# SELECTING THE BEST RHEOLOGICAL AND PIPE TURBULENT FLOW PREDICTION MODELS FOR NON-NEWTONIAN FLUIDS – USE OF *RMSE* and $R^2$ vs. *AIC*

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Most rheological and turbulent flow models for non-Newtonian fluids are nonlinear and deciding which one best represents the experimental evidence is not always obvious. Goodness-of-fit of non-linear models is often evaluated on the basis of root mean squared error (*RMSE*) or coefficient of determination ( $R^2$ ) which can be misleading and inappropriate for non-linear models. Pipe test data from the Flow Process and Rheology Centre, Cape Peninsula University of Technology were used to compare the power law, Bingham plastic, Herschel-Bulkley and Casson rheological models for 5% carboxymethyl cellulose (CMC) laminar data, and the Dodge and Metzner, Darby, Torrance, Wilson & Thomas, Slatter and El Emam models for bentonite and sludge turbulent flow data. The models were compared on the basis of *RMSE*,  $R^2$  and the Akaike Information Criterion (*AIC*). The *RMSE* and  $R^2$  criteria were useful in ranking models, but did not always distinguish between them, whilst the *AIC* approach clearly indicated the best model(s) in the candidate group.

KEY WORDS: Akaike information criterion (AIC), model selection, non-Newtonian, RMSE,  $R^2$ , turbulent flow

## **1. INTRODUCTION**

Much experimental work in turbulent pipe flow of non-Newtonian fluids has been reported over the years, but fundamental understanding is not complete. There are no generally applicable theories, and suitable mathematical and computational models are still under development [Rudman et al. (2004)]. As a result, the different analytical, semiempirical and empirical correlations (explicit and implicit) that have been proposed to predict turbulent pressure losses [see for example Dodge & Metzner (1959), Heywood & Cheng (1984), Wilson & Thomas (1985), Slatter (1994), El-Emam et al. (2003), Gao & Zhang (2007)] continue to be used. Generally these models were developed for a specific type of material and/or are based on a particular set of results, from which the coefficients of the correlation are derived. Rarely have these been corroborated by using independent data and consequently they are not universally applicable [Slatter (1994)]. The turbulent flow models use rheological parameters derived from laminar flow data, assuming these to still hold at the much higher turbulent wall shear stresses, which may not always be true. Also, extending laminar rheology to turbulent flow shear rates results in different wall shear stresses for different rheological models. This can greatly influence turbulent flow predictions [Slatter (1994), van den Heever et al. (2014)].

It seems sensible then to identify the most appropriate rheological model for the material and to compare experimental turbulent flow results with the predictions of several different correlations, most of which are nonlinear. Choice of model should be based on its general applicability, not just goodness-of-fit. This can be done by applying some criterion that additionally accounts for model complexity. Any such criterion, however, says nothing about the functional form of the candidate models – it cannot identify whether or not a better model exists [Myung (2000), Burnham & Anderson (2002)].

Generally two methods are used to determine model parameters, maximum likelihood estimation (MLE) and least-squares estimation (LSE). MLE is a standard technique to estimate parameters in statistics and requires that the distribution the data follows be known (or assumed). LSE is associated with the statistical concepts of linear regression, residual sum-of-squares (*RSS*), coefficient of determination ( $R^2$ ) and root mean squared error (*RMSE*). It does not require any distribution assumption and is useful in summarising experimental data, but does not have the properties of MLE. It is usually regarded as the approach used with linear regression models, not as a general parameter estimation method [Myung (2003)]. In LSE, parameter values are found that most accurately describe the data (how closely the model fits the data) by minimising *RSS*, whereas MLE finds the parameters that are most likely to have produced the data. However, when the data are (or are assumed to be) independent and to follow a normal distribution with constant variance, then LSE gives the same parameter estimates as MLE for linear models [Burnham & Anderson (2002; 2004; 2011), Myung (2003), Symonds & Moussalli (2011)].

To identify the "best" model once the parameters have been found, several criteria are used [Myung (2000), Spiess & Neumeyer (2010)]. Here, only three of these are considered, namely *RMSE*,  $R^2$  and the Akaike information criterion (*AIC*). MLE is a prerequisite for the *AIC*. These criteria, described in more detail below, include only the number of model (regression) parameters p to account for model complexity. In this paper only these criteria are compared. Experimental errors are assumed to follow the normal distribution and the merits of the various rheological and turbulent flow models are not considered.

