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Analysis of Some Common Theoretical and Empirical Relationships between Settling Velocity of a Sediment Particle as a Function of Particle Size and Water Temperature and Development of New Empirical Nonlinear Regression Equations

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ABSTRACT: One of the most important problems in irrigation canals is sedimentation of floating particles which, in the long-run may inhibit the canal's flow debit. Up-to-date the sedimentation science argues about the proper laws that govern the physics of the sedimentation process, namely, the settling velocity v_s of a particle in a fluid flow, which is very dependent on the interaction between the fluid (e.g. water) and the sediment. Although the fundamental law describing this settling velocity, i.e. Stoke's law, has been known for quite some time, many scientists have been working in this field since then to come up with more precise descriptions of the sedimentation process. One essential key to do this properly is the exact definition of the physical properties of the fluid (water) and of the solid particles. In this study, eight related equations describing the settling velocity v_s of a particle in a fluid have been studied and compared to each other. More specifically, for each of these eight equations, v_s as a function of the diameter d_s of the sedimentary particle has been computed for water temperature of 20°C. The range of d_s from 0.005 cm to 1 cm has been divided into three separate categories. Polynomial regression models of second order are fitted to the mean theoretical fall velocities in each diameter category using classical- and weighted least squares, with the latter allowing to better incorporate the heteroscedastic errors into the model. Very good model fits as indicated by $R^2 > 0.99$, but more clearly, by low values of the AIC are obtained. Finally, to generalize the results to other temperatures, linear corrections to the regression predictors of the fall velocities are proposed.

Keywords: Sediment transport, Fluid flow, Empirical equation, Settling velocity

1 INTRODUCTION

The fall velocity of sediment particles, also called the terminal or settlement or more often settling velocity is one of the most important particle characteristics in sediment transport studies and plays important role for the understanding of suspension, deposition, mixing and other physical as well as chemical and biological exchange processes. This settling velocity is directly related to the relative flow conditions existing between the sediment particle and the motion of the water. It depends in a certain form on the size, shape, and the surface roughness of the particle and the viscosity of the fluid (Yang, 1996).

Owing to the fact that sediment transport in rivers is sensitive to the settling velocity of the sedimentary particles, many attempts to estimate the latter , starting with Stokes in (1851) and followed by, among others, Oseen (1927), Rubby (1933), Rouse (1938), Zanke (1977), Yalin (1977), Hallermier (1981), Dietrich (1982), Van Rijn (1989), Concharov [cited in Ibad-zadeh 1992], Julien (1995), Cheng (1997), Brown and Lawler (2003) and She *et al.* (2005), who all developed empirical or semi-empirical relations for estimating the settlement velocity of sediment particles. In a useful attempt, the US Interagency Committee on Water Resources (1957) summarized the data obtained by several researchers by that time and published a graphical relation to estimate the drag coefficient which, subsequently, allows to calculate the fall velocity (Vanoni, 1957).

More recently, Jimenez and Madsen (2003) presented a simple formula to calculate the fall velocity of natural particles with grain sizes ranging between 0.063 and 1mm. these authors thencompared their formula with several other empirical formulas proposes by the references cited above and showed performed

best – as measured by the standard error of the estimation - for fine sediments with nominal diameters d_N ranging between 0.063 and 0.25 mm, for which sediment suspension in natural conditions is most likely to occur.

Fenite *et al.* (2004) used two sets of measured fall velocity data for comparing seven formulae. The results showed for the dataset of (VanRijn 1997), the formula of Cheng (1997) performed best, However, the formula of Dietrich (1982) did better in the finer-sediment-size range, while that of Zhang (1989) applied better in the medium- and coarser- size ranges. Therefore, the choice of suitable formula depends on the sediment-size range.

Wu and Wang (2006) examined again the relations of the US Interagency Committee (1957) mentioned above, but used a wider range of data and included the equation proposed by Cheng (1997) and came up with an explicit mathematical expression for the fall velocity of natural sediment particles which include also a (Corey) shape factor S_f , describing the deviation from a spherical (S_f *=1)* particle shape. They reported that by considering the effects of viscosity and this shape factor, their formula has a relative mean error of 9.1%, but, surprisingly, when the variation of S_f is neglected and set to a constant (=0.7, i.e. slightly ellipsoid) this error decreases to 6.8%. In conclusion, Wu and Wang (2006) pretended that their fall velocity relationship performs better than nine other existing formulae referenced in the literature.

