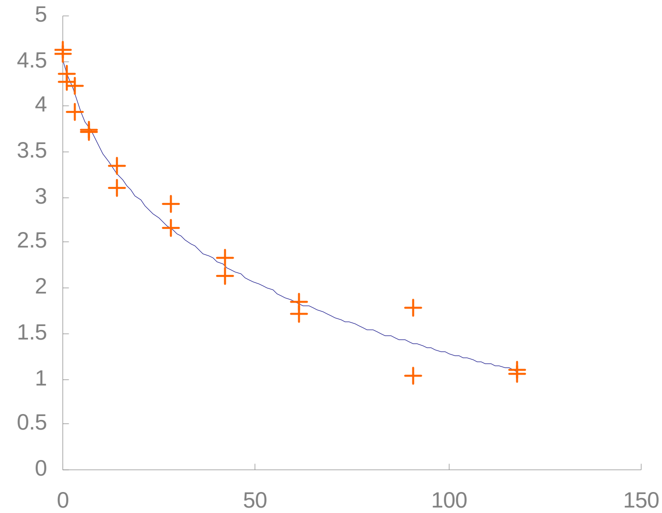
lack-of-fit test after Neter *et al*. 1990	
g	10
p	3
SSLF	0.072989781
SSPE	0.436733504
F(LOF)	0.23875
F test	3.13546
P-value	0.964995608
Optimal	

Check residual plots for equal variance

PFO: This model does not fit well. P<0.01
GH: This model fits acceptably. But check assumptions and residuals.

There is strong evidence from the lack-of-fit test that the GH model fits well : the P-value is nowhere near the threshold of 0.01, the F value due to lack-of-fit (F_{LOF}, 0.239) is very small – much less than the threshold F-test value (3.135) and to summarize this a text message is given to clarify the meaning of these numbers: "This model fits acceptably. But check assumptions and residuals". As always with fitting a statistical model you must check whether your underlying assumptions have been adhered to, or violated. So this direction is emphasized here.

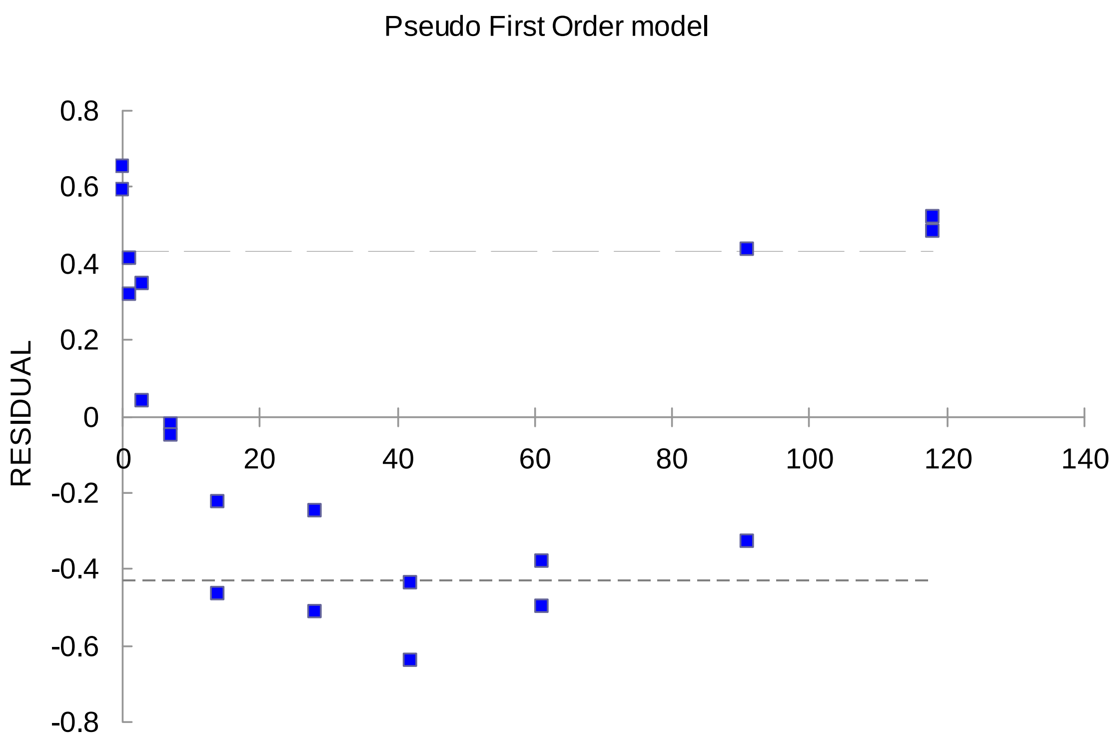
Also it is very clear from the predicted vs. observed chart that this model does indeed fit the data very well. It looks like this model will be the model of choice for estimating DT50 and DT90 values.



But before we jump ahead and just accept this model let's examine whether our assumptions hold, especially that of equal variance.

