Using the Microsoft Excel 'Solver' Tool to Perform Non-Linear Curve Fitting, Using a Range of Non-Newtonian Flow Curves as Examples.

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Abstract:
The Microsoft Excel 'Solver' tool is a very simple but powerful procedure, even in the hands of the mathematically disadvantaged. It has very good application for quickly fitting experimental flow-curve data to non-Newtonian flow models with any number of parameters, and can cope with data from a number of sources. Examples are given for a range of industrially important examples ranging from standard non-Newtonian liquids, through detergent solutions to gels, pastes, and filled polymer melts, often measured on different viscometers.

Zusammenfassung:
Das Microsoft Excel Makro 'Solver' ist eine sehr einfache aber auch effiziente Berechnungsmethode, um experimentelle Daten von Fliesskurven an nicht-Newtonsche Fliessmodelle mit beliebiger Anzahl von Parametern zu fitten. Desweiteren kann das Makro auch Daten verschiedener Rheometersoftware einheitlich bearbeiten. Aus einem Bereich industriell wichtiger Anwendungen werden hierzu Beispiele gegeben, wie von nicht-Newtonschen Standardfluiden, über Waschmittellösungen bis zu Gelen, Pasten, sowie gefüllten Polymerschmelzen, welche oft mittels verschiedenen Viskosimetern gemessen werden.

Resumée:
L'outil Microsoft Excel "Solver" est une procédure très simple mais aussi très puissante, même pour les personnes désavantagées en mathématiques. Il présente de très bonnes solutions pour l'ajustement rapide de données expérimentales, telles que des courbes d'écoulement, avec des modèles d'écoulement non-Newtonien possèdant un nombre de paramètres quelconque. Il peut venir à bout d'un ensemble de données provenant de différentes sources.Une gamme d'exemples industriellement importants est présentée. Ces exemples vont des liquides non-Newtonien standards, jusqu'aux gels, pâtes et fondus de polymères chargés, en passant par les solutions de détergent, tous souvent mesurés avec différents viscosimètres.

1 INTRODUCTION

There are good reasons why one should want to fit experimental data to empirical mathematical expressions. Not only will such an exercise provide the most economical way of describing any particular physical behaviour, it also - in the case of rheology - gives us the possibility of predicting how a particular liquid will behave in new and more complex situations. A simple example would be the description of the flow curve of a non-Newtonian liquid measured in a simple cone-and-plate geometry, and then the prediction - using appropriate mathematical formulae - of its flow in pipes, in draining etc. We could go even further, and use the same mathematical expression as an input into a computational fluid dynamics (CFD) program to describe flow in even more complex situations such as mixers, pipe bends, etc. Also, in some situations, curve-fitting yields parameters that can be compared to theoretical models that can provide some kind of description of the liquid microstructure, see for instance [1].

The simplest descriptions of non-Newtonian liquid behaviour are the two-parameter Bingham and power law models with formulae Bingham, $\sigma = \sigma_0 + \eta_p\dot{\gamma}$ and $\sigma = \kappa\dot{\gamma}$, respectively. If these are plotted in the appropriate way - linear for Bingham and log-log for power-law - then the parameters can be immediately read off the plots as slopes and intercepts. This can be done manually from a graph or else using the simplest graph plotting routines in graphical packages (i.e. the trendline in Microsoft Excel). However, fitting more complex models is not so easy, and various mathematical manipulations are necessary. We have previously used such routines to fit non-linear data, see [2] where we had to develop a complex simplex routine for the purpose, which involved the simultaneous fitting of both simple-shear and extensional viscosity/rate-of-deformation curves. Commercial software can be bought to perform these fits, see for instance www.multisimplex.com/. However, there are simpler and cheaper ways to proceed, and here