Zhiyao *et al*. (2008) established a new relationship between the Reynolds number (Re) and a dimensionless particle parameter and developed a simple formula for predicting the fall velocity of natural sediment particles that is applicable over a wide range of Re-numbers, i.e. from low Re, Stokes flow to high Re, turbulent flow. The precision of their formula was tested against experimental data and it was shown that the perdition accuracy of their formula is higher than that of other formulas with relative error of 6.36% and that it is applicable to Re- numbers less than 2×10^5.

Sadat *et al*. (2009) examined and re-evaluated 22 fall velocity relationships that had been published by 17 researchers during the period 1933-2007. They developed a new formula and verified it with two sets of laboratory data - one of these already reported by Zegzhda (1934) and the other measured by Raudkivi (1990) - and proved a good agreement between the observed and calculated data over a wide range of particle sizes (0.01-100mm).

In this study, eight published equations describing the sinking velocity v_s of a particle in a fluid, i.e. that of Stokes (1851), Rubby (1933), Zanke (1977), Chang (1984), Zhang (1989), Van Rijin (1989), Julien (1995) and Soulsbey (1999) - have been used to develop more easily applicable 2^{nd} -order polynomial regression model using classical and, to better account for the model errors, a sophisticated weighted least squares approach. The regression equations found are then corrected for the effects of temperature.

2 THEORY OF FALL VELOCITY CALCULATION (STOKES' LAW)

Consider a sphere falling through a viscous fluid. As the sphere falls so its velocity increases until it reaches a velocity known as the fall velocity. At this velocity the frictional drag due to viscous forces is just balanced by the gravitational force and the velocity is constant (Fig. 1).

The fall velocity is derived by balancing drag (F_D), buoyancy (F_B), and gravity (F_W) forces that act on the particle, i.e.

$$F_D = F_W - F_B \tag{1}$$

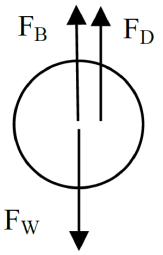

Figure 1. Drag, buoyancy and gravity force acting on a particle in a fluid.

The drag force F_D on a particle traveling in a resistant fluid is (Prandtl and Tietjens, 1957)

$$F_D = \frac{C_D v_s^2 \rho A}{2} \tag{2}$$

where C_D= drag coefficient that is a function of *Re* and shape factor (S_f) - S_f = 0.7 for natural sediment particles -, v_s= fall velocity(cm/s), ρ = mass density of water, and A= projected area of particle in direction of the flow.

$$F_W - F_B = \frac{4}{3}\pi r^3(\rho_s - \rho)g \tag{3}$$

where r = Particle radius, and ρ_s, ρ densities of sediment and water, respectively.

The fall velocity is then calculated from Eqs. 2 and 3:

$$v_s = \sqrt{\frac{8g(\rho_s - \rho)\pi \mathrm{r}^3}{3C_D\rho A}} \xrightarrow{\text{spherical particle}} v_s = \sqrt{\frac{4g(\rho_s - \rho)\mathrm{d_s}}{3C_D\rho}} \tag{4}$$

where, d_s = 2r, the diameter of particle.

Once the drag coefficient has been determined, the fall velocity can be calculated. Stokes (1851) derived an expression for the drag force F_D on a small spherical particle – with particle diameter d_s equal to or less than 1mm – for *Re<<1* (sub-laminar or creeping flow) by solving the Navier-Stokes equations (Graf, 1971) and came up with the famous Stokes' law:

$$F_D = 6\mu\pi r v_s \xrightarrow{Eq.2} C_D = \frac{24}{\mathrm{Re}} \tag{5}$$

and putting this in Eq. 4 results in

$$v_s = g(G_s - 1)d_s^2 / 18\mu \tag{6}$$

where μ= the dynamic viscosity of the fluid (N·s/m²) and $G_s = \frac{\rho_s}{\rho}$ is the specific gravity of soil ~ 2.65.

