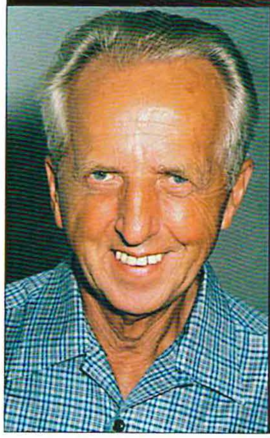

Computer-Based Saturation Curve Analysis

by Dr. David Kirk, Coventry University, U.K.

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INTRODUCTION

Computer-based curve-fitting procedures are now almost universally available. They offer several advantages over manual procedures. Apart from greater speed of execution, they are objective – rather than subjective – so that a given, fixed, procedure will always yield the same values from the same set of data. This paper examines and explains the several stages that are involved in establishing and applying an appropriate procedure. These stages have been incorporated into an Excel program that is available as an example of the principles involved.

The several stages that are involved in acceptable computer-based saturation curve analysis can be expressed as: **Curve Selection**, **Curve Fitting** and **Parameter Analysis**.

A table containing ten sets of Almen arc height versus peening time data is included (Table 1). These data sets, representing a wide range of practical peening conditions, are being promoted by the SAE as a 'test for acceptability' for saturation curve-fitting programs. Each 'target value' in Table 1 represents the average of calculations made by several different organisations.

Table 1
Data Sets for Curve-Fitting Acceptability.

Data Set	Arc height data							Target Saturation Time**	Target Intensity*
1	Minutes	4	6	8	12			4.8	
	Inch A	0.0060	0.0069	0.0070	0.0070				0.0064
2	Minutes	2.5	5	10	20			6.5	
	Inch A	0.0030	0.0036	0.0044	0.0044				0.0040
3	Cycles	3	6	12	24			5.65	
	Inch N	0.0065	0.0081	0.0088	0.0090				0.0080
4	Cycles	1	2	3	4			1.87	
	Inch A	0.0036	0.0051	0.0052	0.0053				0.0048
5	Minutes	4	6	8	12			4.82	
	Inch A	0.0062	0.0070	0.0072	0.0072				0.0066
6	Minutes	1.13	2.25	4.5	9			4.12	
	Inch N	0.0046	0.0087	0.0101	0.0107				0.0098
7	Minutes	2	3	4	6			2.8	
	Inch N	0.0055	0.0066	0.0067	0.0068				0.0063
8	K/Feed	0.25	0.5	0.75	1	2	4	0.43	
	Inch A	0.0081	0.0096	0.0100	0.0103	0.0108	0.0113		0.0093
9	K/Feed	0.25	0.5	0.75	1	2	4	0.66	
	Inch A	0.0108	0.0129	0.0137	0.0144	0.0157	0.0164		0.0137
10	K/Feed	0.25	0.5	0.75	1	2	4	0.47	
	Inch A	0.0045	0.0054	0.0059	0.0058	0.0062	0.0064		0.0054

*Acceptability requirement ±0.0005-inch, **Acceptability suggestion ±20%

CURVE SELECTION

This is the most important stage of curve analysis. We have to decide which is the 'best curve' for the problem in hand. Curve fitting itself, using a computer, is simple – anyone can do it in less than 10 minutes with no prior experience! Open Excel®, click Tools, then Add-ins and tick the boxes marked "Analysis ToolPak" and "Solver". Entering the Data Set No.1 values from Table 1 into an Excel spreadsheet, highlighting the data, clicking 'Chart', selecting XY (scatter), 'Finish', clicking 'Chart' again and selecting 'Add Trendline', immediately gives access to curve fitting equations. Excel offers six different types of equations that can then be used for curve fitting. The 'default' equation is 'Linear' (already highlighted) so that clicking 'OK' immediately gives us a straight line fitted to Data Set No.1. If we had wanted to know the equation of that straight line we could have clicked the 'Options' button *before* clicking 'OK' and ticked the 'Display equation' box. On clicking'OK' we now get the equation displayed on the (printable) graph. Alternatively we could have selected any one of the five other options (Logarithmic, Polynomial, Power, Exponential and Moving Average) and the corresponding curve will be fitted.