## 2. BACKGROUND AND METHODS

#### 2.1 ROOT MEAN SQUARED ERROR

Root mean squared error (*RMSE*) is an estimate of the standard deviation of the random component in the observed data, and is defined as [Myung (2000)]:

$$RMSE = \sqrt{\frac{RSS}{(N-p)}} ; RSS = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$
(1)

where N = number of data points,  $y_i =$  experimental values,  $\hat{y}_i =$  model (predicted) values, p = number of regression parameters and (N-p) = number of degrees of freedom of the

model. *RMSE* is minimised during parameter estimation, so smaller values imply a better model fit to the data.

### 2.2. COEFFICIENT OF DETERMINATION

The coefficient of determination ( $R^2$ ) is often used to quantify how well a model fits a data set and will usually have a value between 0 and 1. It is useful in linear analysis as it indicates how much of the variance in the data is due to the fit, but in nonlinear analysis it doesn't have this interpretation since the total sum of squares (TSS) does not equal the regression sum of squares plus the residual sum of squares, as it does in linear analysis.  $R^2$  can be improved by adding independent model parameters to get a better fit, but this does not necessarily improve the model. A high value for  $R^2$  can be misleading and means only that the fitted curve came close to the observed data points, not necessarily that the model is good or meaningful. What value of  $R^2$  distinguishes a "good" from a "bad" model is not defined, so  $R^2$  gives no insight for choosing the best model [Burnham & Anderson (2002), Spiess & Neumeyer (2010), GraphPad software (1995-2015)].  $R^2$  is defined as [Spiess & Neumeyer (2010)]:

$$R^{2} = 1 - \frac{RSS}{TSS} ; TSS = \sum_{i=1}^{N} (y_{i} - \bar{y}_{i})^{2}$$
(2)

where  $\bar{y}_i$  = average of experimental values. To account for the number of parameters in the model the adjusted  $R^2$  value,  $R^2_{adj}$ , is used, as [Spiess & Neumeyer (2010), GraphPad Software (1995-2015)]:

$$R_{adj}^{2} = 1 - \frac{(N-1)RSS}{(N-p)TSS}$$
(3)

 $R^2$  will be negative if RSS > TSS which can happen if the model fits the data very poorly.

#### 2.3. AKAIKE INFORMATION CRITERION

Akaike's information criterion (*AIC*) is an "information – theoretic" approach based on Kullback-Leibler (K-L) information. Akaike (1974) found the link between K-L information and the maximised log-likelihood, which enabled the definition of his information criterion as [Akaike (1974), Burnham & Anderson (2002; 2004; 2011)]:

$$AIC = -2\ln(ML) + 2k \tag{4}$$

where ML = maximum likelihood estimate and k = number of estimable parameters in the model. *AIC* is a numerical value or metric that enables simultaneous comparison of proposed models. It is an estimate of how much better the best approximating model (lowest *AIC* value) is than the next best models in a set, and favours less complex models i.e. those with fewer parameters. *AIC* does not identify the best fit model, but for a given set of data determines a trade-off between variance and bias for the fitted parameters of each model. Parameter estimation for all the models must always be done with the same data set. The *AIC* value for each proposed model is calculated using either its *ML* or, if

for all the models, errors follow a normal distribution with constant variance, the least squares regression statistic *RSS*. In this case k = (p + 1) (to account for model variance,  $\sigma^2$ ) [Burnham & Anderson (2002; 2004; 2011), Symonds & Moussalli (2011)] and the *AIC* is given by:

$$AIC = N \ln\left(\frac{RSS}{N}\right) + 2k \tag{5}$$

Additionally, when N is small relative to k (taken as N/k < 40), a second order bias correction term should be added to the AIC value to give a corrected value,  $AIC_c$  as [Burnham & Anderson (2002)]:

$$AIC_{c} = AIC + \frac{2k(k+1)}{N-k-1}$$
 (6)