Both the density and the dynamic (i.e. also the kinematic viscosity ν=μ/ρ) of water are functions of the temperature (Streeter and Wylie, 1985). The kinematic viscosity is calculated by (Yang, 1996).

$$v = \frac{1.792 \times 10^{-6}}{1 + 0.0337T + 0.000221T^2} \tag{7}$$

where *T*= temperature in ^oC. The range of variations of these water characteristics is shown in Table 1.

Table 1. Water characteristics

T (^oC)	ρ (kg/m^3)	μ (N-s/m)^2	ν (m^2/s)
0	999.8	1.781 * 10^{-3}	1.785 * 10^{-6}
10	999.7	1.307 * 10^{-3}	1.306 * 10^{-6}
20	998.2	1.002 * 10^{-3}	1.003 * 10^{-6}
30	995.7	0.798 * 10^{-3}	0.800 * 10^{-6}
40	992.2	0.653 * 10^{-3}	0.658 * 10^{-6}

3 EMPIRICAL EQUATIONS FOR THE FALL VELOCITY

As stated in the previous section, Stokes law is valid only for a small range of particle sizes and sub-laminar flow (Re<<1). When Re is greater than 1, no explicit closed relationship exists anymore, so that one must rely on one of the many empirical formulae established over more than a century by the various researchers referenced in the introduction. Among these we analyze further in this study the experimental relationships for the fall velocity as listed in Table 2. The range of particle diameters investigated in the following is 0.005 to 1 cm and the shape factor S_f - defined as $S_f = c/(ab)^{1/2}$, where a,b,c, are the major axis of an equivalent ellipsoid, i.e. S_f = 1 for a spherical particle - has been fixed to 0.7, i.e. the value recommended by Wu and Wang (2006), as discussed earlier.

Once the fall velocity v_s has been calculated for all particles diameters d_s for an individual water temperature, the mean fall velocity $\bar{x}$ for each d_s obtained with the eight relationships is computed. To account for the often large differences in the theoretical predictions by some of the formulae, outlier data is

determined by a Boxplot method and subsequently eliminated in the classical least squares polynomial regression.

Table 2. Experimental relationships for fall velocities in water as a function of particle size and water viscosity

Author	Equation
Stokes (1851)	$v_s = g(G_s-1)d_s^2 / 18\,\nu \quad Re << 1$
Rubby (1933)	$v_s = F\,[d_s\, g(G_s-1)]^{0.5}$ $F = [\,2/3 + (36\nu^2/\, g(G_s-1)\, d_s^3)\,]^{\,0.5} - [36\nu^2/\, g(G_s-1)\, d_s^3]$ $d_s > 0.02$ cm
Zanke (1977)	$v_s = (10\,\nu / d_s)\,[(1+ 0.01\, g(G_s-1)\, d_s^3/\, \nu^2)^{0.5} - 1]$ $0.1\text{mm} \le d_s \le 1\text{mm}$
Cheng (1984)	$v_s = (\,\nu / d_s\,)\,[\,(25+1.2D_*^2)^{0.5} - 5\,]^{1.5}$ $D_* = d_s\,[g(G_s-1) / \nu^2]^{1/3}$
Van Rijn (1989)	$v_s = g(G_s-1)d_s^2 / 18\,\nu \qquad d_s < 0.01$ cm $v_s = 1.1\,(g(G_s-1)\, d_s)0.5 \qquad d_s \ge 0.1$ cm $v_s = (10\,\nu / d_s)\,[\,(\,1 + 0.01\, D_*^3)^{0.5} - 1\,] \quad 0.01 \le d_s < 0.1$ cm
Zhang (1989)	$v_s = [(13.95\,\nu/\, d_s)^2 + 1.09 g(G_s-1)\, d_s]^{0.5} - 13.95\,\nu/\, d_s$
Julien (1995)	$v_s = (8\,\nu / d_s)\,[(1 + (0.222\, g(G_s-1)\, d_s^3) / 16\nu^2)^{0.5} - 1]$
Soulsbey (1999)	$v_s = (10.36\,\nu / d_s)\,[(1 + (0.156\, g(G_s-1)\, d_s^3\,) / 16\nu^2)^{0.5} - 1]$