The major problem is to decide what type of equation *should* be fitted. To illustrate the problem, consider two curve-fitting choices for Data Set No.1, 'Linear' and 'Polynomial', presented in fig.1. The 'Number' for the Polynomial in Excel was increased from its default value of 2 to become 3 – a cubic equation. Neither of the two choices of fig.1 is appropriate, even though the cubic equation is a 'perfect' fit! To get to a *good* choice we have to consider the relationship between the variables that the data points represent. We know, from experience, that peening tends to affect Almen arc height in a way that resembles an exponential type of behaviour. As shot peeners we also know that there is another data point that is not included in any of the Data Sets of Table 1. That is 0, 0 – representing the fact that if we have peened for zero time we will have zero *added* curvature (the as-supplied strips might be slightly curved but we will have corrected for that). A good choice of equation will, therefore, be one that passes through the origin (0,0) and has a familiar 'exponential-type' shape. *Continued on page 18*

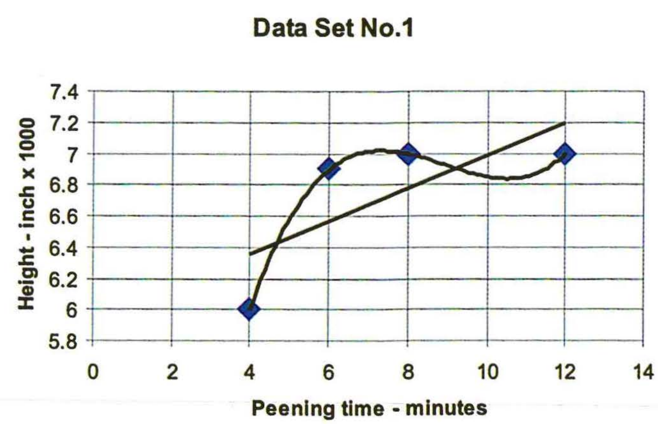

Fig.1 Linear and Cubic equations fitted to Data Set No.1.

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The author has previously proposed that the actual shape of Almen saturation curves can be expressed using any of the three following equations:

$$\mathbf{h = a(1 - exp(-b*t)} \quad (1)$$
$$\mathbf{h = a(1 - exp(-b*t^c)} \quad (2)$$
$$\mathbf{h = a(1 - exp(-b*t^c) + d*t} \quad (3)$$

where **h** is arc height, **t** is peening time and **a**, **b**, **c** and **d** are parameters.

Equations (1) to (3) are progressively more exact in terms of expressing 'true shape' and all three must pass through the point 0, 0 (h equals zero when t is zero). Each equation requires at least one more data point than there are parameters – if we are to avoid distorting a curve by forcing it to pass through every point. With only four data points, as in Data Sets Nos.1-7 for example, equation (1) would be suitable but equations (2) and (3) would be subject to distortion. On the other hand, for the three six-point Data Sets (8, 9 and 10) of Table 1 any of the three equations *could* be used. Turning to Data Set No.2 and modifying it to include the extra point 0, 0 we can now try to select an appropriate equation. Fig.2 shows the effect of applying equation (1). This curve is much more appropriate than either of those shown in fig.1. Having selected an equation that appears to be appropriate, we now have the mechanical problem of actual curve fitting.

CURVE FITTING

Curve fitting is the determination of the parameters of an equation that accurately describes the relation between the variables that the data points represent. The parameters are determined by minimising the differences between a set of data points and the equation that has been chosen to represent those data points. According to the 'Theory of Least Squares' the "best" curve is one that minimises the sum of the squares of these differences.