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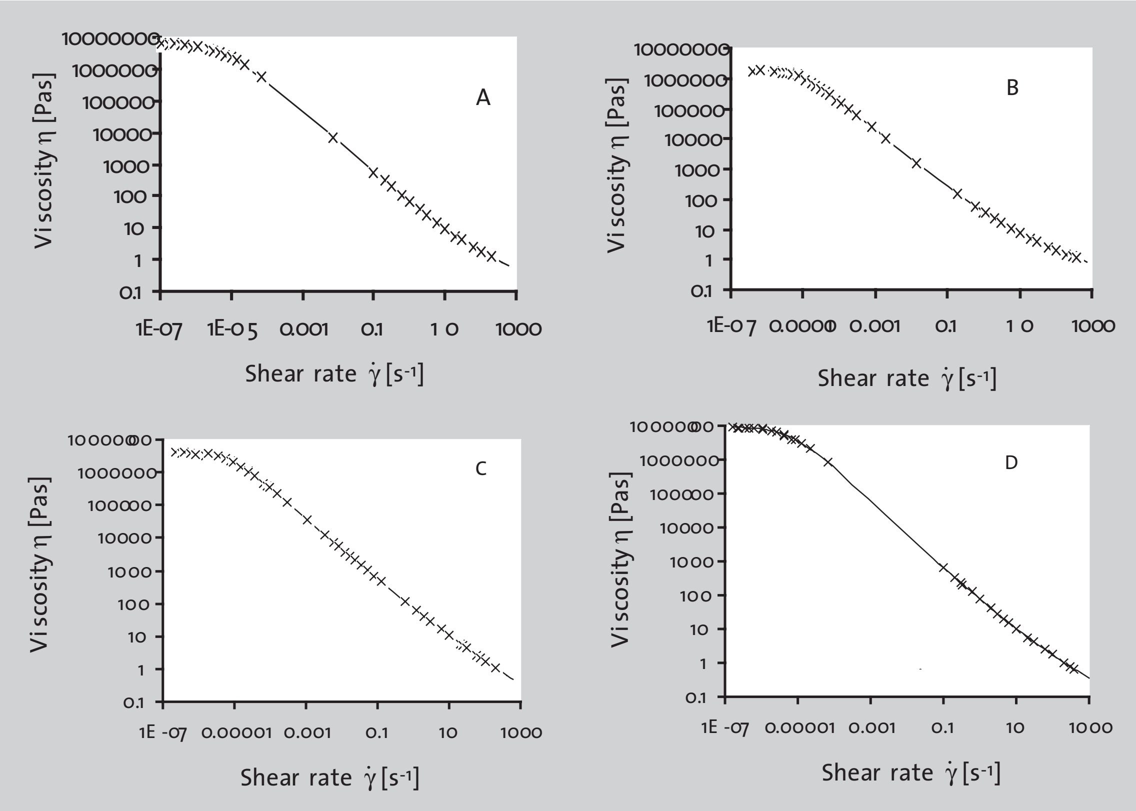

Figure 7 (above): Viscosity/shear-rate curves for four commercial shower gels, fitted to the five-constant simplified Cross model plus power-law model fitted using the parameters given in Table 3.

Product code	η_0	K	m	κ	n
A	6,058,747	158,948.5	0.960	6.49	0.6144
B	2,104,306	119,451.2	0.975	13.38	0.569
C	4,167,970	132,609.3	0.957	19.50	0.3825
D	9,156,628	156,457.2	0.997	15.45	0.4229

