

### **S3.1.2 LIQUID FILTRATION MODELING OF DISORDERED FIBROUS FILTERS UNDER UNFAVORABLE CONDITIONS**

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The CFD simulations of disordered fibrous filters under unfavorable conditions were conducted to investigate the effects of interactions between particles and randomly distributed fibers with different solid volume fractions (SVFs) on the filtration performance. We employed discrete phase model (DPM), which is the Lagrangian particle tracking method in ANSYS Fluent. User-defined functions (UDFs) were developed to consider the particle deposition via interception and interaction energy calculations for particle attachment. Besides, we included the torque analysis for determining the particle detachment during the DPM process. This DPM process using UDFs was validated by performing the single collector (sphere and fiber) simulations for the wide range of collector size and fluid velocity under favorable and unfavorable conditions. The results of filtration and collision efficiencies of the single collectors were compared to the theoretical models, correlation and experimental data and we found our CFD simulations showed good agreement with the existing expressions and data. By employing our CFD simulations using the developed UDFs, the filtration and collision efficiencies of the disordered fibrous filters were studied. From the results obtained under unfavorable conditions, we concluded that solution chemistries, e.g., ionic strength and zeta potential, had a significant impact on particle deposition. Moreover, we found that the hydrodynamic drag (or torque) had an important role in preventing particle deposition, especially for larger particles at low ionic strength.