INSTITUTE FOR POLYMERS AND COMPOSITES

ML DRIVEN MODELS TO PREDICT THE DRAG COEFFICIENT OF A SPHERE TRANSLATING IN SHEAR-THINNING VISCOELASTIC FLUIDS

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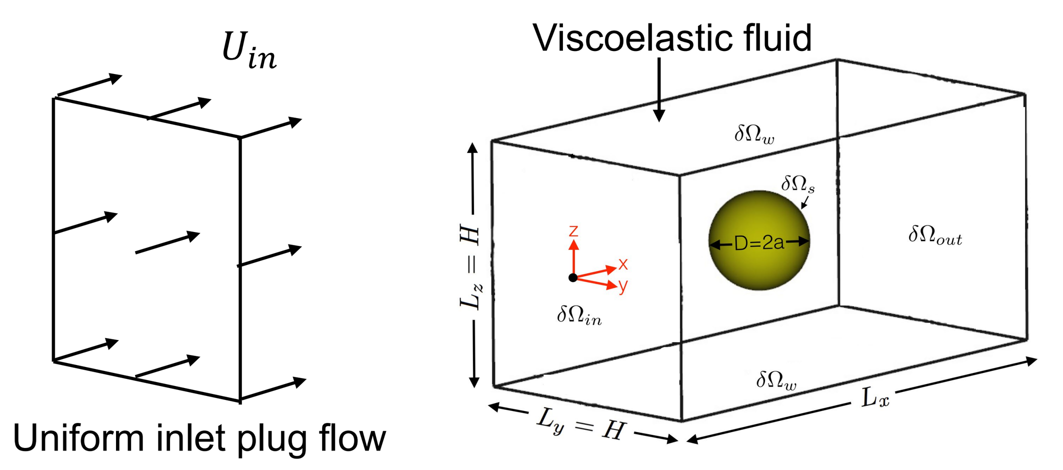
INTRODUCTION

- Non-Newtonian fluid suspensions are widely used in several areas of our daily life, from toothpastes to drilling muds to injection molding of filled polymers melts.
- However, an efficient numerical solver capable of simulating such processes is still missing in the scientific literature.
- For this purpose, a 3D CFD-DEM viscoelastic solver is developed in this work to handle particle-laden viscoelastic flows using a new approach, based on machine learning (ML) models, to compute a particulate-phase drag model valid for a wide range of material parameters.



$$Re = 2Re_a = \frac{2a\rho U_{in}}{\eta_0}$$

$$Wi = \frac{\lambda U_{in}}{H}$$

$$\zeta = \frac{\eta_P}{\eta_0}$$

- To calculate the dimensionless viscoelastic drag correction factor, χ (Wi), we begin with 3D direct numerical simulations (DNS) of unconfined viscoelastic flows (with the shear-thinning Giesekus fluid model) over a wide range of parameters, specifically for Reynolds number $Re \leq 50$, Weissenberg number $Wi \leq 5$ (λ is the relaxation time), retardation ratio $0 < \zeta < 1$, (η_0 is the viscosity in the limit of vanishing shear rate and η_P is the polymeric contribution to the viscosity) and the mobility parameter $0 < \alpha < 1$.
- A total of approximately 3000 DNS were performed and the results obtained enable the development and validation of machine learning models which relate the input data (specifically *Re, Wi*, ζ and α) to the output (response) variable, here the dimensionless viscoelastic drag correction factor on the particle, χ (Wi).
- A number of different ML algorithms are considered, including the Random Forest (RF) [1], Gradient Extreme Boosting (XGBoost) [2] and Deep Neural Network (DNN) [3].
- The data set is divided into training and testing subsets to compare with the predicted data, in percentage 80/20, respectively.
- To train and compare the performance of aforementioned models, the accuracy is evaluated based on three common statistical indicators, R^2 (R-squared), RMSE (root mean squared error) and MAPE (mean absolute percentage error).

$$R^2 = \frac{\sum_{i=1}^{n}(y_i - y_i^*)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i^*)^2}\ ,\quad RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - y_i^*)^2}\ ,\quad MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i^* - y_i|}{y_i} * 100\%$$

