Development of CFD Models for Adsorbent Hollow Fibres for Gas Separations

Scott Allan[1], James M. Pinwill[1], Y.M. John Chew[*1,2], Semali P. Perera[1,2]

[1] Department of Chemical Engineering, University of Bath, UK
[2] Centre for Advanced Separations Engineering (CASE), University of Bath, UK

Introduction

Volatile Organic Compounds (VOCs) are a class of air pollutant that cause adverse environmental and health related side effects such as thinning of the ozone layer, global warming and respiratory problems [1]. Conventional separation and adsorption systems used in the treatment of VOC emissions are performed using packed beds. Unfortunately, packed beds have the distinct disadvantage of high operating costs due to high pressure drop and the potential maldistribution of flow (e.g. channelling).

Interest has surrounded the use of adsorbent hollow fibres (HF) as an alternative to existing adsorption technology because of their comparatively low pressure drop and efficient sorption cycles. This research focuses on developing a series of computational models to improve the understanding of transport phenomena within adsorbent HFs designed and commissioned in the Department of Chemical Engineering, Bath. Analysis of the effect of factors, such as Reynolds number, adsorption and desorption coefficients, adsorbent capacity and diffusion coefficient, on the adsorption process are investigated.

Adsorbent Hollow Fibres

Fig. 1 shows a double layer circular spinneret, electron micrograph of a single channel HF and a 50 mm cartridge bundle developed at the University of Bath. The HFs are prepared by dissolving a polymer (polyethersulfone (PESF)) into a solvent (N-methyl-2-pyrrolidone (NMP)) to form a viscous solution [2]. Adsorbent powder (e.g. Zeolite 13X) is added and mixed until a homogeneous mixture is prepared. Pressure is then applied to extrude the mixture through a spinneret of different dimensions and into water. Phase inversion occurs as the hydrophilic solvent is drawn into the water, leaving behind the adsorbent HF.

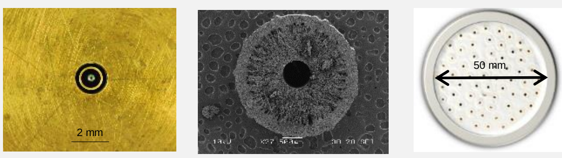

Fig. 1 : Image of a double layer circular spinneret (left), electron micrographs of the single channel HF (middle), cartridge made up from single channel HFs (right).

Numerical Modelling

Computational fluid dynamics (CFD) were applied to resolve the conservation equations involving continuity, momentum and species transport. Convective and diffusive transport were assumed within the fibre bore whereas in the porous media transfer occurred by diffusion and adsorption, modelled using the Langmuir isotherm. The numerical models were built using a commercial CFD platform, COMSOL Multiphysics™. The governing equations, boundary conditions and bore geometries are shown in Figure 2.

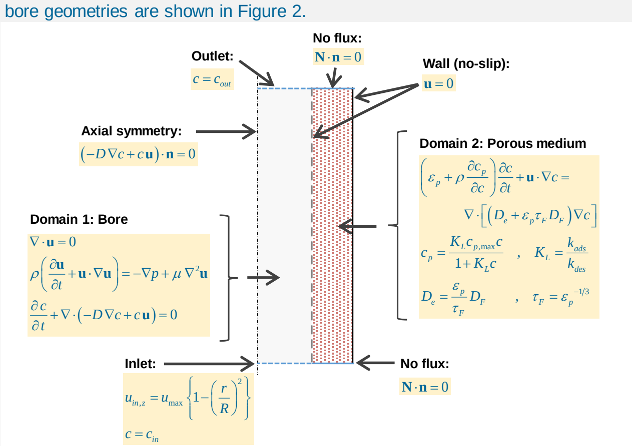

Fig. 2(a): Schematic of half a circular HF showing the lumen, adsorption surface and porous medium.

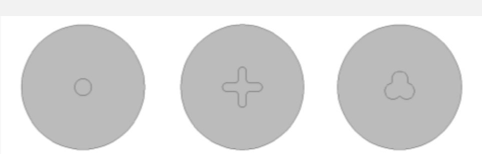

Fig. 2(b): Hollow fibre of circular (right), clover (middle) and trilobal (right) shape.