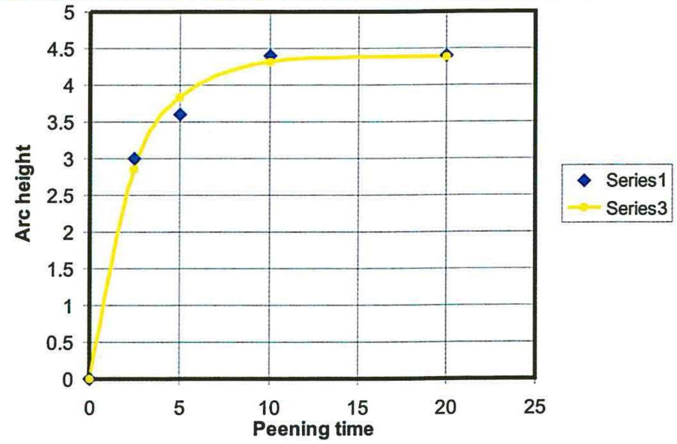

Fig.2 Equation (1) fitted to Data Set No.2.

A facile solution to the problem of curve fitting would be to purchase a dedicated curve-fitting computer program and use it to apply an equation of one's choice. That is acceptable for those who are experienced in curve fitting. The drawback is that such programs assume both expertise and understanding on the part of the user. An alternative for those who wish to develop an understanding of curve fitting – and/or save money – is to utilise the facilities available in Excel. The subsequent sections are dedicated to the latter alternative.

Table 2
Data set and differences between measured arc heights and equation (1) predictions.

Strip No.	Peening time	Arc height	Predicted arc height	Residuals	Residuals squared
1	2	5	6.3212	1.321	1.74558
2	4	8	8.6466	0.647	0.41815
3	8	9	9.8168	0.817	0.66723
4	16	10	9.9966	-0.003	0.00001
					Total = 2.83098

One problem with Excel is that the 'Add Trendline' function does not incorporate any suitable equation for our Almen saturation curves. This problem is easily overcome by using the 'Solver' function (fig.2 was produced using that function). At the heart of curve fitting is the need to minimise the differences between our data points and those predicted by the equation that we have chosen. Let us first assume that equation (1) has been chosen as being appropriate. Secondly, consider, as an example, the Almen arc height data shown in Table 2. Column 1 shows the strip number, column 2 the peening time and column 3 the corresponding arc heights (the arc heights have been deliberately 'rounded' to whole numbers equivalent to 'thousandths of an inch').

The next step is to produce arc heights that would be predicted by equation (1). We must first substitute some real values for **a** and **b** into that equation **(h = a(1–exp(-b*t))**. Let us substitute: a=10 and b=0.5 to give:

$$\mathbf{h = 10(1-exp(-0.5*t))} \qquad (4)$$

as the equation that we fit to the data points. The values obtained by substituting the four *peening time values* into equation (4) are given as 'Predicted Arc Heights' in column 4 of Table 2 (we could have obtained these predicted values by using either a calculator or Excel). The differences between the Predicted Arc Height and the corresponding measured Arc Height are termed "Residuals" in Table 1, column 5. These 'residuals' have then been squared and totalled in the last column. The data set values, equation **h = 10(1-exp(-0.5*t))** and the predicted arc heights are plotted in fig.3. The data points are 'Series 1' and the predicted arc height values and the curve are presented as 'Series 3'. We see from fig.3 that the equation that we have used has a reasonable shape but is *not a particularly good fit*. The "best fit" is the one for which the 'total of residuals squared' is a minimum. With our 'first guess' at the values for **a** and **b** of **10** and **0.5**, the total of residuals squared is **2.83098**. Our problem is to get that total down to a minimum (which cannot be zero unless all of our data points lie *exactly* on the equation curve).