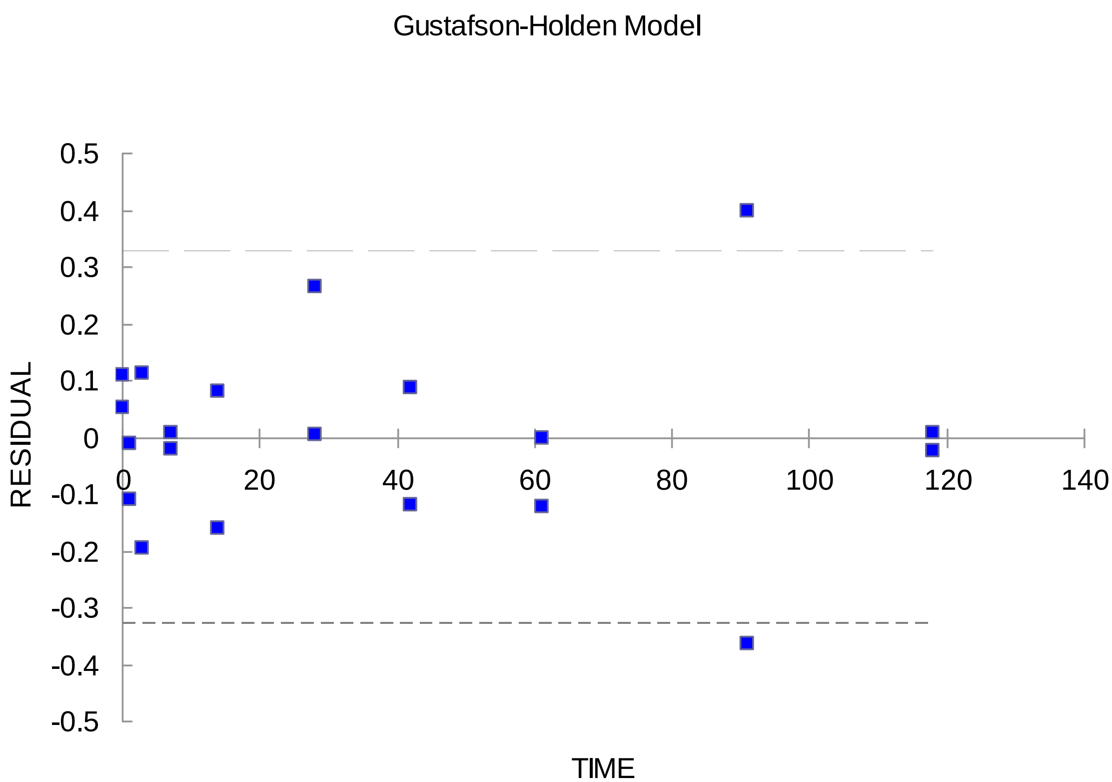
Using the Fitter Menu let's go to see what the residuals look like. Click the 'Residuals' button.

This will take you to the 'Residuals – Transformed' tab of the fitting tool workbook. Here let's first examine the residuals of the PFO model:



These clearly violate the assumptions of the model – that the variances are balanced and of approximately equal magnitude at the different measurement points. Here it is obvious that there is systematic error (mode under predicting to start with, then over predicting, then under predicting again), and that the variances are not balanced. Based on an examination of these residuals you should reject this model as unsuitable *even if the GOF test indicated it was 'acceptable'*.

The GH model (shown on the same page) does however show a much better distribution of residuals and gives good confirmation that this model is definitely acceptable.



There are only two points lying outside the two standard deviation lines (dotted, positive and negative), the variance is even across the measurement range and there are no systematic errors.

You can feel confident that the GH model fit to the example 2 data is definitely the best model (of the two tested). It will give good estimates of the DT values you may need. The summary shows the differences in the estimates very clearly: the PFO model over-estimates the DT50 and DT90 values because it does not fit the data well.

Estimates	PFO	GH
DT50	24.1	6.0
DT75	48.1	16.6
DT90	79.9	43.2
Confidence Limits		
$DT90_{LCL}$	–	33.3
$DT90_{UCL}$	–	53.1

An Extra Consideration

One additional step of the analysis you may wish to consider is indicated on the summary tab. It's whether or not you have *too much* data to obtain good estimates of the DT90 or DT50. If, after the GH model fits well, the last data point is at a time that is more than twice the upper 95% confidence limit of the DT90 this is an indication that the estimates of DT90 (and DT50) *may* be influenced by data much beyond that upper bound. This may or may not affect the results, and this will be a judgment you have to make in each case. However, if such a situation occurs the summary tab will give you that suggestion.

Confidence Limits				
$DT90_{LCL}$	–	33.3	–	–
$DT90_{UCL}$	–	53.1	–	–
Comment	Based on the GH transformed fit consider truncating your data and refitting because your data goes on beyond twice the DT90 upper 95% confidence limit			
	Number of data points beyond DT90UCL		6	
	Percent of data points beyond DT90UCL		30%	
	Percent of experimental time-course beyond DT90UCL		55%	

In this case twice the $DT90_{UCL}$ is at 86 days. The data extends to 118 days. There are two measurement times beyond 88 days – at 91 and 118 days. Visual examination of the model fit shows that in the region of the DT90 estimate (43 days) there is no indication that the model either over or under-estimates the measured values. Thus in this case there is probably no improvement in the model to be had by truncating the data after 86 days and refitting. However other data will differ and this option should be considered. In particular if you wish to examine the effect of data truncation on the estimates example data set no. 4 is a good one to do this with. That's the data used in the original Aldworth & Jackson paper – please see that paper for a full discussion of these points.

User Guide version 1.0 (April 11th, 2008)
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The Aldworth-Jackson Fitting Tool (Implementation in Excel)
Author : Adrian Wadley, Stone Environmental Inc, San Francisco, CA

Acknowledgments
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