D*= dimensionless particle coefficient

4 DATA ANALYSIS

4.1 *Boxplot outlier test*

In a boxplot, introduced by Tukey (1977), the main elements are the median, the lower quartile (Q_1) and the upper quartile (Q_3). The boxplot contains a central line (median) and extends from Q_1 to Q_3. Cutoff points, known as fences, lie at *1.5* (Q_3-Q_1) below the lower quartile and above the upper quartile define the lower and upper limit of fences, LIF and UIF, respectively, i.e.

$$LIF = Q_1 - 1.5IQR, UIF = Q_3 + 1.5IQR \tag{8}$$

where the inter quartile range IQR is equal to Q_3-Q_1. In the present study, when using ordinary least squares regression, 37 data points (equal to 5% of the total data) have been eliminated by the outlier test.

4.2 *Least Squares (LS) and Weighted Least Squares (WLS) regression methods*

The goal is to fit the theoretical predictions of the various Stoke's formulae for the fall velocities *v (=y)* as a function of the particle diameter *d* (=*x*) by more generally usable simple polynomials of order two:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i \tag{9}$$

This equation can be written in matrix notation as

$$y = X\beta + \varepsilon \tag{10}$$

where X is an *N x 3* predictor matrix whose three columns consist of $(1, x_i^2, x_i^3)$ $(i = 1,..,N)$, β is the vector of unknowns and ε is a random error vector, assumed to be normally distributed, with expectation $E(\varepsilon)=0$ and a variance matrix $\psi = V\sigma^2$, where V is a diagonal matrix (i.e., the errors are uncorrelated) and σ^2 is an unknown common variance. This means that $\varepsilon \sim N(0, V\sigma^2)$. Such an error distribution is called heteroscedasdic (Beck and Arnold, 1977) and this is often not taken care of in regular least squares. In such a case, the classical least squares estimator (see Eq. 15, later) is then not any more a BLUE (best linear unbiasted estimator), i.e. not optimal (Beck and Arnold, 1977).

In fact, the general linear model (10) for the unknown parameters β is solved by a least-squares approach (Draper and Smith, 1998). However, because of the heteroscedasticity, ordinary least squares is not valid, so that the maximum likelihood estimation (MLE) method must be applied (DeGroot and Schervish, 2002). In MLE the probability density function f(β,Y), i.e. the likelihood function L(β,Y) , is maximized or, more conveniently, its logarithm is ln f(β,Y) = ln L(β,Y) is minimized. For the estimation problem (10) and the statistical assumptions ln L(β,Y) can be written as (Beck and Arnold, 1977):

$$\ln L(\beta,Y) = \ln f(\beta,Y) = -\frac{1}{2}\left[N\ln(2\pi) + \ln|\psi| + S_{ML} \right] \tag{11}$$

where S_{ML} is the function to be minimized by the linear model:

$$S_{ML} = (Y - X\beta)^T \psi^{-1} (Y - X\beta) \tag{12}$$

As the first two terms in Eq. (11) are constant, its minimization is equivalent to minimizing Eq. (12) which results in the general heteroscedastic ML least squares estimator:

$$b_{MLE} = (X^T \psi^{-1} X)^{-1} X^T \psi^{-1} Y \tag{13}$$

or, with $\psi = V\sigma^2$, in the so-called weighted least squares estimator:

$$b_{WLS} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y \tag{14}$$

wherefore the elements of the diagonal matrix V^{-1} are associated with the weights w_i of the observations.

For the case that the weights w_i are equal (=1), Eq. (14) becomes the ordinary least squares estimator:

$$b_{LS} = (X^T X)^{-1} X^T Y \tag{15}$$

Both weighted (WLS) and ordinary (LS) least squares fitting will be applied to the means $\bar{x}_i$ of the fall velocities predicted by the various Stokes formulae (usually seven or eight) in Table 1. For WLS the weights w_i are set to $w_i = 1/s_i^2$, where s_i^2 are standardized variances of the mean velocities, estimated by $s_i^2 = \frac{\sum_{j=1}^{n}(x_{ij}-\bar{x}_i)^2}{n-1} / \bar{x}_i^2$, and n is the number of formulae used to compute the mean $\bar{x}_i$ of a velocity.