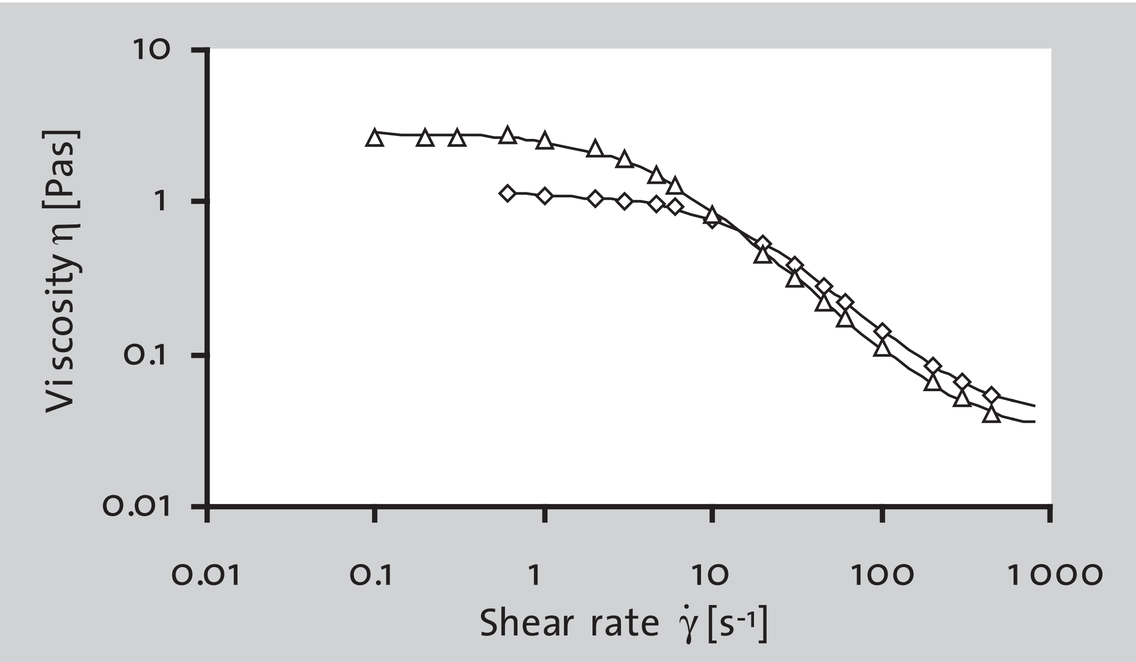

Figure 8 (below): Viscosity/shear-rate curves for two commercial surfactant-thickened bleaches fitted to the Cross model, with the parameters given in Table 4 (sample A has the higher low-shear rate viscosity).

