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Determination of Nusselt Number of Herschel Bulkley Nanofluids by Using CMA-ES Algorithm

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Abstract
Drilling muds are the most applicable fluids in drilling. Two basic types of drilling fluids are used, water based muds (WBM) and oil based muds (OBM). Water based muds are more applicable than oil based muds. One of the most important applications of this fluid is cooling a bit. Chemical engineers try to change drilling mud's rheological property in order to increase heat transfer to the bit. Rheological properties of drilling muds are well described by the Herschel Bulkley model. Adding polyacrylic acid to water changes its rheological property to Herschel Bulkley fluid. Standard equations like Shah and London and Hausen correlations were not able to predict local Nusselt number of non-Newtonian fluids.This study concerns estimating parameters of a local Nusselt number of Herschel Bulkley fluids with CuO nanoparticles in four concentrations of 0.1, 0.3, 0.6 and 0.05% in constant heat flux and laminar region. A nonlinear optimization algorithm (CMA-ES) was used to estimate local Nusselt number. There is good agreement between experimental data and those predicted by proposed correlations with R^2 greater than 0.99.

Keywords: *Drilling Muds, Herschel Bulkley Fluid, local Nusselt Number,CMA-ES Algorithm*

1. Introduction
Numerous industries such as pharmaceutical, petrochemical, food industries and electronic industries deal with the fluid flow behavior of non-Newtonian fluids due to wide applications. Drilling fluid is one of the most applicable ones in chemical engineering. Drilling fluids perform several functions in drilling operations including controlling formation pressures, maintaining hole integrity and stability, cooling and lubricating the drill bit and the drill string, cleaning the bottom hole, and suspending cuttings in the annulus when circulation is stopped or carrying them to the surface during drilling [1]. For having these properties, they follow the Herschel Bulkley rheological model and their rheological properties.

The Herschel Bulkley model is characterized by the following equation:

$$\tau = \tau_0 + K\gamma^n \qquad (1)$$

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τ and τ_0 are shear stress and fluid yield stress, γ is shear strain rate and K and n are fluid consistency and fluid behavior indices.The Herschel-Bulkley model is commonly used to describe materials such as concrete, mud, dough, toothpaste, bentonite-based drilling muds, Minced fish paste, raisin paste, starch, sodium polyacrylate, phosphate and polyethylene oxide. Some researchers investigated heat transfer of Hershel Bulkley material [2-6], the rheological property of drilling fluid [7-9] and estimating parameters using an algorithm[10-13].

The term nanofluid refers to a kind of fluid consisting of nanometer-sized particles with high thermal conductivity dispersed in a common base fluid such as water, a denomination introduced by Choi [14]. Many researchers studied the convective heat transfer of nanofluids in the laminar regime [15-17], in developing region [18], fully developed laminar flow regime [19, 20] and laminar and turbulent region [21, 22]. They found that the heat transfer coefficient enhanced with increasing nanoparticles concentrations. Heat transfer coefficient of MWCNT nanofluids in the horizontal tube under laminar flow regime increase with the axial distance and for fixed axial distance decrease with Reynolds number [23].Researchers investigated the laminar convective heat transfer and viscous pressure loss for alumina-water and zirconia-water nanofluids in a flow loop with a vertical heated tube [24]. They showed that the heat transfer coefficients in the entrance region and in the fully developed region increased by 17% and 27%, respectively, for alumina–water nanofluid at 6 vol.% with respect to pure water. Moreover, heat transfer coefficient of zirconia–water nanofluid increased approximately 2% in the entrance region and 3% in the fully developed region at 1.32 vol%.