The WLS- and LS- fitting models have been programmed in the R® statistical environment. For the selection of the optimal polynomial model, as well as for the comparison of the two model approaches, the coefficient of determination R^2 – which often does not work well for heteroscedastic models (Beck and Arnold, 1977) – and the Akaike's information criterion (*AIC*) (Akaike, 1974) are used. *AIC* is defined as

$$AIC = 2k - 2\ln L \tag{16}$$

where k is the number of estimated parameters in the model and ln L is as above. By minimizing the AIC, models with more parameters which always result in better fit, i.e. smaller residuals, are penalized.

Once the polynomial coefficients have been determinded by the two least squares methods, 90% - confidence intervals for the predictors y_i^{pred} are computed by (Draper and Smith, 1998)

$$CI = y_i^{pred} \pm t_{0.05,N-(k-1)} * \sqrt{s^2 x_i^T (X^T V^{-1} X)^{-1} x_i} \tag{17}$$

where xi denotes the predictand, and $s^2 = S_{ML}/(N-k)$ is the residual variance of the model fit.

As it was not possible to fit the whole the diameter range 0.005 cm$<d_s \leq$1cm of the various Stoke formulae by one polynomial curve, the regressions were carried out for three separate diameter categories - 0.005cm $\leq d_s \leq$ 0.01cm, 0.01cm$<d_s \leq$ 0.1cm and 0.1cm$<d_s \leq$1cm-. Moreover, since the fall velocity depends on the water temperature (Interagency Committee, 1957), all regressions are done for the reference temperature of 20°C. After that, the regressed velocities are linearly corrected for other temperatures.

5 RESULTS AND DISCUSSION

For 20°C water temperature, the fall velocities as a function of the particle diameter are calculated by the eight relations given in Table 1, wherefore the specific formula restrictions as noted in the table have been respected, so that for some diameters the fall velocity could not be calculated by all eight relations. Next, iutlier velocity data for a particular diameter are determined by the Boxplot test (Eq, 8) and thus eliminated from the subsequent regression analysis.

The left panels of Fig. 2 show the fall velocity points generated in this way for the three particle size categories, as discussed. For each category the mean data for each particle size has been calculated and a regression line is fitted to this mean data by LS and WLS where, moreover, the constant term β_0 in Eq. (9) has been omitted in the least squares regression.

