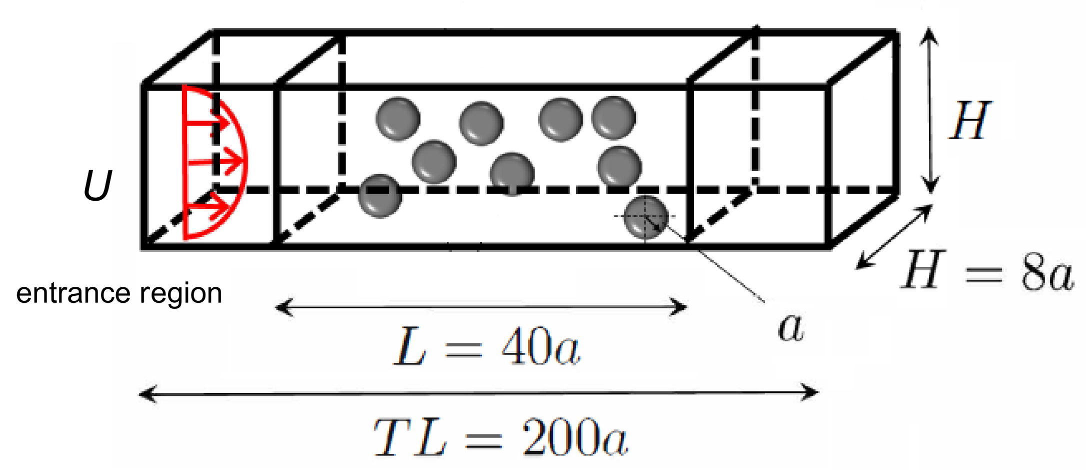
Digital-twin for particle-laden viscoelastic fluids: ML-Based models to predict the drag coefficient of random arrays of spheres

C. LOIRO[1], C. FERNANDES[1], G. H. MCKINLEY,[2] S. A. FAROUGHI[3,*]

INTRODUCTION

- The dependence of normalized average fluid-particle force F on solid volume fraction and on the rheology of non-Newtonian fluids needs to be characterized.
- Direct numerical simulations (DNS) were performed to obtain the drag coefficient of random arrays of monodisperse spherical particles translating in shear-thinning viscoelastic fluids, described by the Giesekus model.
- The normalized average fluid-particle force F is obtained as a function of the volume fraction of dispersed solids $0 \le \phi \le 0.2$, Reynolds number $Re \le 50$, Weissenberg number $0 \le Wi \le 4$, retardation ratio $0 < \zeta < 1$ and mobility parameter $0 < \alpha \le 0.5$.
- The numerical results obtained from the large-scale computations enable us to develop a meta-model, based on Machine Learning (ML) models, specifically, Random Forest [1], Deep Neural Network [2] and XGBoost [3], for the fluid-particle drag force to be used in particle-laden viscoelastic flows.



