



Adsorption Simulator Software

ID# 2024-058

HIGHLIGHTS

- Computational fluid dynamic (CFD) simulation software to predict the gas adsorption on various geometries of monolith (honeycomb) adsorbents.
- The model facilitates the optimization of monolith adsorbent bed designs.
- Potentially enables reduction in raw material usage and minimizes disposal of exhausted adsorbents.

OPPORTUNITY

While numerous studies have explored the modeling of adsorption on monoliths, none have specifically examined the impact of monolith structures on adsorption performance. University of Alberta researchers have developed a three-dimensional (3D) coupled mass and momentum transfer model that accounts for the effect of monolith adsorbent structural parameters on the adsorption of volatile organic compounds (VOCs). They have investigated the effect of channel shape (square, triangular, and hexagonal), channel size, wall thickness, and adsorbent length in an effort to enhance the adsorption performance of monolithic adsorbents. By varying the length of the monolith, it was demonstrated that there is an optimum length to adsorb specific concentration of a VOC for a particular duration. On the other hand, the invention advances the functioning of a computer by offering a comprehensive model that includes all the essential coefficients for simulating adsorption in various media and pollutants, a feature missing in previous models.

The developed model can be used for optimizing the design of monolith adsorbent beds for gas adsorption processes. Additionally, customizing the production process minimizes raw material usage while maximizing efficiency for specific applications.

COMPETITIVE ADVANTAGE

- Streamlines the design of custom adsorber structures for enhanced adsorption efficiency, tailored to specific applications.
- Surpasses previous models by allowing general computers to compute results for small models, but high CPU and RAM are necessary for more accurate and larger models.

STATUS

- Patent Pending.
- [Pour SE, Mamaghani AH, Hashisho Z, Crompton D, Arellano H, Anderson JE. Experimental and modeling study of volatile organic compounds adsorption over zeolitic monolith adsorbent. Chemical Engineering Journal. 2024 Feb 15;482:148956.](#)

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