Optimisation of adsorption column processes: the role of adsorbent microstructure and its packing arrangement.

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Abstract: In adsorption column processes, the design of the adsorbent microstructure and its packing arrangement is key to define the optimal conditions for the process to take place. The relation between the void region, the radius of the adsorbent particles and the size of the pores determine the adsorption capacity of the column, as well as the energetic cost of the process. The pollutant is captured in the adsorbent micropores, which can be accessible either directly through the external surface in contact with the fluid flow, or through the internal surface of the pellets. To reach this region, an intraparticle diffusion phenomenon drives the contaminant molecules through mesopores and macropores to the inside of the adsorbent. These wider pores distribute the pollutant to the micropores located in the inner regions of the adsorbent, where they are finally captured. In this talk, we describe a new mathematical model that considers a representative cell accounting for the dimensions of the column void region and the pellet structure. The advection-diffusion-reaction equation is coupled with the momentum equation to describe the motion of the pollutant through the fluid flow and through the mesopores and macropores. The effect of the variation of the parameters defined in these equations is not trivial, since the mechanisms present in the model are inter-related. The behaviour of the model under certain changes is explained, and the optimal dimensions of the adsorbent particles to obtain the maximum removal efficiency after a certain time are provided. Energetic considerations are also taken into account, defining a trade-off between outlet concentration levels and energetic cost. The final aim is to show the potential of this new model, which can be useful when designing new adsorption materials for the filtering of pollutants.

References:

[1] The role of adsorbent microstructure and its packing arrangement in optimising the performance of an adsorption column. A Valverde, IM Griffiths. Submitted to Discover Chemical Engineering, Apr. 2024. https://doi.org/10.21203/rs.3.rs-3951770/v1