Recently, some researchers studied non-Newtonian nanofluid, where the increased nanoparticles concentration in a solution of carboxymethyl cellulose improved heat transfer [25, 26], thermal conductivity [27], rheological characteristics of non-Newtonian nanofluids [28] and heat transfer of polyacrylic acid nanofluids [29].Some authors use integral transform method in annular duct [30] and circular tube and parallel plate duct [31], Simplified Method [32] and finite volume [33] to calculate Nusselt correlation of Herschel Bulkley fluid. Covariance matrix adaptation evolution strategy (CMA-ES) [34, 35] was evaluated for estimating parameters of Nusselt correlation for Herschel Bulkley nanofluid with constant heat flux boundary condition. As the performance of this method in prediction of complicated equations is high, this method is used for prediction of Nusselt number in Herschel Bulkely nanofluids. CMA-ES has rarely been used in chemical engineering [36, 37]. They found that CMA-ES is a reliable algorithm for estimating parameters. In this article, new local Nusselt correlations were suggested for Hershel Bulkley fluid with CuO nanoparticle by using CMA-ES algorithm.

2. Covariance matrix adaptation evolution strategy algorithm (CMA-ES)

CMA-ES was introduced by Hansen and Ostermeier in 1996. CMA-ES is a state-of-the-art stochastic and iterative optimization algorithm where, at each iteration, population of candidate solution is sampled. The initial population is generated by sampling a multivariate normal distribution. One of the most important properties of the CMA-ES is its invariance [38, 39]. Invariance properties are invariance to order preserving, invariance to angle preserving, scale invariance, invariance to scaling of variable and invariance to any invertible linear transformation of the search space where the first two of them are more important [35].CMA-ES has two methods of derandomized and cumulation, in derandomized mutation distribution changes deterministically. It will happen by gathering information about successful search steps and using them to modify the covariance matrix mutation distribution so that the probability of the previously successful step is increased.With cumulation, the information from the past generations is used in the self-adaptation by considering the search-path the population has undergone [40]. Offspring generation, selection and recombination, adapting the covariance matrix and step size control are four important operators in the process of evolution [41, 35]. A simplified algorithm taken from Hansen [35] is presented in Fig. 1.

Step 1: Set parameters and initialization

Set parameters: population size λ, parent number μ, recombination weights $\omega_{i=1\cdots\mu}$, learning rate for the cumulation for the step size control c_σ, damping parameters d_σ, learning rate for the cumulation for the rank-one update c_c, c_1 and c_μ to their default values. [35]

Set evolution paths p_σ, p_c, covariance matrix $C = I$, and iteration number g=0.

Choose distribution mean m and step size is σ.

Step 2: Evolution loop

Stop when termination criterion is met, g=g+1

Sample new population of search points, for $k = 1, \cdots, \lambda$

$$z_k \sim \mathcal{N}(0, \mathrm{I}) \tag{2}$$

$$y_k = BDz_k \quad \sim \mathcal{N}(0, \mathrm{C}) \tag{3}$$

$$x_k = m + \sigma y_k \quad \sim \mathcal{N}(m, \sigma^2 \mathrm{C}) \tag{4}$$

Selection and recombination

$$\langle y \rangle_w = \sum_{i=1}^{\mu} \omega_i y_{i:\lambda} where \sum_{i=1}^{\mu} \omega_i = 1,\ \ \omega_i > 0 \tag{5}$$

$$m \leftarrow m + \sigma \langle y \rangle_w = \sum_{i=1}^{\mu} \omega_i x_{i:\lambda} \tag{6}$$

Step-size control

$$P_\sigma^{(g+1)} \leftarrow (1 - c_\sigma).P_\sigma^{(g)} + \sqrt{c_\sigma\ (2 - c_\sigma)\mu_{eff}}\, C^{(g)^{-\frac{1}{2}}} \langle y \rangle_w \tag{7}$$

$$\sigma^{(g+1)} \leftarrow \sigma^{(g)}.exp\left(\frac{C_\sigma}{d_\sigma}\left(\frac{\left\| P_\sigma^{(g+1)} \right\|}{E(\|\mathcal{N}(0, I_d)\|)} - 1\right)\right) \tag{8}$$

Covariance matrix adaptation

$$P_C^{(g+1)} \leftarrow (1 - c_c).P_c^{(g)} + H_\sigma^{(g+1)} \sqrt{c_c(2 - c_c)\mu_{eff}} \langle y \rangle_w (9)$$

$$C^{(g+1)} \leftarrow (1 - c_{cov}).C^{(g)} + \frac{c_{cov}}{\mu_{cov}} P_C^{(g+1)} P_C^{(g+1)^T} + c_{cov}.\left(1 - \frac{1}{\mu_{cov}}\right) \sum_{i=1}^{\mu} \omega_i y_{i:\lambda}^{(g+1)} \tag{10}$$

Figure 1. Simplified algorithm of CMA-ES.

