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MACHINE LEARNING PREDICTIONS FOR FLOW BEHAVIOUR OF SILVER NANOSUSPENSIONS

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Abstract

Silver nanoparticles are among the most investigated metal nanoparticle systems due to their high electrical conductivity, peculiar optical properties, and antimicrobial particularity with wide application in electronics, environmental protection, medicine, or agriculture-food industries. The rheological behaviour of nanoparticle suspensions mainly provides the knowledge required in configuring adequate processing conditions for specific applications, namely on the microstructure or interactions particle-to-particle and particle-to-fluid. Simulation and modeling that engages machine learning enable a better understanding and define the entire colloidal dispersions' behaviour. Based on the flow behaviour of colloidal nanosuspensions, predictive models capable of capturing detailed information can be built, and valuable knowledge can be obtained, which may subsequently allow the estimation of the most suitable composition with the desired rheological properties. Twelve colloidal suspensions containing silver nanoparticles in two concentrations were prepared using silver nitrate as a silver precursor, sodium alginate, and alginate/lignosulfonate in different mixing ratios as a dispersion medium. Their flow behaviour investigated through rotational measurements carried out under a controlled shear rate showed that generally, the non-Newtonian (shear thinning) behaviour depended more on dispersion media composition than the silver nanoparticles concentration. The performances of four classification algorithms, namely Adaptive Boosting, Random Forest, K-Nearest-Neighbours, and Support Vector Machine, are studied as a chemical process reverse engineering alternative to assess a nanosuspension composition based on its rheological behaviour. The predictive modeling methodology can be successfully applied to different datasets, bringing valuable insights into their behavior.

Key words: prediction, random forest, rheology, silver nanosuspension, supervised grouping algorithm

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