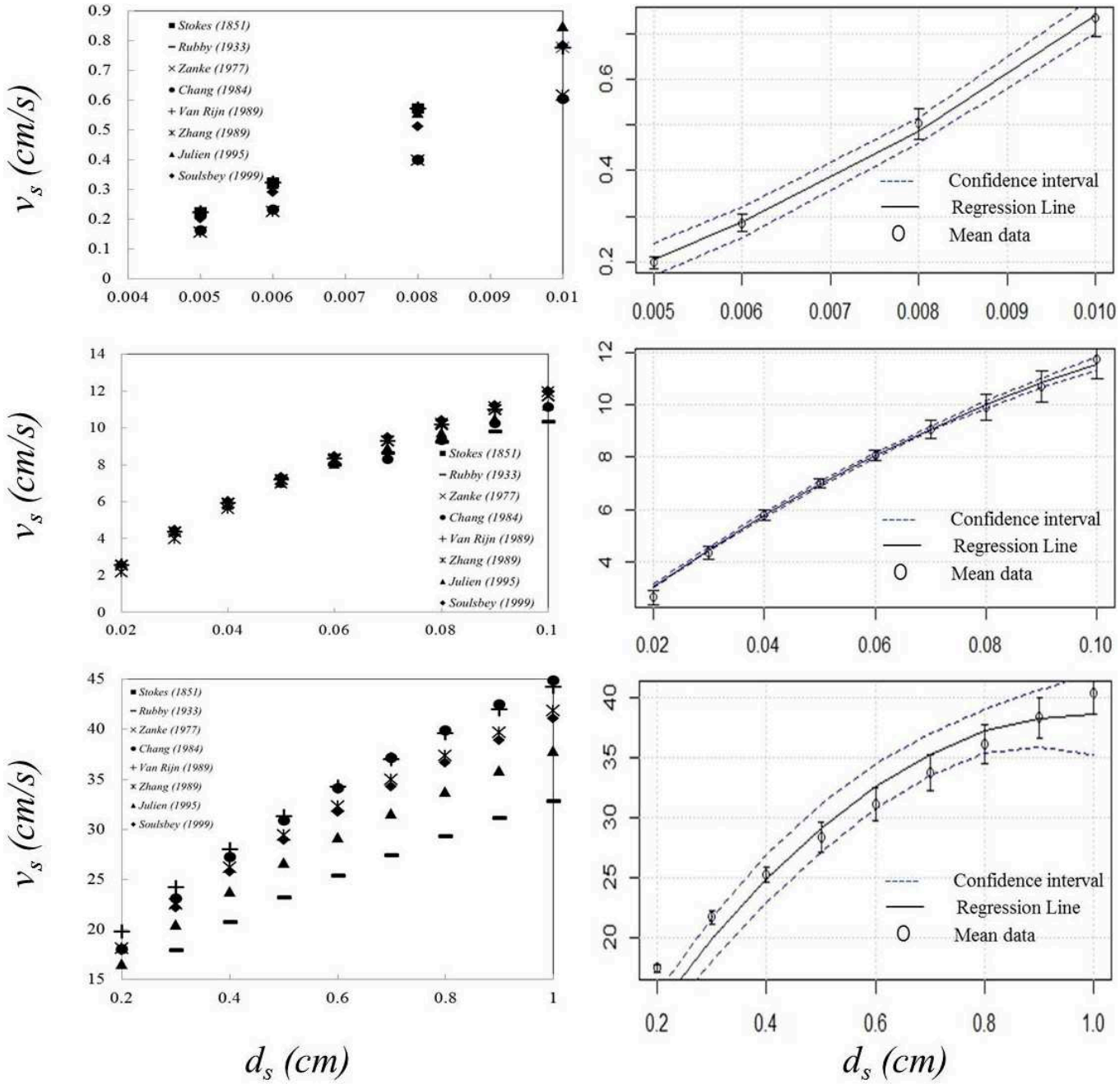

Figure 2. Left panels: Empirically computed velocities (Table 1) for the three diameter categories. Right panels: Mean velocities with +- standard deviation segment, regression curve and 90% confidence lines for the corresponding categories.

Table 3. Statistical results of LS- and WLS polynomial regression model for fall velocities for T=20°C

Diameter interval	Method	Equation $v_s = b_1 d_s + b_2 d_s^2$	R^2	AIC	sd(b_1)	sd (b_2)
$0.005cm \le d_s \le 0.01cm$	LS	$v_s = 8.32\ d_s + 6583\ d_s^2$	0.99	- 20.68	3.74	443.0
	WLS	$\mathbf{v_s = 8.53\ d_s + 6544\ d_s^2}$	0.99	-20.93	3.63	416.7
$0.01cm < d_s \le 0.1cm$	LS	$v_s = 158\ d_s - 415.9\ d_s^2$	0.99	-1.84	3.70	45.55
	WLS	$\mathbf{v_s = 163\ d_s - 473.5\ d_s^2}$	0.99	-8.74	2.21	31.17
$0.1cm < d_s \le 1cm$	LS	$\mathbf{v_s = 78.0\ d_s - 39.36\ d_s^2}$	0.99	40.91	3.98	4.90
	WLS	$v_s = 84.8\ d_s - 47.45\ d_s^2$	0.99	45.71	4.41	5.84

The results of the polynomial regression analysis are summarized in Table 3. Based on the values of R^2 which, as mentioned is not always a good indicator of the goodness of a regression fit, and better, the AIC, the best polynomial is highlighted for each diameter category. Also indicated are the standard-errors of the two estimated regressors b_1 and b_2. The corresponding *p*- values indicate that these regressors are statistically significant, particularly, for the second and third diameter groups which encompass more data than the first one. Table 3 indicates also that for the first two diameter categories WLS provides better results than LS, whereas for the last category the opposite is true. However the differences appear to be only minor. The selected polynomial regression lines are shown, together with the lower and upper confidence lines (Eq. 17), in the right panels of Fig. 2. Also plotted are the error bars, indicating the standardized (normalized) standard deviations s_i of the mean fall velocities, i.e. the predictors.