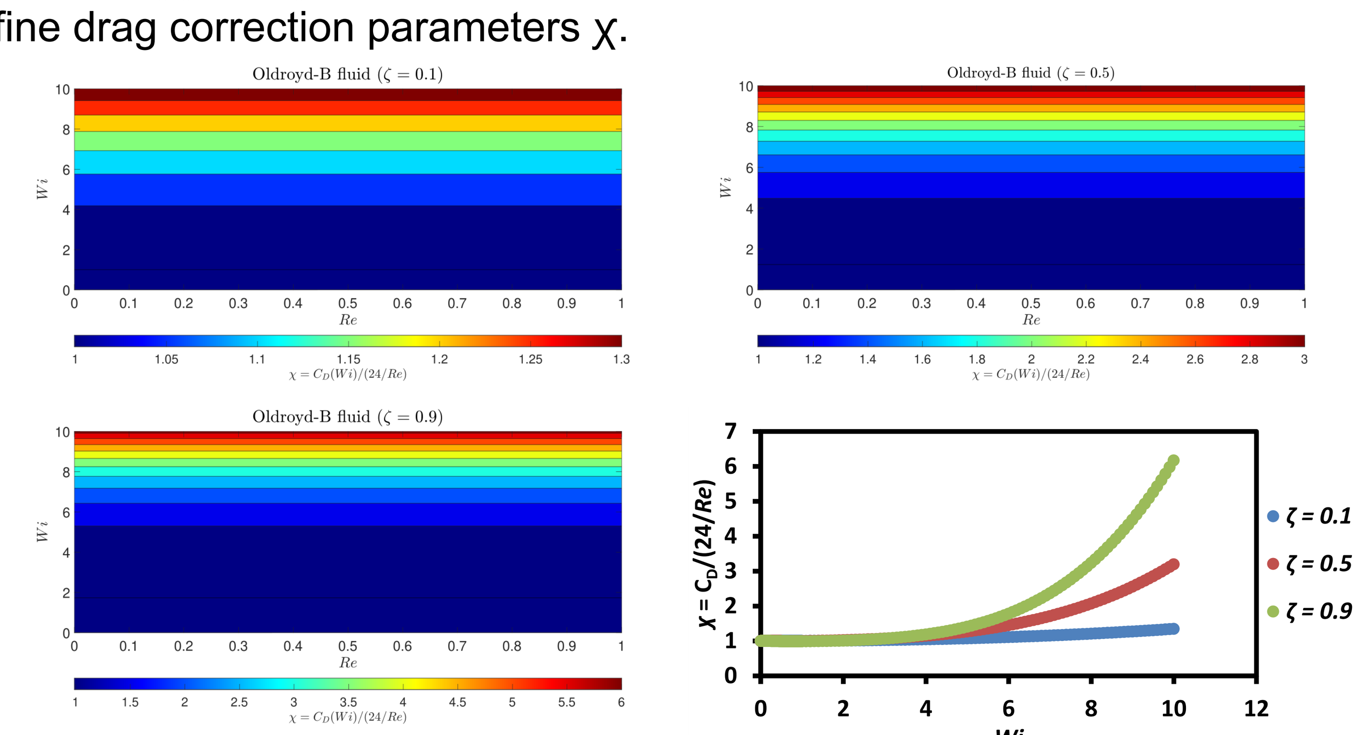
where y_i^* are the observed values, $\bar{y}_i^*$ is the mean of the observed values and y_i are the predicted values.

