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Development of a CFD modeling approach applied to gas separation in hollow fiber membrane module: Pt. 2 - Analysis of mass transfer models

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Abstract

Computational simulations are widely used to represent the gas separation process using membranes. However, the approaches cannot describe the physical effects of the membrane module's geometry [1]. Thus, the Computational Fluid Dynamics (CFD) approach [2] was used to study the flow and mass transfer in a membrane module for separating CO_2 and natural gas. Detailing a large number of hollow fibers within a module is a significant challenge, as the computational effort to mesh and simulate the equipment would be prohibitive. This work presents the development of a CFD model to represent the flow over the hollow fibers as a porous media region, and the mass transport through the membrane is represented as a volumetric sink term. Simulation tests were performed to analyze the different model approaches for the mass transfer sink term.

Introduction

A CFD solution requires the definition of computational geometry and its spatial discretization in non-overlapping volumes. To avoid the complexity of geometrically describing the hollow fibers, a porous media modeling approach is employed to capture the effect of a pack of fibers in each mesh volume. In all, the model development is divided into two scale sizes. The macroscale deals with species transport through the porous media from the flow perspective using CFD conservation equations. Considering a homogeneous fiber packing in the module, the porosity and flow permeability are constant and can be obtained as an equipment parameter.

On the other hand, a well-mixed two-compartment approach [3] is used to model the mesoscale, which determines the mass transport rate through the fibers of the membrane module according to the available surface area. Therefore, developing a geometric model for the fiber distribution on each mesh volume is necessary. It can be assumed that the fibers are cylinders uniformly distributed in a cubic geometry with a volume identical to the mesh element. Figure 1 shows a diagram of the geometry, mesh, and model scales. This work analyzes the mass transfer sink models and their configuration on the ANSYS Fluent CFD package.

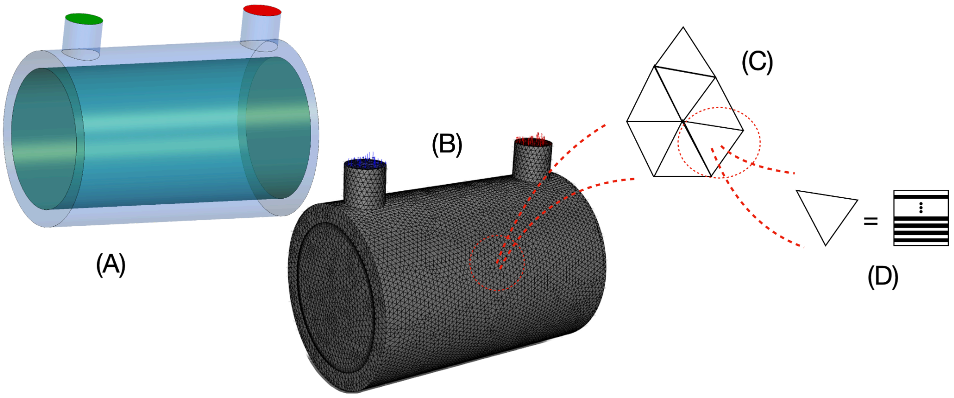


Figure 1: Diagram for the geometry and model scales. (A) Module geometry with packed fiber region in green; (B) Unstructured mesh; (C) 2D representation of the mesh; (D) Equality of mesh volume and representative cube.

Flow and mass transfer models

The mass that transfers from the module to the hollow fiber's interior, S_m, is modeled through a volumetric sink term. For steady and incompressible flow, Eqs. (1), (2), and (3) show the continuity, momentum, and chemical species conservation equations where v is the velocity, p is the pressure, y_A is the mass fraction of species A, ν is the kinematic viscosity, and $D_{A,eff}$ is the effective diffusion coefficient. It is crucial to notice that the interior of the fibers is not considered in this model, and, as such, the sink term must appear in both continuity and species conservation equations. At last, as this work deals with the mass transfer models only, the flow resistance due to the presence of the pack of fibers is neglected.