3. Standard correlations

Heat transfer in the pure liquids is usually characterized by using dimensionless parameters such as Nusselt, Graetz, Reynoldsand Prandtl numbers. The local Nusselt number in laminar flow with constant heat flux can be calculated as a function of the Graetz number. There are some standard correlations for calculating the Nusselt number in the circular tube. In this part, two of them are introduced and used for optimization.

3-1.The Shah and London correlation

Shah and London proposed a correlation to calculate local Nusselt number in thermally developing region with uniform heat flux in 1975[42].

$$Nu = \begin{cases} 1.953\left(Re\,Pr\frac{d}{x}\right)^{\frac{1}{3}} & Re\,Pr\frac{d}{x} \geq 33.3 \\ 4.364 + 0.0722Re\,Pr\frac{d}{x} & Re\,Pr\frac{d}{x} \leq 33.3 \end{cases}$$

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(11)

3-2. The Hausen correlation

Hausen empirical correlation is used for outer tube flow with constant surface temperature, hydrodynamically developed and thermally developing flow. This correlation is good for both liquids and gases [43, 44].

$$Nu = 3.66 + \frac{0.0668RePr\frac{d}{x}}{1+0.04\left(RePr\frac{d}{x}\right)^{\frac{2}{3}}} \qquad (12)$$

4. Optimizations

Both Shah and Hausen correlations were not able to predict non-Newtonian behavior precisely.Their standard deviations (S_D) are 3.334 and 4.6969, respectively.This work is based on constant heat flux and as Shah correlation is suggested for constant heat flux, it has better performance than Hausen, which is suggested for constant temperature. In order to evaluate the local Nusselt correlation, standard correlation forms were selected and separate codes were written for them in MATLAB R2013b. Local Nusselt was estimated in 5, 21, 39, 56, 73.5, 91, 108.5 and 125.5cm of pipe and diameter of 1cm. Reynolds number was in the range of 600 to 2000 and Prantel was in range of 4.412 to 7.083. Estimation was evaluated under 160 data of an aqueous polymer solution of 0.2% w/w polyacrylic acid in water with CuO nanoparticle [29, 45]. Each optimization was done for different concentrations of 0.1, 0.3, 0.6 and 0.05 percent of CuO in an aqueous solution of polyacrylic acid. Less than half of the data were carried out to evaluate the proposed correlations. First, it was checked with Shah, which is simpler and later Hausen. As CMA-ES is a novel and robust evolutionary algorithm, this method is used for prediction. CMA-ES is a reliable method to find the global minimum more dependably and accurately in 50 iterations than Firefly Algorithm(FA)and Shuffled Complex Evolution (SCE) [36].CMA-ES is more robust than Real coded Genetic Algorithm(RGA) and BLT method [46]. CMA-ES implements a principle component analysis of the previously selected mutation steps to determine the new mutation distribution [41]. Each new population forms a new generation until a certain termination criterion is met. Implementation of optimization will stop when four situations happen namely, stop when the fitness value is reached, stop when maximum iteration is reached, stop when the covariance matrix is numerically not positive definite and finally when the all standard deviations are smaller than what was given to tolerance [47]. In CMA-ES population size λ, parent number μ and recombination weight ω_i should be set accurately so that other parameters such as c_c,c_σ, d_σ, c_{cov} and μ_{cov} can be derived from them. Pertinent details of parameters used in this work are summarized in Table 1.

Table 1. Selected value of parameter used in implementation of CMA-ES.

