# CFD (COMPUTATIONAL FLUID DYNAMICS) MODELING TO PREDICT ADSORPTION PERFORMANCE OF FIXED BED & AMC (AIRBORNE MOLECULAR CONTAMINATION) FILTERS & OPTIMIZE GAS PURIFIERS

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A wide variety of process conditions and parameters influence the design of high-performance gas phase contamination control solutions. However, these conditions and parameters are not universally understood, yet play a vital role in the development of effective solutions. While building and testing physical prototypes will result in new solutions, this process is performed at the expense of time-to-market, the exploration of extensive design alternatives, the ability to optimize iterations, and ultimately total cost. Virtual prototyping of gas filtration and purification solutions using Computational Fluid Dynamics (CFD) can be used to simulate process conditions, chemical kinetics and thermodynamics, while avoiding the compromises of solely empirical testing. This presentation will demonstrate how ANSYS® Fluent CFD is used to predict and optimize the performance of gas filtration and purification solutions.

Adsorption performance was first modeled for a flow-through a porous medium with mass, momentum, and energy source terms defined using User-Defined Functions (UDFs). The analysis included the development of the UDFs to model the local adsorption mass transfer within an activated-media of an axisymmetric fixed-bed. This analysis resulted in an understanding of the adsorption capacity throughout the bed, as well as the local adsorption mass transfer. Each modeling result was further validated against experimental data, including breakthrough time.

Building on the success of the fixed-bed adsorption modeling, the second analysis involved predicting the removal efficiencies of AMC (airborne molecular contamination) filters. The application of CFD modeling created an efficient method to estimate the Cost of Ownership (CoO), providing a method to optimize filter life cycle strategies for products that are either exposed to many contaminants or those that utilize multiple filter types.

Finally, the CFD methodology was applied to optimize the design of gas purifiers. Performance optimization is a critical issue in designing gas purifiers that remove VOC (volatile organic compounds) because the adsorption performance varies greatly as a function of process parameters. After initial validation of the CFD model with experimental data, the model was extended to study purifier performance while varying several process parameters, including bed length, contaminant concentration, inlet flow rate and inlet pressure. Based on simulation results, a set of mathematical correlations was developed that predict adsorption breakthrough as a function of process parameters. Furthermore, using these correlations, a simplified optimization calculator was developed that effectively predicts the parametric effects on purifier performance without performing lengthy experiments or requiring designers to learn to use CFD.

The application of CFD to filtration and purification solutions has provided a powerful and valuable new resource to better understand and quickly develop products that can more efficiently control microcontamination. This methodology results in gas phase contamination control solutions that that are modeled effectively to predict future performance in removing damaging elements present in the manufacturing environment.