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

$$Wi = \frac{\lambda U}{H}$$

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

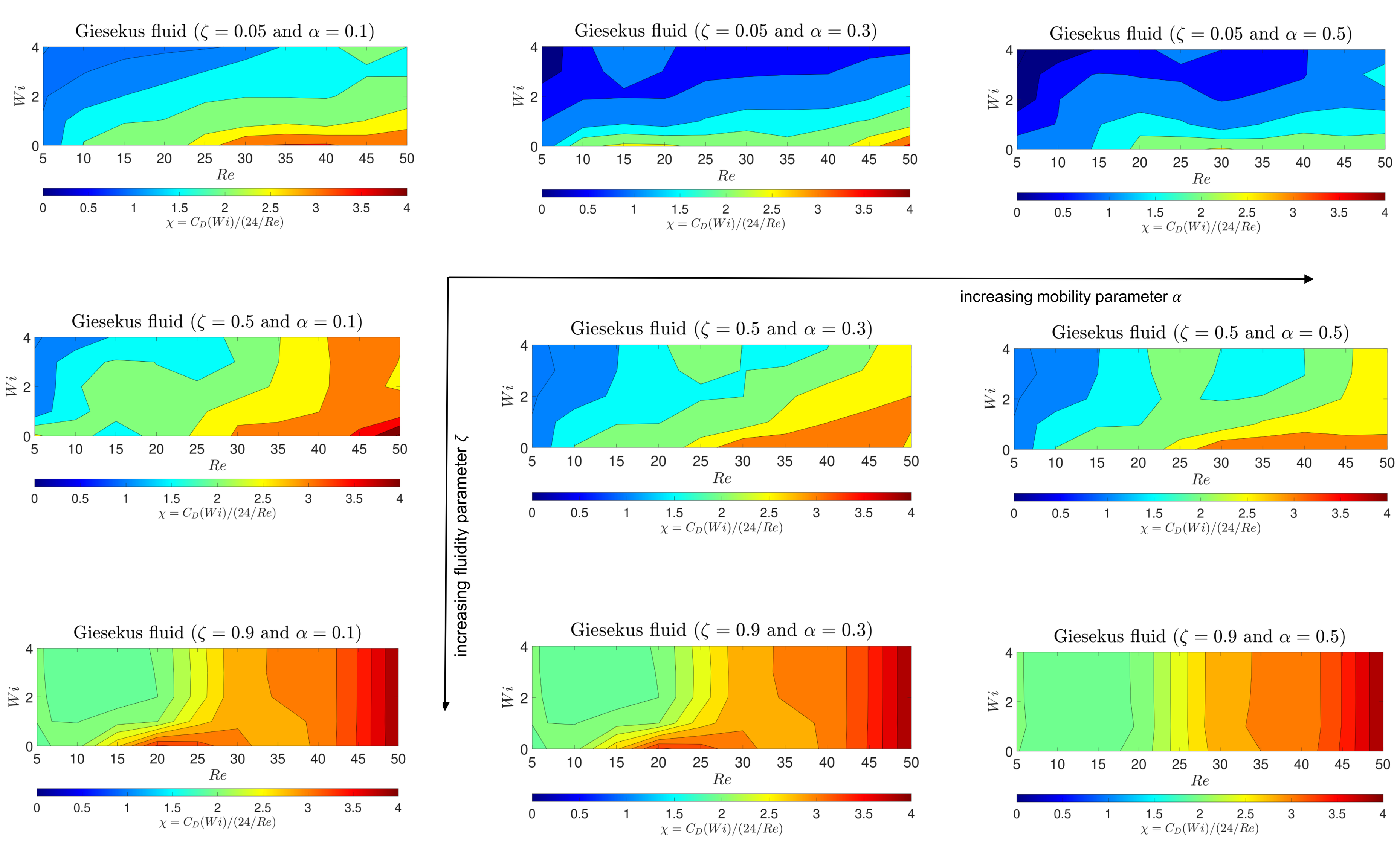
RESULTS AND DISCUSSION

1. DNS RESULTS

- Direct numerical simulations of the viscoelastic drag correction factor, χ, for random arrays of spheres translating in the shear-thinning Giesekus viscoelastic fluid model, were performed.

