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NUMERICAL STUDY OF LAMINAR FLOW AND MASS TRANSFER FOR IN-LINE SPACER-FILLED PASSAGES

Surface 1 (longitudinal cylinders)

Fig. 1. Schematic of CONWED membrane spacer unit

ABSTRACT

Performance calculations for laminar fluid flow and mass transfer are presented for a spacer-filled passage containing cylindrical spacers configured in an inline-square arrangement, typically employed in process industries. Calculations are performed, based on stream-wise periodic conditions for a 'unit cell' and compared with those for 10 rows of units. The method is validated for an empty passage (i.e. a plane duct). Results are presented for normalized mass transfer coefficient and driving force as a function of Reynolds number, and wall mass flux (blowing parameter). Both constant and variable wall velocities are considered, the latter being based on osmotic pressure difference.

INTRODUCTION

Membranes are used for reverse-osmosis, ultra-filtration and nano-filtration. Permeate-retentate mixture flows between two parallel membranes through which the permeate (transferred substance) passes, but not the retentate. Spacers are employed to provide structural integrity, and promote mixing. An assembly involves hundreds/thousands of unit cells. Flow and concentration can be presumed to be fully-developed. Understanding and optimizing fluid flow and mass transfer in such assemblies can be achieved by means of CFD. Various geometries were previously studied [1-4]. The mass transfer problem is rationalized here in terms of dimensionless numbers consistent with the standard mechanical engineering formation in this article. The selected spacer considered here is the CONWED geometry [1-2].

Mathematical Considerations

A theoretical methodology for fully-developed periodic heat/mass transfer was described by Beale [5,6]. Primitive variables are employed throughout. Method is quite general ie not limited to only Neumann or Dirichlet wall conditions, as was true for earlier approaches, Patankar et al. [7].

Transport equations solved for steady incompressible laminar fluid flow and binary mass transfer with constant properties,

$$\text{div}(\rho \mathbf{u}) = 0 \quad (1)$$

$$\text{div}(\rho \mathbf{u} \mathbf{u}) = -\text{grad } p + \text{div}(\mu \text{ grad } \mathbf{u}) \quad (2)$$

$$\text{div}(\rho \mathbf{u} \mathbf{y}) = \text{div}(\Gamma \text{ grad } y) \quad (3)$$

In the finite-volume method these are converted to linear algebraic equations

$$\sum a_{NB} (\phi_{NB} - \phi_P) + S = 0 \quad (4)$$

where $S = C(\phi_w - \phi_P)$ (NB: Patankar [8] employs $S = a_p \phi_P + a_s$). For convective mass transfer, wall boundary condition may be written

$$\dot{S} = \dot{m}'' A (y_i - y_w) \quad (5)$$

y_i is the *transferred substance-state* [9]. For a fine grid, $y_p \approx y_w$ and $C \approx \dot{m}'' A$. Otherwise wall-value and C computed as harmonic averages (see paper for details).

For *fully-developed flow* [5,6] the upstream boundary condition is:

$$y(0) = c_1 y(l) + c_2 \quad (6)$$

$$c_1 = (y_w(0) - y_w(0)) / (y_w(l) - y_w(0)) \quad (7)$$

$$c_2 = y_w(0) - c_1 y_w(l) \quad (8)$$

Mass transfer driving force $B(x) = (y_w(x) - y_w(x)) / (y_w(x) - y_i)$
Periodicity equivalent to driving force being cyclic namely $B(l) = B(0)$

For *low-flux mass transfer*, situation is analogous to heat transfer with constant wall flux (Neumann). Depends on *blowing parameter* $\bar{b} = \dot{m}'' / \bar{g}^*$ where $\bar{g}^* = g / \lim_{\dot{m}'' \rightarrow 0} \dot{m}'' \rightarrow 0$ ie ratio of convection to diffusion For $\bar{b} \ll 1$, mass transfer is so small that both continuity and momentum effects due to injection/suction at the wall may be ignored. For finite-rate mass transfer, inlet/outlet velocity fields differ and may be presumed periodic with $u(0) = cu(l)$. Then introduce a wall momentum-source $\dot{S} = \dot{m}'' A (v_i - v_w)$ in the cross-wise velocity field, with associated periodic terms in v at the inlet/outlet.

CFD code PHOENICS version 2008 was used to perform calculations. Tests conducted by removing cylindrical obstacles. Values very close to $f^* = 0.24$ and $Sh^* = 8.235$ (plane duct) obtained. Figure 2 shows g/g^* , as a function of b . In contrast to classical heat transfer problem where g/g^* varies from 1 to 0.916, for $Nu = 7.541$. For latter v -velocity is negligible. For high mass transfer rates, cross-wise velocity important, as are continuity effects. Figure 4 shows comparison of periodic problem with 10-unit-cell entry length case. Agreement is very good.

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Fig. 2. Benchmark studies for plane duct.

Fig. 3. Flow visualization for Re = 80.