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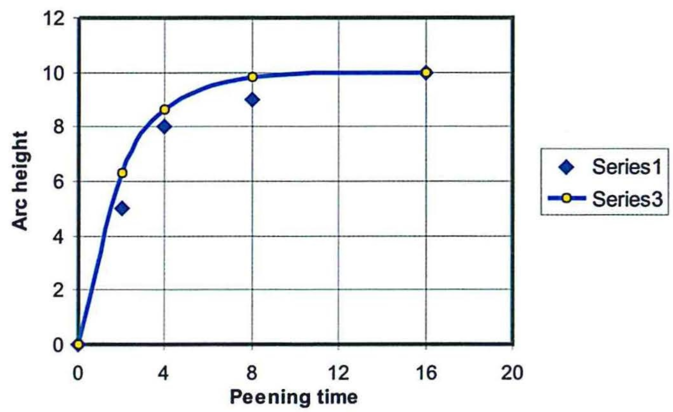

*Fig.3 Data set from Table 2, Predicted Arc Heights and equation h = 10(1-exp(-0.5*t)).*

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There are two ways in which the total of residuals can be minimised. The first way is to use an **iterative approach** (computers use that approach a great deal). Iterative solutions are based on "try, try, try again" until the minimum value is obtained. Computers are essentially stupid (but can be taught to perform very clever tricks). Consider, as an example, finding the answer to the question "What was the population of the USA according to the 1990 census?" Assume that we are sitting opposite someone who knows the exact answer and will only give yes or no answers. We could start by asking "Is it greater than 1?" Having been told, "Yes", we could then ask "Is it greater than 2?" This could go on for years until eventually we got a "No". A more intelligent iterative approach would be to start with 200,000,000, followed by 300,000,000, then 250,000,000, 225,000,000, 240,000,000 and so on until we converged on the correct answer (248,709,873), in a matter of minutes. Computers can 'ask questions' at a phenomenal speed - which means that they can usually converge very quickly onto the required answer to any mathematical question.

Returning to the problem of minimising the total of residuals squared, we usually solve our problem by getting the computer to use an iterative approach to obtaining the 'best' values for our **a** and **b** parameters. The computer will have a built-in mechanism to stop it from trying to perform more than a set number of iterative attempts. That is why we must help it by giving it reasonably-close start values. The second way of minimising residuals is to use what are called "normal equations". Many generations ago, mathematicians derived normal equations because they speeded up curve-fitting enormously. Each type of equation has a corresponding set of 'normal equations'. *If* these are built into the computer program being used then we do not need start values. A very small number of calculations are required – by comparison with the iterative approach.

We can use the 'Solver' function to provide a solution based on iterative calculations. That solution, for the data in Table 2, is that **a = 9.86** and **b = 0.37** with the total of residuals squared now being reduced to **0.31946** (from the **2.83098** given previously using 'first guesses' for a and b of 10 and 0.5). Fig.4 shows this 'best-fitting' equation: h = 9.86(1-exp (-0.37*t)), which is an obvious improvement on that given in fig.3. Again "Series 1" is the data points and "Series 3" is the fitted curve and the points on that curve at exactly the same peening time values. We now have both a'good curve' (but not necessarily the best curve) and a 'good fit'.

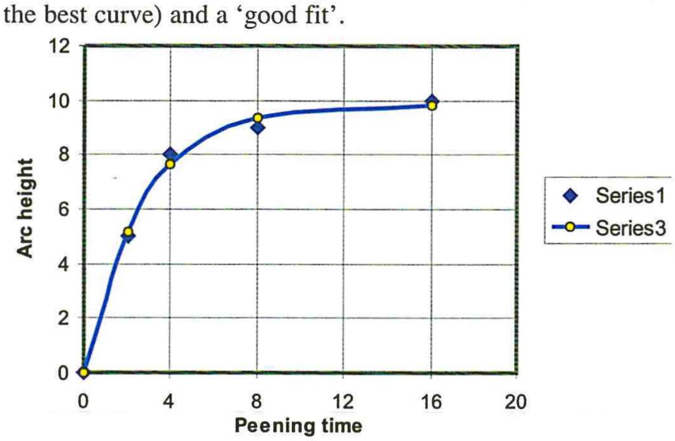

Fig. 4 'Best-fitting' two-parameter equation (1) fitted to Table 2 data.