$$\chi = C_D(Wi)/C_D(Wi=0) = C_D(Wi)/(24/Re)$$

$$\phi = 0.04$$



2. DATA DRIVEN MODELS

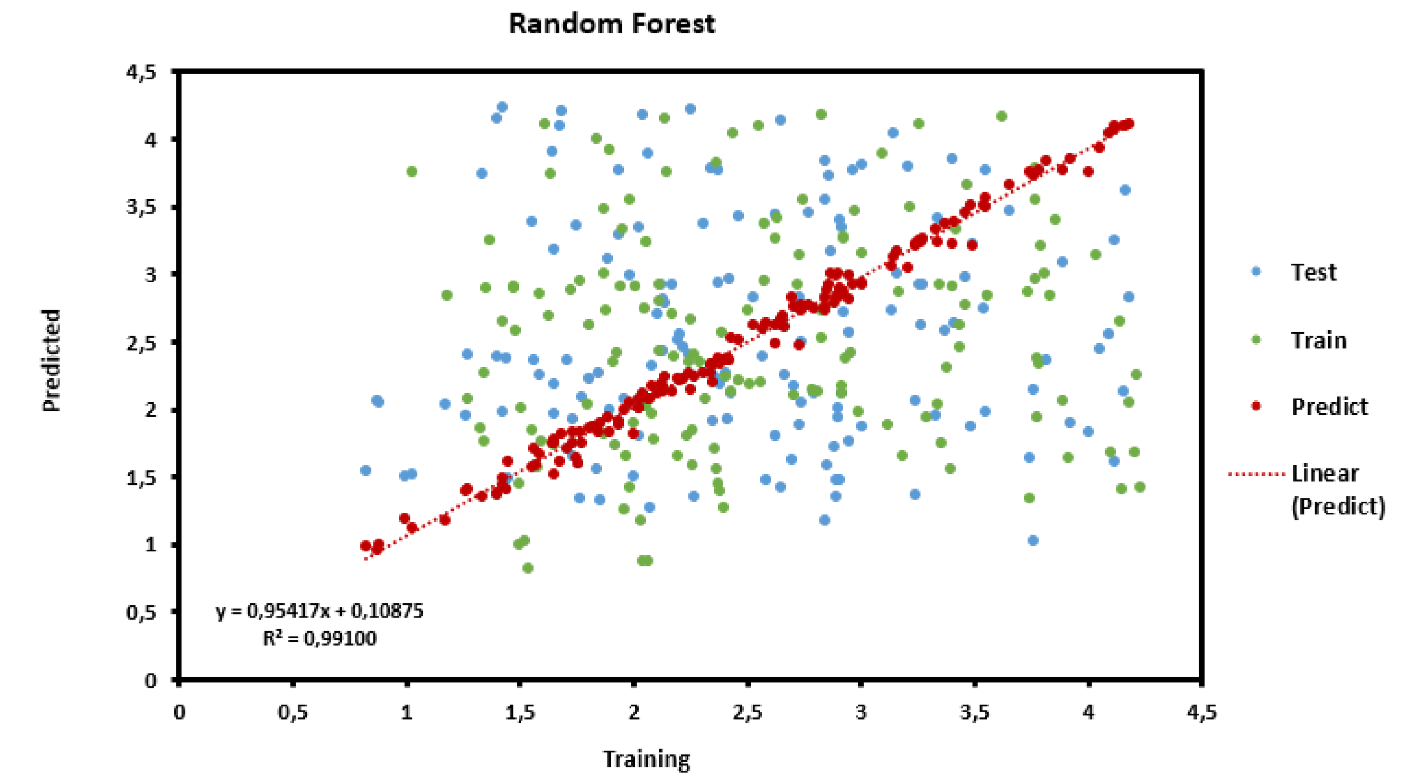
- In these models, Random Forest (RF) [1], Deep Neural Network (DNN) [2] and Extreme Gradient Boosting (XGBoost) [3] are considered. The dataset was divided into training and validation subsets and then compared with the predicted drag coefficient with a percentage 80/20, respectively.
- In order to train and compare the performance of this three models, the accuracy is evaluated with statistical indicators, RMSE (root-mean-square error), R^2 (R-squared) and MAPE (mean absolute percentage error).
- To evaluate the performance of the ML models, we present these indicators in the following table:

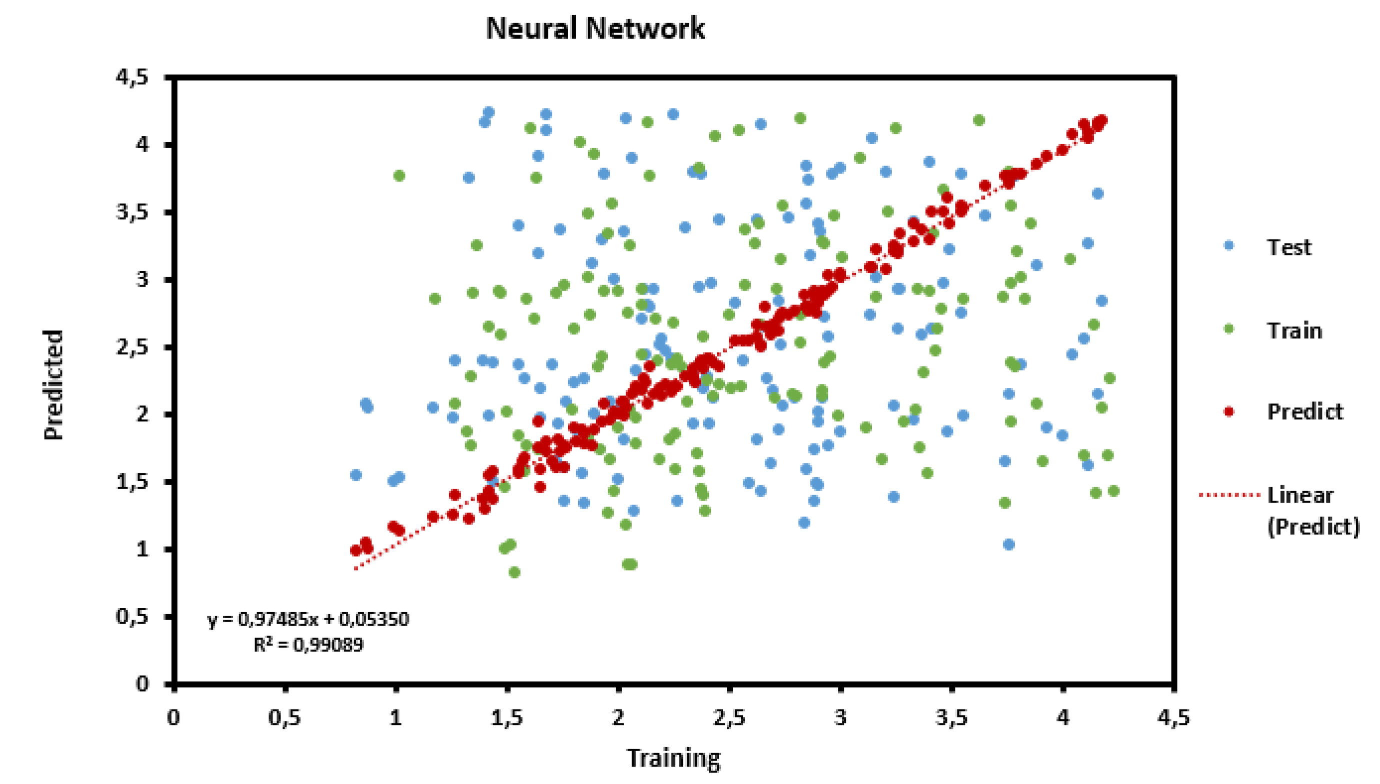
$$R^2 = \frac{\sum_{i=1}^{n}(y_i - y_i^*)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i^*)^2}, \quad RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - y_i^*)^2}, \quad MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i^* - y_i|}{y_i} * 100\%$$