Method	Parameter	Selected value
CMA-ES	σ N	0.5 3D (Shahand London correlation) 4D (Hausen correlation)

5. Results and discussion

All optimizations were carried out with CMA-ES algorithm code obtained by Hansen [35]. CMA-ES is shown as a reliable method for estimating parameters. Correlation (13) was obtained after 121 iterations and 728 NFE and correlation (14) was obtained after 347 iterations and 2778 NFE. Increasing the population in many cases, considerably increases the performance of the algorithm [48]. In Table 2 the modified correlations derived by CMA-ES algorithm for Herschel-Bulkley nanofluid containing CuO particles are listed. Figs.2 and 3 show the comparison of modified correlations in six different Reynolds numbers with standard deviation (S_D) and R square (R^2).

Table 2. Correlations derived by CMA-ES.

Correlation	Correlation name	Correlation number
$Nu_{Local} = 2.8505\left(Re\,\mathrm{Pr}\frac{d}{x}\right)^{0.31317} - 1.0489$	Modify Shah	(13)
$Nu_{Local} = 0.69247 + \frac{0.99711\left(d/x\right)Re\,Pr}{1+0.35757[\left(d/x\right)Re\,Pr]^{0.69045}}$	Modify Hausen	(14)

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_{exp} \tag{15}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(y_{exp}-y_{cal}\right)^2}{\left(y_{exp}-\bar{y}\right)^2} \tag{16}$$

$$S_D = \sqrt{\frac{1}{n}.\sum_{i=1}^{n}\left(q_{cal(i)} - q_{\exp\,(i)}\right)^2} \tag{17}$$

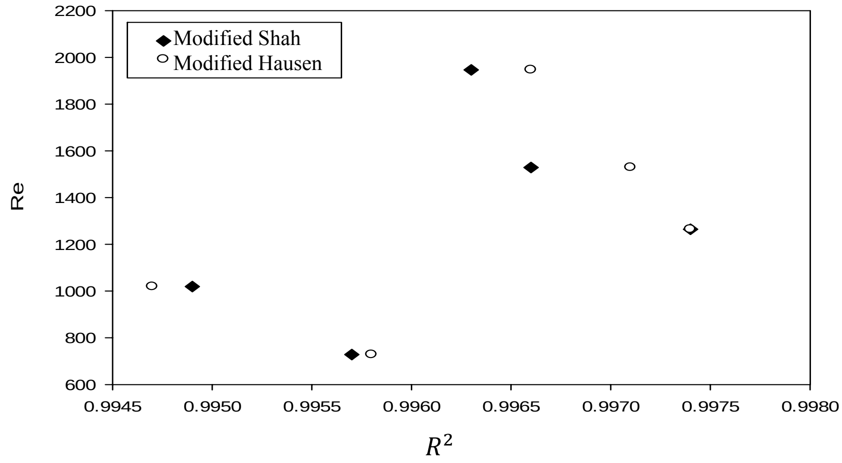


Figure 2. Comparing R^2 of derived correlations with different Reynolds number.

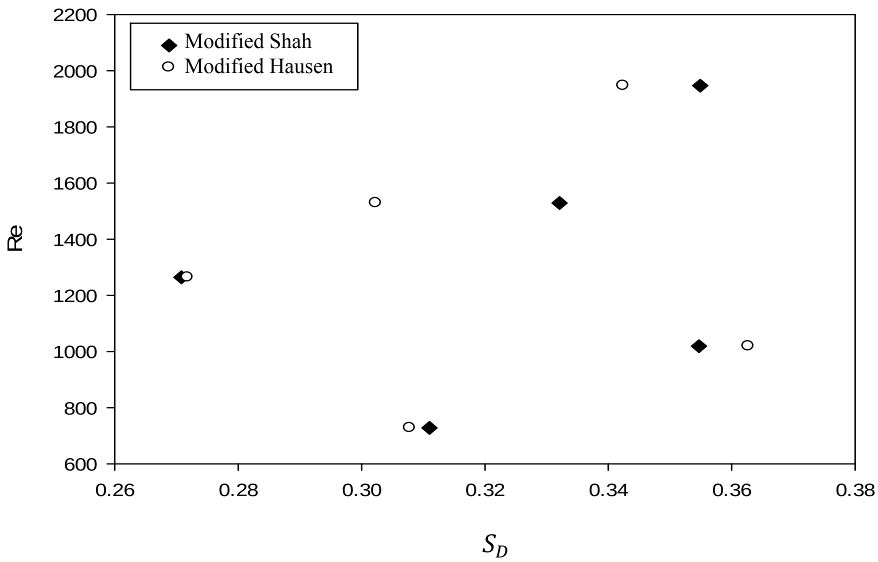
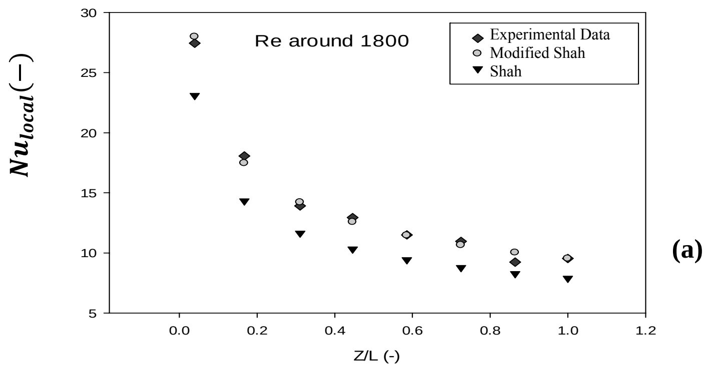


