Prediction of attachment efficiency using machine learning on a comprehensive database and its validation

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Abstract

Colloidal particles can attach to surfaces during transport, but the attachment depends on particle size, hydro-dynamics, solid and water chemistry, and particulate matter. The attachment is quantified in filtration theory by measuring attachment or sticking efficiency (Alpha). A comprehensive Alpha database (2538 records) was built from experiments in the literature and used to develop a machine learning (ML) model to predict Alpha. The training (r-squared: 0.86) was performed using two random forests capable of handling missing data. A holdout dataset was used to validate the training (r-squared: 0.98), and the variable importance was explored for training and validation. Finally, an additional validation dataset was built from quartz crystal microbalance experiments using surface-modified polystyrene, poly (methyl methacrylate), and polyethylene. The experiments were per -formed in the absence or presence of humic acid. Full database regression (r-squared: 0.90) predicted Alpha for the additional validation with an r-squared of 0.23. Nevertheless, when the original database and the additional validation dataset were combined into a new database, both the training (r-squared: 0.95) and validation (r-squared: 0.70) increased. The developed ML model provides a data-driven prediction of Alpha over a big database and evaluates the significance of 22 input variables.

Keywords

Author Keywords: Attachment efficiency; Machine learning; Missing data; Colloid deposition

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