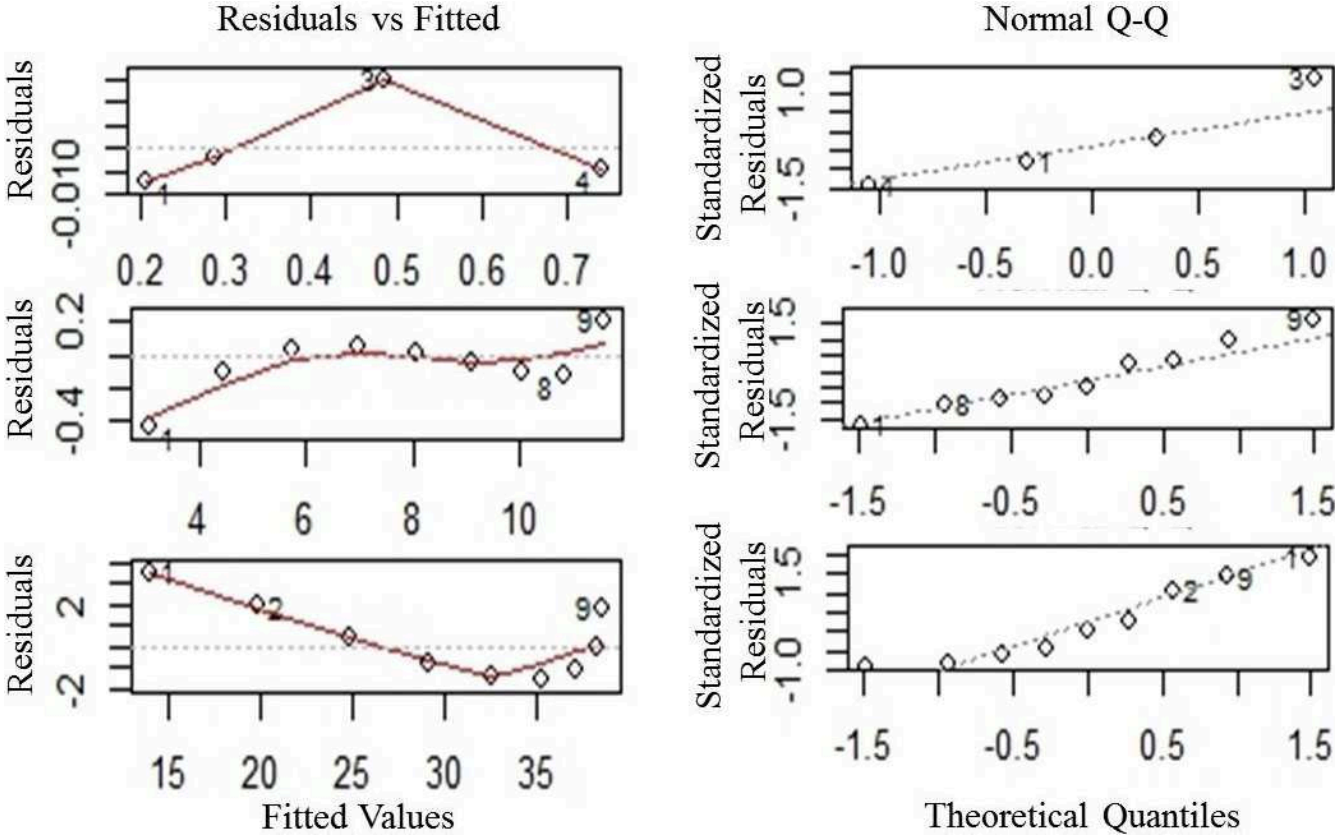

Figure 3. Left panels: Regression residuals for the three diameter classes. Right panels: Corresponding normal Q-Q plots.

One can notice that these are becoming steadily larger with increasing particle diameter or fall velocity, i.e. heteroscedasticiy is clearly present in the data.