Figure 3. Comparing standard deviation of derived correlations with different Reynolds number.

The maximum S_D of the modified Shah and modified Hausen were 0.4439 and 0.4284, respectively. In general, the modified Hausen equation was found to be superior to the modified Shah, even though their difference is negligible.

The local Nusselt number decreases with the increase of axial distance because the boundary layer thickness increases with axial distance. Suspended particles in a fluid migrate from the high shear rate region to the low shear rate region [16]. Due to this phenomenon, nanoparticles concentration and thus apparent viscosity of the nanofluid decrease near the wall and as a result, cause smaller boundary layer thickness [29]. Furthermore, the stochastic movement of particles causes the increase of temperature difference and rate of heat transfer will increase.

Fig.4 (A, B) shows difference between the modified correlations, Herschel Bulkley nanofluid experimental data and base correlations. The equations derived by CMA-ES have a good agreement with experimental data. CMA-ES used derandomization to increase the probability of producing previously selected mutation steps again[41]. The unique feature of CMA-ES is the mutation procedure. It is carried out each generation after the best search points are selected and, during the recombination step, their weight is computed. By mutation, Gaussian noise is added, which is determined by a correlated sample distribution that is continuously adapted during the optimization procedure. Later, CMA-ES learns the pair-wise dependencies of the decision parameters by updating a covariance matrix of the sample distribution [47]. This way, it adapts to the structure of the objective function and quasi exploits second-order information. It is implemented in a way that this updating mechanism is independent of the coordinate system, which makes this evolution strategy an efficient and robust solver and enables it to predict data in a better way. Power law index (n) of TiO_2 and Al_2O_3 of Herschel Bulkley nanofluid decreases with increasing particle concentration, however CuO increase. Thermal conductivity and consistency indices of TiO_2, Al_2O_3 and CuO nanofluids increase with increasing particle concentration [29]. Proposed correlations for CuO were evaluated for TiO_2 and Al_2O_3 particles in Fig. 5. Fig. 5 shows the proposed correlations were able to predict other nanoparticles local Nusselt well.



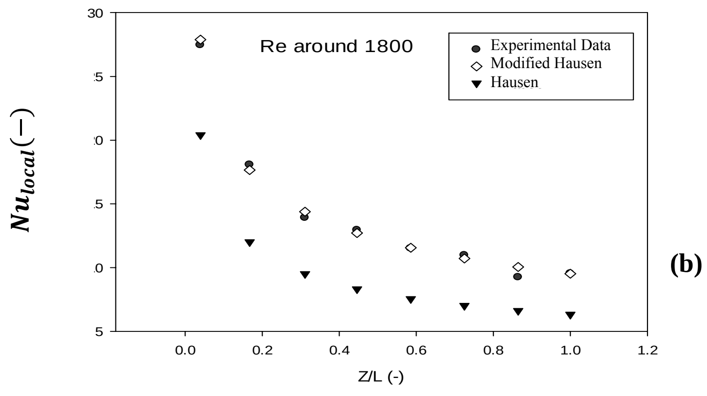


Figure 4. (a, b). Comparing proposed correlations with experimental data.