Since  $AIC_c$  tends to AIC as N increases it is recommended to simply use Eq. (6) consistently for all the models considered [Burnham & Anderson (2002)]. Individual  $AIC_c$  values do not help to rank models and implicitly contain constants (not shown in Eqs. (4) to (6)) which depend on N, although not on the fitted model.  $AIC_c$  differences account for these, and are the key to interpretation of the  $AIC_c$  values and ranking of the models [Burnham & Anderson (2011)]. The differences are calculated as:

$$\Delta_i = AIC_{ci} - AIC_{cmin} \tag{7}$$

where  $AIC_{cmin}$  is the smallest of the  $AIC_c$  values of the proposed models. Thus for the "best" model  $\Delta_i = 0$  and all other  $\Delta_i$  are positive. The larger  $\Delta_i$  is the more unlikely it is that model i is the best approximating model. As a rough guide, models with  $\Delta_i \leq 2$  are effectively equal to the best model and have substantial support, models with  $\Delta_i$  up to about 7 have less support but are plausible and should be considered. Models with  $\Delta_i > 14$  are probably not plausible and can be discarded [Burnham & Anderson (2002; 2011), Symonds & Moussalli (2011)]. Two additional quantities can be obtained from the  $\Delta_i$  for model i:

$$ER_i = \frac{e^{\left(-\frac{\Delta_{best}}{2}\right)}}{e^{\left(-\frac{\Delta_i}{2}\right)}} ; \ \Delta_{best} = 0$$
(8)

which defines how much more likely the best model is than model i. It can also be used to compare any two models in the set. The second is the Akaike weight  $w_i$  for model i:

$$w_{i} = \frac{e^{\left(-\frac{\Delta_{i}}{2}\right)}}{\sum_{r=1}^{R} e^{\left(-\frac{\Delta_{r}}{2}\right)}} \quad for \ R \ models \tag{9}$$

 $w_i$  lies between 0 and 1 and gives the probability that model i is the best approximating

model for the given data. The  $w_i$  values must sum to 1 [Burnham & Anderson (2002), Symonds & Moussalli (2011)]. Even if all candidate models are "bad" a "best" model will be identified - the analyst must ensure the use of meaningful models. Examples of the use of *AIC* versus other measures can be found in Burnham & Anderson (2002), Thayer et al. (2007), Spiess & Neumeyer (2010) and Symonds & Moussalli (2011).

#### 2.4. EXPERIMENTAL FACILITIES, TEST MATERIALS AND DATA

The data of the examples presented here were all obtained in the pipe test loops of the Flow Process and Rheology Centre (FPRC) of the Cape Peninsular University of Technology (CPUT). Details of these loops and the estimated experimental errors for each are summarised in van den Heever (2013). In all the tests, flowrate was set and pressure gradient measured. Experimental data used to evaluate the model selection criteria are for carboxymethyl cellulose (CMC), bentonite and sludge in pipes ranging from D = 0.013 to D = 0.211 m at 8V/D values from 20 to  $1740 \text{ s}^{-1}$  (V = average velocity (m/s), D = pipe diameter (m)) and Metzner-Reed Reynolds numbers ( $Re_{MR}$ ) between 8 and 79650.

## **2.5. RHEOLOGICAL MODELS**

The Herschel-Bulkley, Bingham plastic, power law and Casson rheological models were used. The rheological parameters of each were determined using MS Excel<sup>®</sup> by iterating the appropriate flow equation to find wall shear stress  $\tau_w$  (in Pa) at each experimental 8V/D value, whilst simultaneously minimising RSS over all the test points. In each analysis different initial values were used and convergence to the same final values checked, to be reasonably sure of a global solution. RMSE,  $R^2$ ,  $R^2_{adj}$ ,  $AIC_c$ ,  $\Delta_i$ ,  $ER_i$  and  $w_i$  were calculated for each model according to Eqs. (1) to (3) and (5) to (9). The rheological and flow equations for these models are summarised in several books, for example Chhabra and Richardson (2008), and in van den Heever (2013).

## 2.6. TURBULENT FLOW MODELS

To evaluate the model selection criteria for turbulent flow, seven (arbitrarily chosen) models were used with selected data for Bingham plastic (as per §2.5) bentonite suspensions and sludges. These seven were the logarithmic and Blasius correlations of Dodge & Metzner (1959), and the models of Torrance (1963), Wilson & Thomas (1985), Slatter (1994), El Emam et al. (2003) and Darby (as given in Chhabra & Richardson (2008)). Iteration was done for the implicit models to find  $\tau_w$  at each experimental 8V/D value, after which the selection criteria metrics were calculated.

## **3. RESULTS AND DISCUSSION**

### **3.1. RHEOLOGICAL MODELS**

Fig. 1 shows the rheological model fits to a set of 5% CMC data. The equations of these fits are listed in Table 1(a).