PARAMETER ANALYSIS

The final objective, having obtained the parameters of a suitable 'best-fitted' equation, is to determine the required values for Almen Intensity and the corresponding peening time. We know that we have to determine the coordinates of a point for which, when the time coordinate T, is doubled, will lead to a 10% increase in the arc height coordinate. This requirement is illustrated by fig. 5.

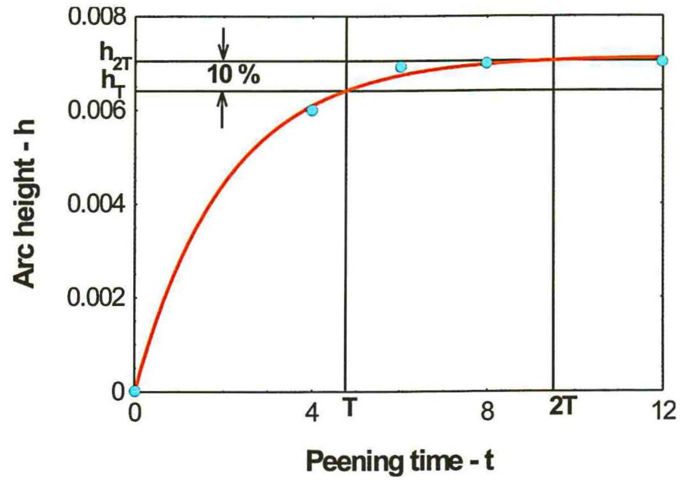

Fig. 5 10% increase criterion applied to Data Set No. 1.

The '10% increase' criterion is expressed mathematically, for equation (1), by:

$$\mathbf{f(t) = 1{\cdot}1a(1\text{-}exp(\text{-}b^*t)) - a(1\text{-}exp(\text{-}b^*2t))} \qquad (5)$$

We need to find the value of t that will make **f(t)** a minimum. Again we could use the 'Solver' function in Excel. There is, however, a simpler solution. The following 'proof' for equation (5) is presented because the statements derived are useful in our context and because the author cannot resist presenting the only time that he has found a practical use for the factorisation principles drummed into him at school! We have that h_{2T}/h_T = 1·1 so that a(1-exp(-b*2T))/(a(1-exp(-b*T)) = 1·1 giving that:

$$\mathbf{exp(\text{-}b^*2T)\text{-}1{\cdot}1exp(\text{-}b^*T) + 0{\cdot}1 = 0} \qquad (6)$$

If we let x = exp(-b*T) we can write equation (6) as: $x^2 - 1{\cdot}1x + 0{\cdot}1 = 0$ which factorises to: $(x - 1){\cdot}(x - 0{\cdot}1) = 0$ giving the solutions that x can be either 1 or 0·1. The solutions to equation (6) are therefore that exp(-b*T) = 1 or 0·1. Taking natural logarithms we have that –b*T equals either ln(1) or ln(0·1), so that T equals either – ln(1)/b or – ln(0·1)/b. The first solution corresponds to the origin (0,0) - because ln (1) = 0 so that T = 0. Therefore the 'real' solution is that:

$$\mathbf{T = \text{-}ln\ (0{\cdot}1)/b\ or\ T = 2{\cdot}303/b} \qquad (7)$$

If we now substitute T = -ln (0.1)/b for t in equation (1) we get that:

$$\mathbf{h_T = 0{\cdot}9a} \qquad (8)$$

Hence, for the example given in fig.4 where a = 9.86 and b = 0.37, the critical arc height is 8.87 at a peening time of 6.22. Equations (7) and (8) are the required 'parameter solutions' for equation (1) curve-fits.

In the case of the three-parameter and four-parameter equations (2) and (3) we must minimise the f(t) of equation (5) iteratively to give T and then substitute into the corresponding equation to yield hT.

EXCEL SOLVER PROGRAM

The principles described in the preceding sections have been encapsulated into an Excel program, "Almen Solver", that is available (free) from either the author (shotpeener@btinternet.com) or the Shot Peener web site (www.shotpeener.com). Detailed instructions are included that should enable every (computer literate) shot peener to use the program. By using the program, the effects of using the Solver function to minimise the residuals and display fitted curves can be visualised directly. The program meets the requirements included in Table 1 for all 10 data sets.