RESULTS AND DISCUSSION

1. VALIDATION OF THE DEEP LEARNING METHODOLOGY WITH THE CLOSURE DRAG MODEL FOR THE OLDROYD-B FLUID

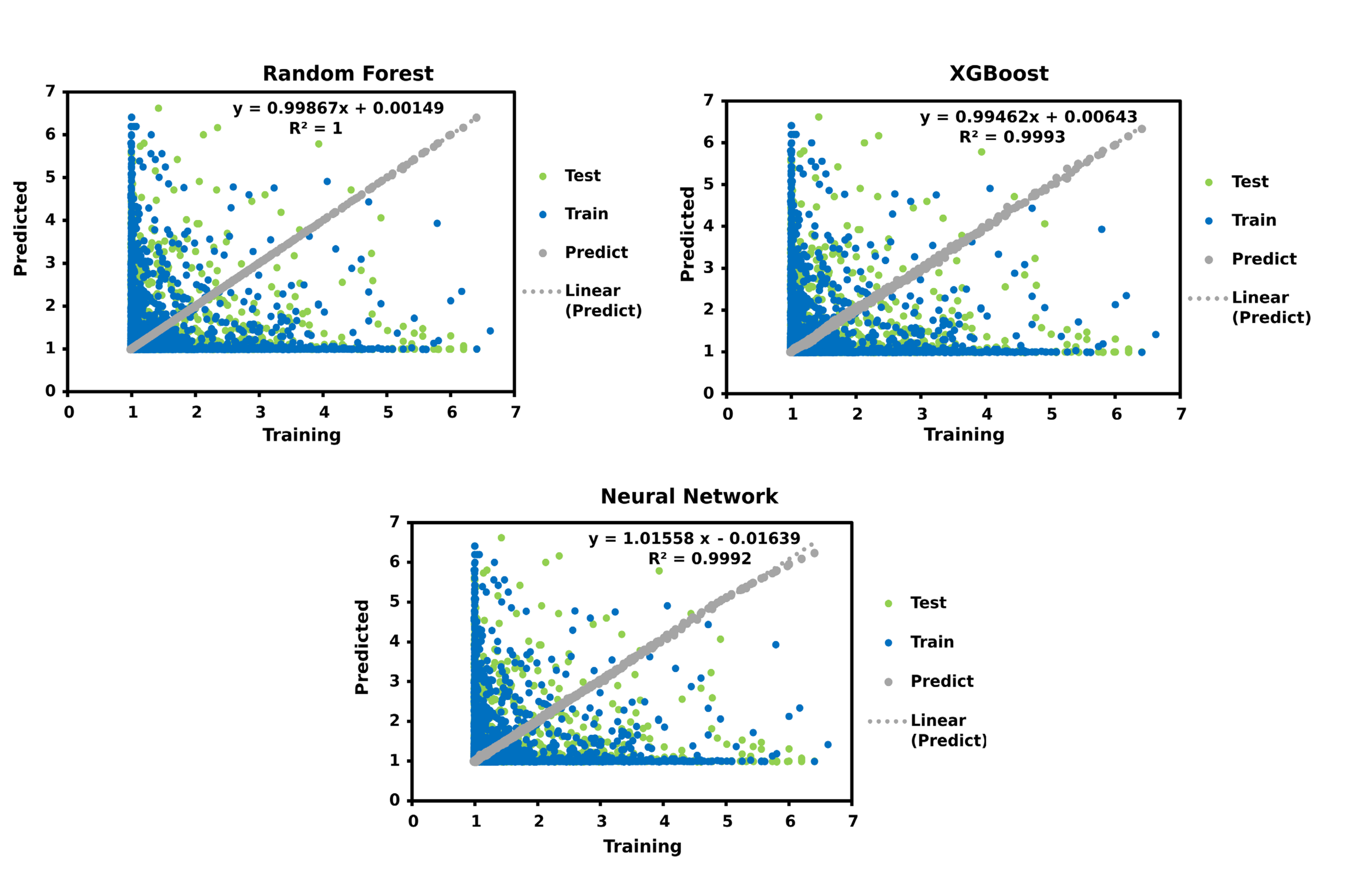
1.1. DNS RESULTS

- The data obtained from the closure drag model existent for the Oldroyd-B fluid [4] are represented for three different retardation ratio (ζ = 0.1, 0.5 and 0.9).
- The evolution of the dimensionless drag coefficient behavior is self similar, for $Re \leq 1$, suggesting the dependence on inertia can be factored out and we can define drag correction parameters χ.