Fig. 4. Developing vs. 'fully-developed' solutions

Low constant-rate mass flux

Figure 5 illustrates local retentate/solute wall mass fraction profiles, and local Sherwood number, Sh_1 and Sh_2 , for suction with constant wall velocity $v_w = -5 \times 10^{-4}$ m/s, imposed at both walls. Retentate mass fractions maximum in stagnation zones where the cylindrical spacers touch the walls, and minimum in regions where stream-wise convective transport is high. Mass fractions are higher on surface 2 than on surface 1. Surface 1 is exposed to a shear layer due to the locally accelerated flow which increases the concentration gradient compared to surface 2 which is shaded by the lateral cylinders. Local values are negligibly small directly under the cylinders, where there is little mass transfer. Magnitude of B is proportional to Δy , so B is a maximum and g a minimum in regions of low concentration. Sh_1 is a maximum in the free shear layer, where velocity and concentration gradients are maximum. Sh_2 is influenced by the inter-tube vortex, Fig. 3, which at low Reynolds numbers is relatively quiescent, therefore effecting more uniform mass fraction gradients at the wall and resulting in lower overall Sh_2 values.

Low variable-rate mass flux

In practical reverse osmosis membrane situations, wall mass flux is coupled to concentration through *osmotic pressure*.

$$v_w = L_p (\Delta p - \Delta \Pi) \quad (9)$$

L_p is membrane permeability, Δp is the pressure change across the membrane and $\Delta \Pi$ is the osmotic pressure difference; itself a function of the concentration difference across membrane. Pharaoh [10] proposed a linear approximation for dilute NaCl brine, which was compared with data from Perry et al. [11].

$$v_w = v_0 + A y_w \quad (10)$$

y_w refers to the retentate, and A is source-term coefficient, C , is now a linear function of y_w , and the source term therefore displays a quadratic dependence on y_w .

Figure 6 shows wall mass flux at surfaces 1 and 2. It can be seen that near the cylinders where the solute concentrations are relatively high the magnitude of the wall velocity is reduced due to the osmotic pressure. For the very dilute mixture and associated small mass flux considered here, this effect is second-order and the impact upon the wall mass fractions and Sherwood numbers is negligible, however for larger values the changes in the concentration will significantly affect the local wall velocity and hence mass fractions and Sherwood numbers. Thus the local Sh distribution will become problem specific.

Fig. 6. Mass fraction and local Sh at surfaces 1 and 2, $Re = 80$, constant v_w .

Fig. 6 Permeate mass flux, $Re = 80$, $v_w = v_0 + A y_w$.

Decreases in solute mass fraction can also lead to substantial changes in the magnitude of the transpiration velocity over the length of the entire membrane assembly. Although the variation over a single periodic element is typically small, the difference between the inlet and the outlet of an entire module will often result in a significantly different blowing parameter between inlet and outlet. It is, straightforward to adopt higher-order regression polynomials, etc.

High constant mass transfer

For low Re_w , the velocity profile is unaffected by injection or suction at the wall. Thus the mass transfer problem is not affected by the flow-field distortions. Under such circumstances it is not necessary to account for either continuity or momentum effects for the fully-developed problem, i.e. injection/ejection of the transferred substance is presumed to occur entirely independently. The converse is true for high mass transfer rates where it is necessary to modify the stream-wise periodic algorithm to take these effects into consideration. At high Re_w , the streamwise velocity field can no longer be considered cyclic, but instead is periodic. In addition sources of mass and momentum at the walls, and equal and opposite sinks across the periodic boundary condition must be prescribed. This was successfully implemented in the code, and the manuscript shows values of g/g^* for high mass flux. For $\bar{b} \ll 0$, (strong suction), mass transfer enhancement is significantly higher than for the plane duct case, Fig. 2. At sufficiently high lateral mass flux rates the notion of stream-wise periodicity becomes questionable due to cross-wise pressure gradients arising. This is unlikely to be an issue for moderate wall Reynolds numbers typical of practical membranes employed in process industry.

CONCLUSIONS

Streamwise periodic boundary conditions for mass transfer problems involving a non-trivial geometry and flow regime were implemented, based on a primitive variable formulation. Comparison of the fully-developed algorithm with a 10-cell developing flow regime showed the developing case asymptotically approached the periodic case. The following problems were considered; (a) constant low- Re_w wall velocity, (b) the variation of wall velocity due to the local osmotic pressure, and (c) constant high- Re_w wall velocity with continuity effects. The stream-wise periodic methodology was readily applied to all of these situations. Convergence as measured by spot values and RMS residuals, was readily achieved, though for $Re > 100$, tests showed the solutions to be transient.

Future Work

Important considerations not given in this paper, which should be addressed in the future include; studies of transient flow and mass transfer, and the impact of free-stream turbulence upon drag and mass transfer. Correlating Sherwood number as a function of Schmidt number is important as the latter can be quite large. Local variations in Sc near the membrane walls are also significant. Comparisons of the present numerical results with those of reliable flow visualization experiments are ongoing and will be presented in future work by the authors.

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