$$\nabla \cdot (\underset{\sim}{v}) = S_m \tag{1}$$

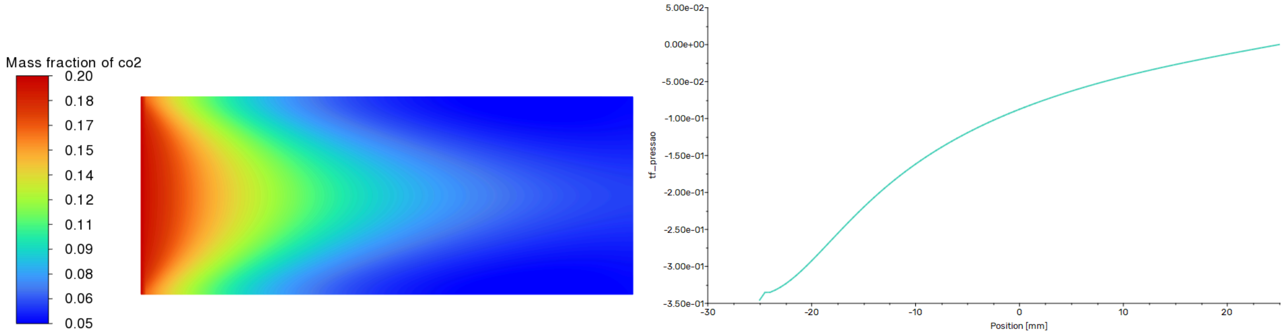
$$\nabla \cdot (\underset{\sim}{v}\underset{\sim}{v}) = -\frac{1}{\rho}\nabla p + \nu \nabla^2 (\underset{\sim}{v}) \tag{2}$$

$$\nabla \cdot (y_A \underset{\sim}{v}) = D_{A,eff} \nabla^2 (y_A) + S_m \tag{3}$$

The sink term was modeled with four approaches: (i) a constant ($S_m =-\ 0.04$ s^{-1}), (ii) a variable value (dependent on position, $S_m =-\ 2.5|x|$ s^{-1}), (iii) the use of 3 species, and (iv) mass rate modeled by the well-mixed two-compartment theory [3]. The latter depends on the membrane permeance, ideal selectivity, and pressure in the hollow fiber, where arbitrary values, 2x10^{3} s/m^{2}, 2x10^{-3}, and 0.0 Pa, respectively, were used. A hexahedral mesh was used for a 2D rectangular geometry (50 mm vs 20 mm), considering it is packed with hollow fibers that can capture one of the chemical species. A CO_2/CH_4 (20%/80% mass fraction) mixture was fed through the left side with a 0.01 m/s velocity, and the outlet was on the right side. The CO_2 was selected as the main species, and the sink term was applied to its equation. Finally, the overall mass balance was checked, subtracting the inlet mass rate from the sum of the outlet mass rate and the overall sink term.

Results

The first tests with model approaches (i) and (ii) have shown that the CO_2 mass fraction decreases due to the sink term as the CH_4 mass fraction increases. Still, the closure of the overall balance was not achieved. By default, the ANSYS Fluent includes the species conservation, shown in Eq. (3), as an additional equation. In other words, it does not affect the continuity equation, which means that despite the sink term being active in Eq. (3), it is null for Eq. (1). Furthermore, only the CO_2 mass fraction equation was solved as the CH_4 mass fraction was obtained by difference from unity. Thus, the sink term also does not directly affect the CH_4 quantity. To confirm this behavior, a ternary mixture ($CO_2/CH_4/N_2$) was fed with 20%/80%/0% mass fractions where the first two species were selected to be solved. The solution showed a decrease in CO_2 and an increase in N_2, which is physically inconsistent. The sink term must be manually checked for the continuity equation to overcome this issue. Doing this and repeating the simulations for model approaches (i) and (ii) were physically consistent, and the overall mass balance was achieved. Figure (1) shows the results of the CO_2 mass fraction and the sink term value obtained by model approach (iv) on a central line along the channel.



(A) (B)

Figure 1: (A) CO2 mass fraction contour and (B) model approach (iv) sink term along the channel.

It can be noticed that the CO_2 is mainly consumed at the beginning of the channel. It occurs since the sink term depends on the difference in the local pressure and the set pressure in the hollow fibers (0 Pa). As the flow pressure is higher at the beginning of the channel, the sink term value has more influence on the CO_2 consumption as it becomes less relevant as the fluid flows. The results are physically consistent, and the last sink term can be used in CFD simulations for hollow fiber membrane modules.

Acknowledgments

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