Figure 1 Rheological model fits to 5% CMC pipe laminar data (test pipe diameters:  $\Box$  0.0577 m,  $\Diamond$  0.0812 m,  $\Delta$  0.1506 m,  $\circ$  0.2110 m)

Clearly the Bingham plastic fit is not appropriate, but the differences between the other models are not easy to quantify visually. The power law and Herschel-Bulkley models look similar and appear to fit the data well, while the Casson model has a reasonably high (unexpected) yield stress and does not fit the data as well in the lower 8V/D region. Referring to Table 1(b) the RMSE and  $R^2_{adj}$  values rank the models as would be expected for this material. The  $R^2_{adj}$  values are all quite high and similar. They suggest, as do the RMSE values, that the Bingham plastic and Casson model fits are not as good as the power law and Herschel-Bulkley fits, but can't quantify this observation. Comparison of the RMSE and  $R^2_{adj}$  values for the power law and Herschel-Bulkley models shows the small effect of (N-p) as suggested by Spiess & Neumeyer (2010). The AIC related values, however, give a clearer picture. The  $\Delta_i$  values immediately require the Bingham plastic and Casson models to be discarded. The Herschel-Bulkley model could be considered, but its  $ER_i$  value reveals it has considerably less empirical support than the power law model, with only a 0.2% probability of being the best model, while the power law model has a 99.8% probability of being the best model in the set, for the given data. This example clearly illustrates the ability of the AIC method to discern between models.

Table 1

5% CMC results (a) fitted rheological model parameters (b) model selection criteria values

(a)					
Model	Fitted parameters				
Power law	$\tau_w = 0.6915 \dot{\gamma}^{0.731}$				
Herschel-Bulkley	$\tau_w = 0.47 + 0.6272 \dot{\gamma}^{0.746}$				
Casson	$\tau_w^{0.5} = 3.11^{0.5} + (0.0779\dot{\gamma})^{0.5}$				
Bingham plastic	$\tau_w = 1.0 + 0.1514 \dot{\gamma}$				

	Model	k	RMSE	$R^{2}_{adj}$	AIC <sub>c</sub>	$\Delta_i$	w <sub>i</sub>	$ER_i$
1	Power law	3	0.6658	0.9988	-56.7	0.0	0.998	1.0
2	Herschel-Bulkley	4	0.7179	0.9986	-44.2	12.5	0.002	519.1
3	Casson	3	2.4368	0.9837	137.9	194.6	0.0	1.8E42
4	Bingham plastic	3	4.2767	0.9499	222.3	279.0	0.0	3.8E60

(b)

#### **3.2. TURBULENT FLOW MODELS**

Fig. 2(a) shows the rheological model fits to pipe test measurements for a 9% bentonite sample. They are similar, except to some extent the power law fit at higher 8V/D values, and cannot easily be differentiated visually. The *AIC* approach (§2.3) confirmed the models are similar and any one of them could be used, with  $\Delta_i$  values of 0 to 3.2 and corresponding Akaike weights of 0.45 to 0.09, indicating that no single model is particularly favoured. This probably results from the fact that there are not many data points at low 8V/D values, and agrees with the findings of Malkin et al. (2004). The Bingham plastic rheology (yield stress  $\tau_y = 32.19$  Pa, Bingham viscosity K = 0.0100 Pa.s) was selected for use in the turbulent flow predictions.



Figure 2. (a) Rheological model fits to 9% bentonite pipe data (b) Dodge & Metzner, Slatter and Wilson & Thomas turbulent model flow predictions (test pipe diameters:  $\Box 0.0577 \text{ m}$ ,  $\diamond 0.0812 \text{ m}$ ,  $\Delta 0.1506 \text{ m}$ )

Table 2 gives the selection criteria for turbulent flow model predictions, three of which are shown in Fig. 2(b). All the criteria rank the models identically, with the first three models having quite similar *RMSE* and  $R^2_{adj}$  values. The *AIC* values though indicate that only the Dodge and Metzner correlations (logarithmic and Blasius form) should be considered, with probabilities of being the best model of 95.54 and 4.42% respectively. The next best model, that of Slatter, has only a 0.04% probability of being the best model, which isn't what Fig. 2(b) suggests. The Wilson & Thomas model, for example, is ranked fifth with an average error of -15% (-6 to -23%), but within this group has no chance of being considered a suitable candidate. As indicated by the  $ER_i$  values the empirical support for the Dodge & Metzner model is overwhelmingly greater than it is for the for Wilson & Thomas model. Such information is useful, but can't be inferred

from Fig. 2(b). Note that these example results are based on data over all pipe sizes.