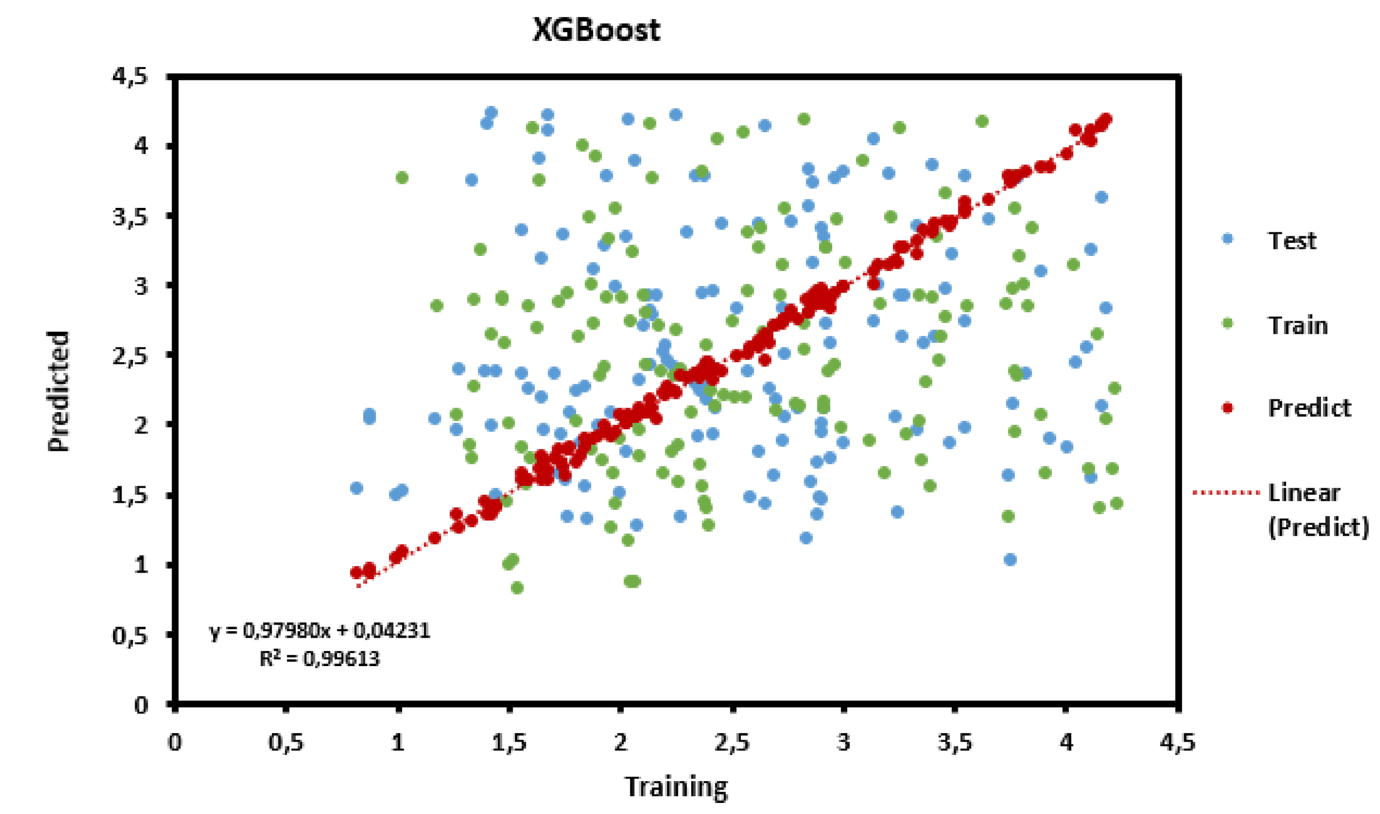
where y_i^* are the observed values, $\bar{y}_i^*$ is the mean of the observed values and y_i are the predicted values.

	Neural Network	XGBoost Model	Random Forest
RMSE	0.0786	0.0525	0.0823
R^2	0.9908	0.9961	0.9910
MAPE	3.0875	1.9935	2.9586

- The model that best suits our case study is the XGBoost Model with the highest value of R^2 and lowest RMSE.
- The table shows that the ML models are accurate ($R^2 \ge 0.98$ in all cases) with low error values.
- We show the tested values (blue points), training values (green points) and the predicted values (red points) and regression line (red line) for each model.







CONCLUSIONS

- The ML models applied to predict the drag force of monodisperse spherical particles translating in shear-thinning viscoelastic fluids, described by the Giesekus model had good performance results. The model that best suits our case study is the XGBoost model with the highest value of R^2(0.9961) and the lowest RMSE (0.0525).
- ML models can be a valuable predictive tool. Numerical simulations combined with ML techniques can coexist (e.g. Eulerian-Lagrangian viscoelastic solver where the drag coefficient $C_D(Re, Wi, \zeta, \alpha, \phi)$ is given by a ML model) for the development of new promising possibilities in computational science and engineering problems.

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[1]Institute for Polymers and Composites, Department of Polymer Engineering, University of Minho, Portugal
{b12374@dep.uminho.pt, cbpf@dep.uminho.pt }
[2]Hatsopoulos Microfluids Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, USA
{gareth@mit.edu}
[3]Petrolern LLC, Atlanta, USA {faroughisalah@gmail.com}

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