membrane modelling in carbon capture technology.

DEMCON MULTIPHYSICS

CORE COMPETENCIES

1. Porous medium modelling
2. Overlapping medium approach
3. Flow calculation
4. Design optimization

Capturing carbon with fibers

Aqualung Carbon Capture provides membrane modules that capture carbon, to aid in the decarbonization of heavy industry and transport. These modules filter CO_2 from process gas streams with minimal additional pressure drops. Aqualung approached us to simulate the behavior of these modules.

We supported Aqualung by aiding in the improvement of a membrane module containing more than 2000 filtering fibers. Using CFD simulations we determined the optimal distribution of fibers (fiber density) as well as the optimal length and thickness of the module.

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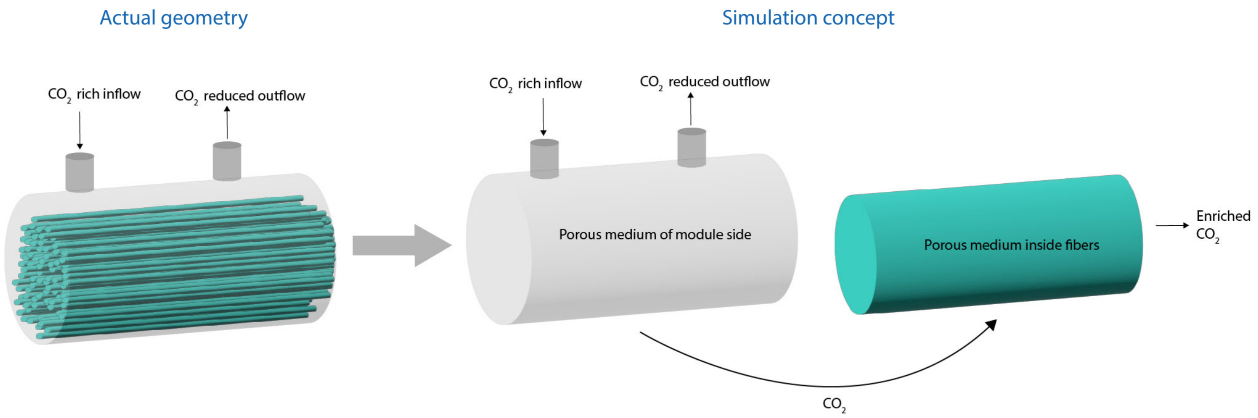

Figure 1 Left: actual geometry with the fibers inside the model. Right: simulation concept. The module and the fibers are modelled as two porous media and simulated with a CO_2 sink term in the module and a production term in the fiber domain.

Simulation description

The relevant physical quantities that were considered in the simulation are the local pressure and CO_2 concentration, both in the module (p_m and c_m) and in the fibers (p_f and c_f). These four terms together determine the amount of CO_2 captured by the fibers. Hence, the fiber domain and the module should both be included in the simulation (Figure 1). The sink term, which is the amount of CO_2 that is entering the fibers per m^3 of module can then be calculated locally. The sink term *m* (in kg/m^3/s) into the membrane fibers is

$$m = \alpha A' \,\Delta(cp),$$

where α is the membrane permeance in kg/s/m^2/Pa/mol, A' is the fiber area per volume of module, and $\Delta(cp)$ is the difference in partial pressure:

$$\Delta(cp) = c_m p_m - c_f p_f$$

Using these governing equations in the simulation, the flow within the module and the fiber was calculated.

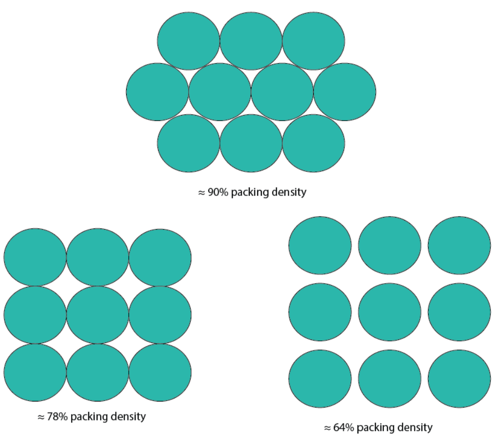

Figure 2 Different packing densities, with the maximal packing density achieved arranging fibers in a hexagonal lattice.

Simulating the pressure drop over 2000 fibers is computationally intensive, thus we simplified the simulation by modelling the fibers as a porous medium. Furthermore, only a small cell of the geometry was simulated in detail, to then use the calculated permeability in a macro model (micro/macro model approach). General information on micro/macro approaches can be found here. In the case of the fibers, the flow resistance is anisotropic. The flow along the fibers has a different resistance to flow compared to the flow perpendicular to the fibers. Both of these properties were calculated for different packing densities to determine the pressure drop over the module (Figure 2). Hence, the packing density is an explicit choice in the module design, and depends on the amount of fibers and the space available inside the module.

Combining the calculated permeability of the fibers with the larger geometry of the module results in a functioning macro model of the membrane. The inputs are the mass fraction and flow rate of CO_2 at the inlet, the pressure at the outlet, and the pressure of suction at the end of the fibers. The outputs are the full flow field, pressure distribution, mass fraction distribution and the amount of CO_2 that is captured within the fibers.

Simulation result

The result of the simulation, when applying all above mentioned boundary conditions, can be seen in Figure 3. The concentration of CO_2 on the module side decreases across the module. At the same time, the CO_2 emerges on the fiber side, locally increasing the concentration before flowing out of the module. This indicates that the module is working as intended and is extracting CO_2 from the feed flow.

Aqualung's use of CFD to optimize module design

Using CFD simulations, input parameters such as module geometry, fiber packing density, and process parameters can be quicky iterated to optimize the module. This means that the module can be tuned for specific industrial processes. In this way, a cost-benefit analysis can be performed, assessing CO_2 capture purity and CO_2 mass flow on the one hand, and the costs such as pumping power and size of the module on the other hand.

In simulations of filtering processes, it is very important to understand the relevant physics driving the membrane filtering. Different membrane processes could for example be driven by pressure, concentration of different species, temperature differences or velocities. We can incorporate this in our simulations. If you have a filtration or membrane technology problem, which you would like to optimize, you can contact us.

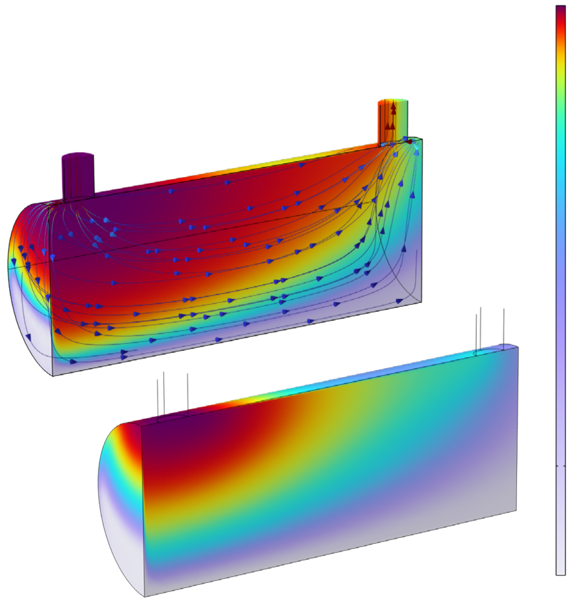

Figure 3 Top: the module domain, bottom: the fiber domain. The arrows in the module domain represent the flow profile on the module side. The color in both domains represents the mass fraction of CO_2.