1.2. DATA DRIVEN MODELS

- The test values (green points), training values (blue points), as well as the regression line and predicted values (points and gray line) for each ML model are presented.
- The regression equation show remarkable accuracy between tested and predicted values, as shown by the large R^2.



- For the Oldroyd-B fluid the ML model that presents the best R^2 (as well as the lowest values of RMSE and MAPE) is the Random Forest model.

	RF	XGBoost	DNN
R^2	1.0	0.9993	0.9992
RMSE	0.0032	0.0177	0.019
MAPE	0.0343	0.5943	0.6958

1.3. COMPARISON WITH CLOSURE DRAG MODEL AND SIMULATED DATA

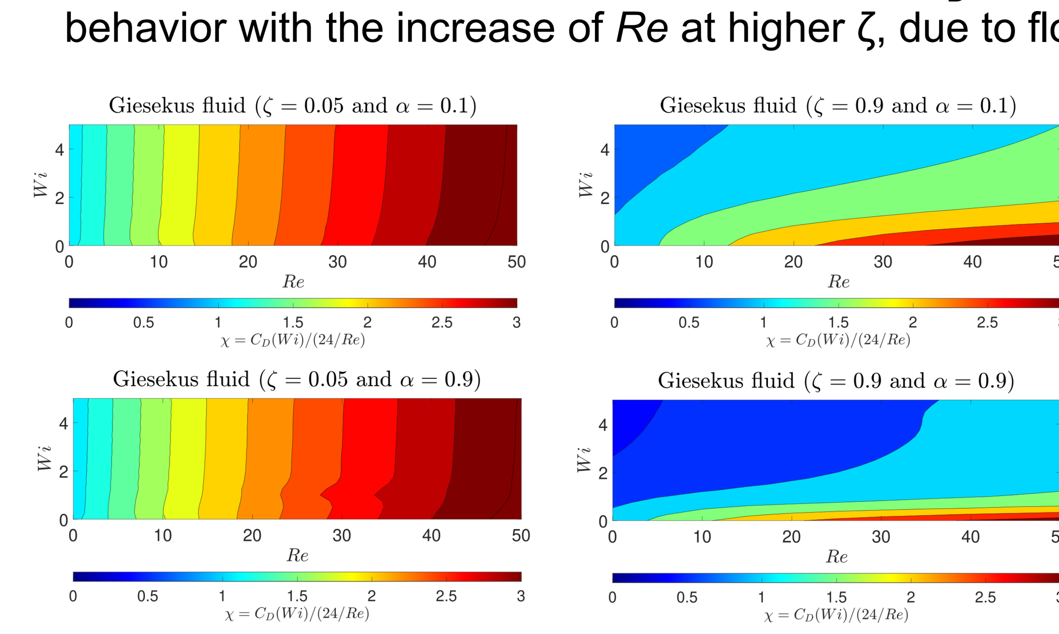
- Relative errors were calculated between the values predicted by the ML models and the actual values given by both a closure drag model [4] and numerical simulations data.
- The first three lines of the table refer to data that were used in the training of the algorithms (from the closure drag model), with a maximum error of 0.67%, and the last two lines show the comparison with data from numerical simulations, with a maximum error of 10.88%.

	ζ	Re	Wi	χ	RF	% Error	XGBoost	% Error	DNN	% Error
Training	0.1	1	3	1.0240	1.0240	0.0005	1.0254	0.1379	1.0303	0.6194
	0.5	0.5	0.5	0.9979	0.9979	0.0004	0.9976	0.0314	0.9942	0.3663
	0.9	0.1	1	0.9882	0.9885	0.0283	0.9942	0.6026	0.9949	0.6739
Validation	0.5	0.3	1.5	1.1154	1.0057	9.8347	1.0021	10.1554	0.9942	10.8765
	0.5	0.3	2	1.1301	1.0198	9.7610	1.0154	10.1440	1.0160	10.0934

2. DEEP LEARNING MODELS FOR SHEAR-THINNING GIESEKUS FLUID

2.1. DNS RESULTS

- For the Giesekus fluid there is an additional constitutive parameter that must be considered, the mobility parameter, with range $0 \leq \alpha \leq 0.9$.
- Compared to Oldroyd-B fluid, we generated data from numerical simulations instead of using a closure drag model, because it does not yet exist for the Giesekus model. The evolution of the drag correction $\chi = C_D$ (Wi, ζ, α)/(24/Re) have a different behavior with the increase of *Re* at higher ζ, due to flow separation.