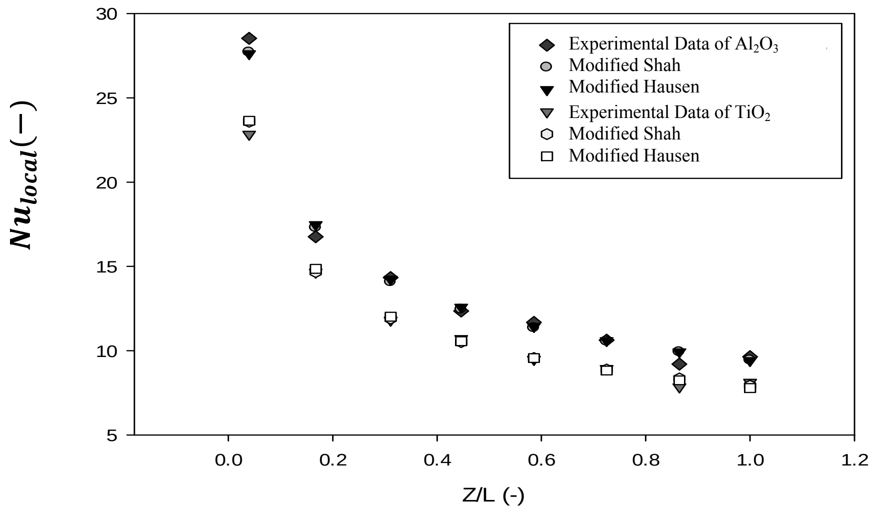


Figure 5. Comparing prediction of proposed correlations for different nanoparticles.

This methodology is not limited to polyacrylic acid, it can be used for other drilling fluids like carboxymethyl cellulose (CMC) and PHPA. New correlations have been determined to predict minimum agitation speed (N_{js}) for solid suspension in non-Newtonian fluids of carboxymethyl-cellulose (CMC+water) and polyacrylic acid (PAA+water) by using CMA-ES algorithm and the method was sufficient for both non-Newtonian fluids [49].

6. Conclusions

Due to the limits of applicability of the Nusselt correlations in predicting Nusselt number of non-Newtonian fluids, two new correlations to handle a local Nusselt number of Herschel Bulkley nanofluid were introduced in this paper. A nonlinear optimization algorithm, CMA-ES was used to estimate the parameters of the Shah and London and Hausen correlations. CMA-ES has a good performance for optimizing simple correlation like Shah and London and complicated one like Hausen. CMA-ES was found to be an effective and reliable algorithm to find the global minimum. In CMA-ES the first population is generated based on the number of dimensions while in selection, best search points are selected. Also, during recombination their weights are calculated and step size and covariance matrix were updated accordingly. This cycle is repeated until one stopping criterion is met.The proposed correlations were not only sufficient to calculate local Nusselt number of an aqueous solution of polyacrylic acid with CuO nanoparticles but also are good for other nanoparticles like TiO_2 and Al_2O_3 in laminar flow with constant heat wall flux at each position of the tube.

Nomenclature

K	Constant in Herschel Bulkley mosel $(Pa\ s^{-n})$
Nu	Nusselt number (dimension less)
Re	Reynolds number (dimension less)

Pr Prantl number (dimension less)
d Diameter of the tube (cm)
x Distance along axis (cm)
n Flow behavior index (dimension less)
C Covariance matrix
D Diagonal matrix
B Orthogonal matrix
R^2 R square
$\bar{y}$ Mean of experimental data
n number of data
SD Standard deviation
NFE Number of Function Evaluations

Greek Symbols

τ Shear stress (Pa)
τ_0 Yield stress (Pa)
γ Shear strain rate (s^{-1})
σ Step size

Subscripts

Exp Experimental
Cal calculated

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