DISCUSSION

There are clear advantages attached to the use of computer-based saturation curve analysis. Sets of Almen height/peening data should in any case be stored in an accessible format – such as Excel or Access worksheets. They can then be readily analysed by pasting into an 'Almen Solver' program. The corresponding analyses can subsequently be checked, stored and used for quality assurance and other procedures. A paramount advantage of computer-based saturation curve analysis is that it is objective. The required saturation height and peening time values are therefore independent of the drawing skill and mood of an operator. It is important, however, to remember that all curve analysis procedures are dependent on the accuracy of the original data. There is an old saying that "You cannot make a silk purse out of a pig's ear."

In introducing computer-based saturation curve analysis it is important to regularise the three basic elements of the analysis - **Curve Selection**, **Curve Fitting** and **Parameter Analysis**. All three elements can be pre-defined by individual organisations so that the only input requirements for an operator are those of entering/pasting data and pressing a defined series of 'buttons'. Any pre-defined procedure can be tested for accuracy against the 'round robin' data sets reproduced as Table 1.

The number of data points in each set restricts the choice of curve equation that is appropriate. With only four Almen height/peening time values in a set, a two-parameter equation should be used. An alternative to equation (1) is to use $h = a*t/(t + b)$. That is a "saturation growth-rate" type of equation and is enshrined in the French specification NF L 06-832 (December 1998). Having fitted that equation the corresponding required parameters are that $T = 9b/2$ and $h_T = 9a/11$. A problem with two-parameter equations is that they do not yield very accurate representations of the 'true shape' of an Almen saturation curve. Their accuracy is, however, generally acceptable. Three- or four-parameter equations are required for very accurate representations of the true shape of Almen saturation curves. Such equations are not, however, appropriate for data sets with only four values. They 'skew' badly with some data sets. An approach to high shape accuracy for data sets with only four values is, however, possible. It can be achieved by using the average of two different two-parameter equations! Fig.6 illustrates an approach that can be used. The values of the two parameters are different for the two equations so that c and d have been shown (instead of a and b) for the 'French specification' curve. Each two-parameter equation 'skews' slightly in opposite directions from the true shape data points, so that a simple average corrects to give a very accurate shape.

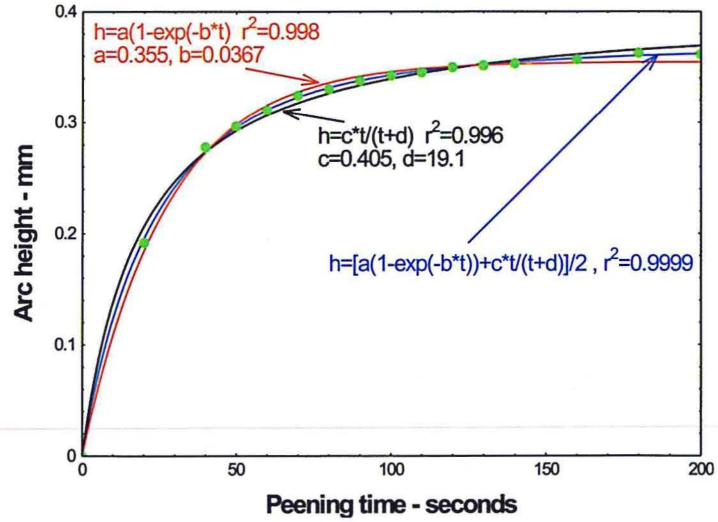

Fig. 6 Combination of two two-parameter equations.

With five Almen strip values a three-parameter and with six values a four-parameter equation are more appropriate fitting equations (than simple two-parameter equations). If only one equation has to be applied to all sets of data then a two-parameter equation is the best choice.

In conclusion it can be argued that computer-based saturation curve analysis should be mandatory, given the ready availability of appropriate procedures.