Table 2

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	Model	k	RMSE	$R^{2}_{adj}$	AIC <sub>c</sub>	$\Delta_i$	w <sub>i</sub>	$ER_i$
1	D & M (log) <sup>@</sup>	2	5.2538	0.9680	122.8	0.0	0.9554	1.0
2	D & M (Blasius)	2	5.7219	0.9620	128.9	6.1	0.0442	21.59
3	Slatter	2	6.5200	0.9507	138.3	15.5	0.0004	2.4E03
4	Darby	2	10.814	0.8643	174.8	52.0	0.0	1.9E11
5	Wilson & Thomas	2	14.257	0.7642	194.7	71.9	0.0	4.1E15
6	Torrance	2	16.046	0.7013	203.2	80.4	0.0	2.9E17
7	El Emam et al.	2	27.636	0.1140	242.3	119.	0.0	9.0E25
<u>a</u> .								

Turbulent flow model selection criteria results for 9% bentonite (Bingham plastic rheology)

 $(^{(a)} D \& M = Dodge \& Metzner)$ 

The results shown in Fig. 3 are the predictions of the turbulent flow models (except the Dodge & Metzner Blasius form, omitted for clarity) for a Bingham plastic sludge ( $\tau_y = 8.19 \text{ Pa}, K = 0.0138 \text{ Pa.s}$ ). They are included to provide an example in which the models all follow the shape of the experimental data well, but over- or under-predict by varying amounts.



Figure 3. Wilson & Thomas, Darby, El Emam, Dodge & Metzner, Slatter and Torrance turbulent model flow predictions for a 5% sludge (test pipe diameters: □ 0.027 m, ◊ 0.052 m, △ 0.063 m)

The Wilson & Thomas, Darby and El Emam results are quite tightly grouped around the experimental values for both diameters. The Slatter and Dodge & Metzner predictions are similar and over-predict wall shear stress by about 20% on average. The Torrance model over-predicts the shear stresses by just over 33% on average. These groupings are clear from the *RMSE* and  $R^2_{adj}$  values given in Table 3, which suggest that the first three models are essentially as good as each other, the Dodge & Metzner and Slatter models are less accurate but could be considered, and the Torrance model is just too inaccurate. However, none of the models appears to be completely implausible and the choice, especially between the first three ranked models, is not clear-cut. Use of the *AIC* provides

greater insight. In this case the  $\Delta_i$  values indicate the Wilson & Thomas model to be the best, but also that the Darby and El Emam models must be considered. Their Akaike weights and the evidence ratios though show the Darby and El Emam models to be much less likely (1.4 and 0.5% respectively) than the Wilson & Thomas model which is 98.1% likely to be the best model. The other models can all be discarded, but note that using individual evidence ratios shows for example that the empirical support for the Dodge & Metzner model is about 12 times that for the Slatter model, or for the Darby model is 2.9 times that for the El Emam model. Such information is useful, but is not at all evident from the plots.

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	Model	k	RMSE	$R^{2}_{adj}$	AIC <sub>c</sub>	$\Delta_i$	w <sub>i</sub>	$ER_i$
1	Wilson & Thomas	2	3.0271	0.9300	48.0	0.0	0.981	1.0
2	Darby	2	3.7462	0.8929	56.5	8.5	0.014	71.0
3	El Emam et al.	2	3.9501	0.8809	58.6	10.6	0.005	205.0
4	D & M (Blasius)	2	6.8371	0.6431	80.6	32.6	0.0	1.2E07
5	D & M	2	6.9500	0.6312	81.2	33.2	0.0	1.7E07
6	Slatter	2	7.8911	0.5246	86.3	38.3	0.0	2.1E08
7	Torrance	2	12.3871	-0.172	104.3	56.4	0.0	1.7E12

Turbulent flow model selection criteria (5% Bingham plastic sludge)

## **5. CONCLUSIONS**

Rheological and turbulent flow models for non-Newtonian fluids are generally nonlinear, so in fitting these models to observed data to determine parameters or evaluate how good they are, use of the  $R^2$  statistic is inappropriate. *RMSE* can be used to rank models, but doesn't give much insight. The Akaike information criterion has been presented as an alternative to use when fitting experimental data or evaluating existing correlations for turbulent flow. Sample data from tests conducted in the pipe loops of the FPRC (CPUT) were used to demonstrate the utility of this criterion and how it allows proper comparison of different models in a group, for a given data set, on a theoretically sound basis. Its use enables the best model in the group to be inferred, but does not remove from the analyst the responsibility of ensuring the candidate models are functionally appropriate in the first instance.

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