Product code	η_0	K	m	η_∞
A	2.824	0.206	1.176	0.0285
B	1.109	0.059	1.269	0.0374

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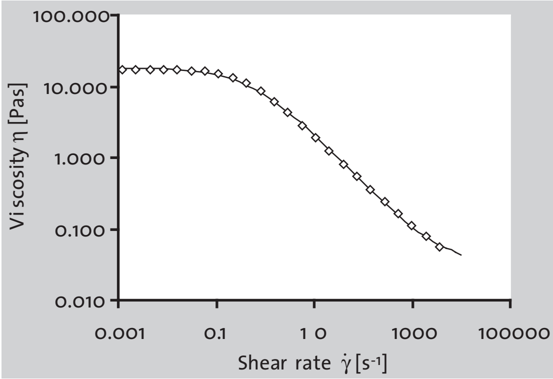
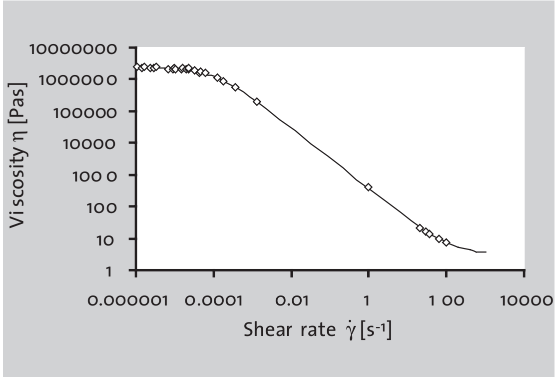
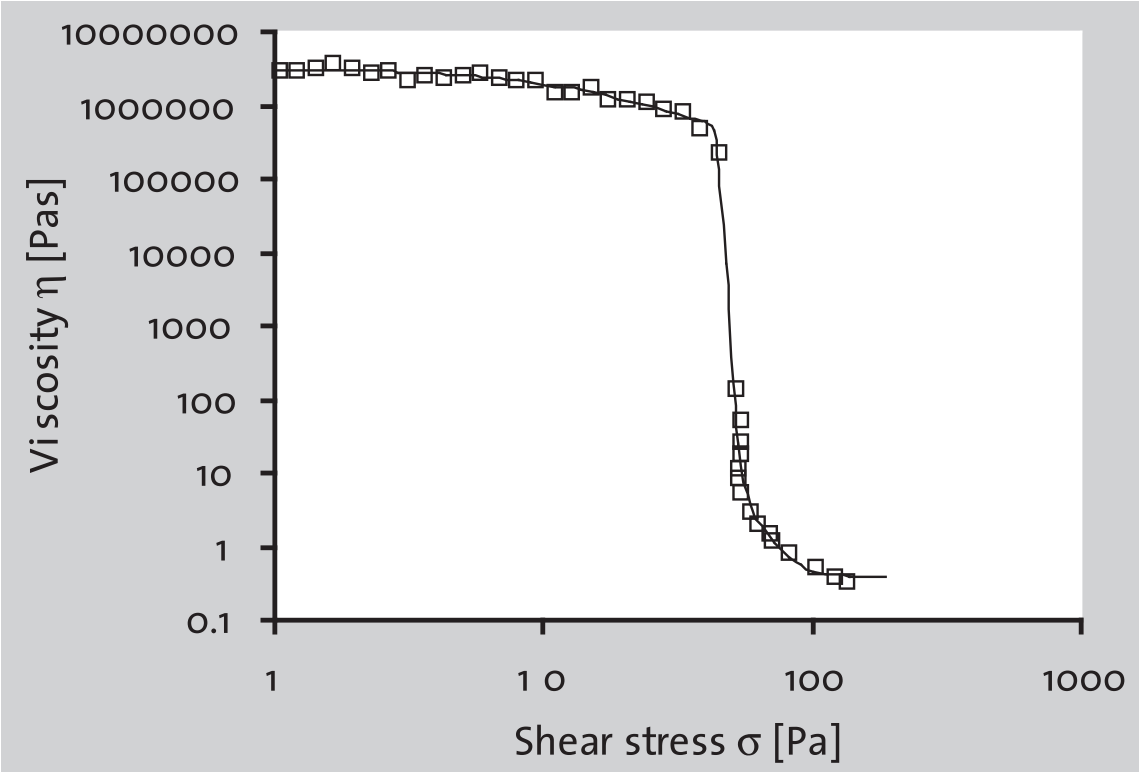
Figure 9 (left): Flow curve for SUA1 non-Newtonian standard liquid, fitted to the Cross model with η_0 = 18.33 Pas, K = 1.472 Pas^n, m = 0.733, and η_∞ = 0.0286 Pas.

*Figure 10 (right): Viscosity/shear-rate data for a toothpaste, fitted to the Cross model, with the following parameters: η_0 = 2.43 * 10^6 Pas, K = 9.440 s, m = 0.964, η_∞ = 3.1 Pas.*

*Figure 11 (below): The flow curve for a skin cream, fitted to an eight-parameter model (as shown above in the text), with the parameters as follows p = 92, σ_1 = 13.81, η_0 = 3.16 * 10^6 Pas, m = 56.05, σ_c = 44.6 Pa, s = -7.22, σ_2 = 79.5 Pa, and η_∞ = 0.39 Pas.*







5 CONCLUSIONS

The Microsoft Excel 'Solver' tool is a very simple but powerful procedure, even in the hands of the mathematically disadvantaged. It has very good application for fitting experimental flow-curve data to standard and non-standard models ranging from a two to an eight parameter model.

One point that should be noticed is that to get the best fit to the high shear rate/stress end of the curve, it is best to plot this data separately and use an appropriate model such as the Sisko model. This fit does not then have to compromise its parameter values by taking very low shear rate data into account.

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