Acknowledgements

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Results

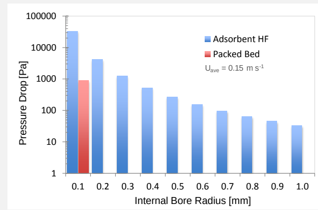

Fig. 3: Comparison of pressure drop in a HF cartridge made up from 15 circular channels and packed bed of equivalent volume of adsorbent. The length of the cartridge and height of packed bed is 200 mm.

The pressure drop, Δp, in the HF cartridge (made up from 15 circular channel) decreases exponentially as the bore radius increases (Figure 3). The Δp in a packed bed with equivalent volume of adsorbent is calculated using Carman Kozenzy equation and is higher than all but three cases where the internal bore radius is < 0.4 mm. Simulations for all bore design were performed using an equivalent radius of 0.5 mm.

Fig. 4 shows that the circular HF has the longest breakthrough and equilibrium times, followed by the clover and trilobal shaped HF. The percentage of HF utilised at the point of breakthrough for the chosen parameters was 37%, 30% and 23% for the circular, clover and trilobal fibres respectively (Fig. 5). Again, the circular fibre is favoured, implying a more efficient adsorption system with less unused adsorbent.

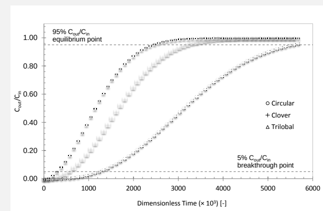

Fig. 4: Breakthrough curves of HFs with different bore shape (equivalent radius for all fibres = 0.5 mm).

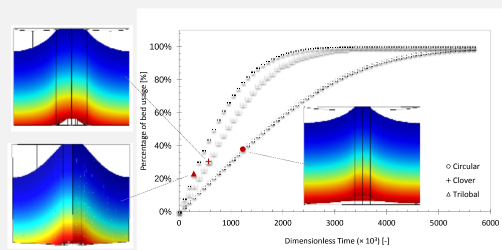

Fig. 5: Percentage of used HF for different bore shape. The red symbols indicate the % of HF usage at breakthrough time.

Conclusions

- Computational models for three fibre bore geometries of circular, clover and trilobal were successfully built and parametric studies for factors affecting the adsorption efficiency were also performed.
- Parametric studies show the most significant effect on the shape of breakthrough curve is the effective diffusivity in the porous media.
- The trends in improving the breakthrough and equilibrium times, and percentage of HF usage suggest circular shape to be the most favourable.

Ongoing Work: Multichannel HF

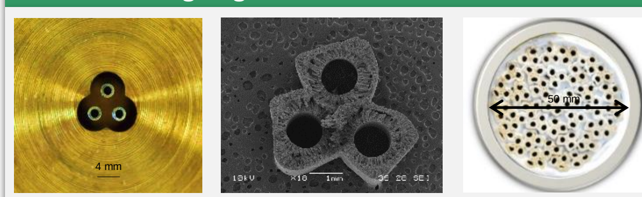

Fig. 6: Image of a multichannel spinneret (left), electron micrographs of the multichannel HF (middle), cartridge made up from 40 multichannel HFs (right).

Fig. 6 shows a multichannel spinneret, electron micrograph of a single multichannel HF and a 50 mm cartridge bundled using 40 HFs. The HF was formed using 13X zeolite as the adsorbent porous material and N-methyl-2-pyrrolidone (NMP), polyethersulfone (PESF) and microporous pore formers. These multichannel HFs allows the preparation of cartridges with more area for flow per unit mass and higher adsorbent capacity. CFD modelling of these multichannel HFs is currently in progress and preliminary studies have shown promising adsorption performance.

References

[1] Harrison R.M. & Hester R.E. (1995), "Sources, Distribution and Fate of VOCs in the atmosphere" in *Volatile Organic Compounds in the Atmosphere*, 1st Ed., Cambridge, UK: The Royal Society of Chemistry.

[2] Jeffs C.A. *et al.* (2013), "A polymer of intrinsic microporosity as the active binder to enhance adsorption/separation properties of composite hollow fibres", *Microporous and Mesoporous Materials*, vol. **170**, pp.105-112.