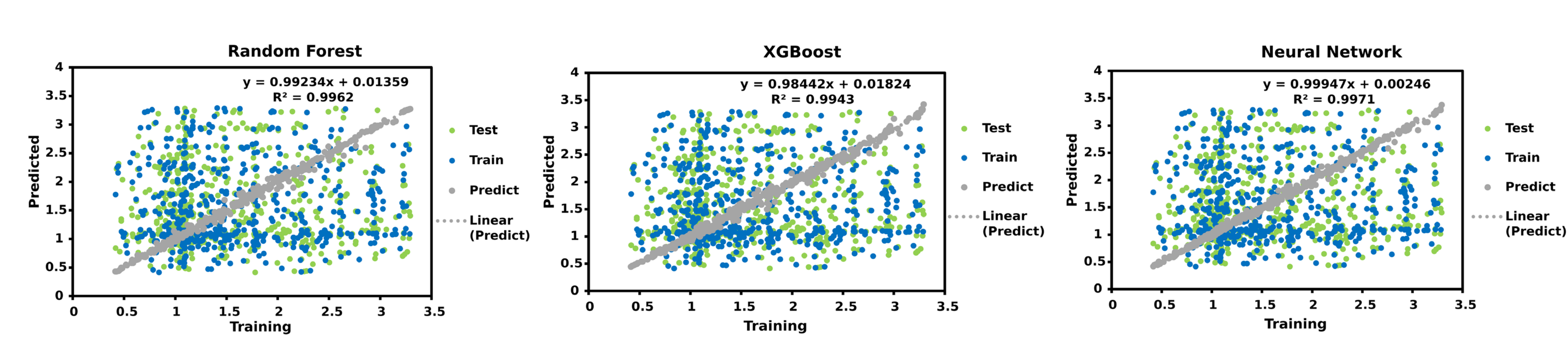


- Drag decreases with *Wi* at *Re* << 1.
- Drag increases with *Re* (even at *Wi* ≈ 0).
- Weaker drag increase with *Re* when *Wi* ≠ 0.

2.2. DATA DRIVEN MODELS

- For the Giesekus fluid the ML model that presents the best R^2 (as well as the lowest value of RMSE) is the Deep Neural Network model.

	RF	XGBoost	DNN
R^2	0.9962	0.9943	0.9971
RMSE	0.0432	0.0529	0.0376
MAPE	1.7058	2.4887	1.8592



CONCLUSIONS

- The ML models applied to predict the drag force on a sphere suspended in an Oldroyd-B and Giesekus fluids showed good performance results, allowing us to conclude that in this context, ML can be a valuable predictive tool for different kinematic conditions.
- For the Oldroyd-B fluid, the ML model with the highest R^2 was the Random Forest, while for the Giesekus fluid it was the Deep Neural Network model. This may be due to the size of the initial database, since for the Giesekus fluid we have less data to train the model.

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REFERENCES

[1] A. Liaw and M. Wiener. Classification and regression by random forest. R News, 2(3):18-22, 2002
[2] T. Chen and C. E. Guestrin. XGBoost: A scalable tree boosting system. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 785-794, 2016
[3] D. F. Specht. A general regression neural network. IEEE transactions on neural networks, 2(6):568-576, 1991.
[4] S. A. Faroughi, C. Fernandes, J. Miguel Nóbrega, and G. H. McKinley. A closure model for the drag coefficient of a sphere translating in a viscoelastic fluid. Journal of Non-Newtonian Fluid Mechanics, 277:104218, 2020.

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