For further model verification residual plots and Q-Q normal plots are shown in Fig. 3. The residual plots, namely that of the largest diameter category, shows variations which might be further evidence for the heteroscedasticiy , with $E(\varepsilon) = 0$, but with no specific trend. The Q-Q plots indicate that the assumption of normally distributed errors $\varepsilon \sim N(0, V\sigma^2)$ is true. Thus, the theoretical statistical properties of the MLE, namely, unbiasedness and minimum variance (Draper and Smith, 1998) appear to be guaranteed.

As the previous regression analyses of the fall velocity have only been carried out for a water temperature of 20°C, corrections for other temperatures have been done by a linear adjustment. More specifically, for temperatures *T* other than 20°C, the fall velocity v_s^T is calculated by

$$v_s^T = v_s^{20} + \Delta v \tag{18}$$

where v_s^{20} is the velocity for 20°C water temperature and Δv is the correction coefficient, which is computed from the difference of the theoretical mean velocity (Table 1), with the corresponding temperature *T,* and of the 20°C- regression predictor (Table 3).

The results obtained for Δv as a function of the particle diameter are listed in Table 4 for temperatures *T*= 0, 20, 30 and 40°C. Values for other temperatures may be estimated by linear interpolation.

Table 4. Fall velocity correction coefficient Δv as a function of the particle diameter for different temperatures.

d_s(cm)	T=0°C	T=10°C	T=30°C	T=40°C	d_s(cm)	T=0°C	T=10°C	T=30°C	T=40°C
0.005	-0.09	-0.05	0.05	0.09	0.09	-0.75	-0.31	0.22	0.37
0.006	-0.12	-0.07	0.07	0.15	0.1	-0.61	-0.25	0.17	0.3
0.008	-0.22	-0.11	0.1	0.23	0.2	-0.39	-0.16	0.11	0.19
0.01	-0.3	-0.16	0.17	0.33	0.3	-0.3	-0.12	0.08	0.15
0.02	-1.01	-0.44	0.36	0.65	0.4	-0.25	-0.1	0.07	0.12
0.03	-1.06	-0.46	0.36	0.65	0.5	-0.21	-0.09	0.06	0.11
0.04	-1.06	-0.45	0.34	0.6	0.6	-0.19	-0.08	0.05	0.09
0.05	-1	-0.42	0.31	0.54	0.7	-0.17	-0.07	0.05	0.09
0.06	-0.94	-0.39	0.28	0.49	0.8	-0.16	-0.06	0.05	0.08
0.07	-0.87	-0.36	0.25	0.44	0.9	-0.15	-0.06	0.04	0.07
0.08	-0.81	-0.33	0.23	0.41	1	-0.14	-0.06	0.04	0.07

6 CONCLUSIONS

The analysis of sediment transport in river engineering problems, such as sedimentation in river courses, morphological changes of river banks, designing the settling basins of water conveyance networks, and sedimentation of dam reservoirs, needs suitable relations to estimate the fall velocity v_s of sediment particles. This fall velocity of a particle in a fluid is computed from a force equilibrium, i.e. in which the sum of the gravity-, buoyancy- and fluid drag force are equal to zero. The fall velocity depends on the density and viscosity of the fluid, and the density, size (diameter d_s), shape, and surface texture of the particle.

In this study eight of the most important relations developed over a period of more than a century for the fall velocity for a range of particle sizes have been evaluated. A mean fall velocity from these proposed relationships is computed and these have been used, after elimination of outliers by a boxplot method, to develop new, but simple, second order polynomial equations for v_s (d_s). Both, classical least squares and a maximum likelihood method have been employed, wherefore the latter allows the incorporation of the heteroscedascity of the model errors by a weighted least squares approach, so that the estimator should theoretically be more reliable. For both methods, very good adjustments of the "observed" mean velocities by the polynomial regressions are obtained, as measured by R^2 of 0.99, but more distinctly, by low values of the *AIC*. We advocate to use these regression equations in future applications of sediment transport as discussed above, as they truly represent a distillation of the many historical, sometimes confusing, empirical relationships between settling velocity and particle size.

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