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Simulation of carbon dioxide transport in different geometrical nanopores

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ABSTRACT: Carbon dioxide (CO_2) transport in porous structures is influenced by the geometrical characters of pores. Applying the laminar flow model, effects of pore shapes such as cylinder, trapezoid, and hourglass, to the CO_2 transport in nano-scale are investigated. Simulated results show that the CO_2 distribution profile is significantly influenced by pore shape and size, but for direction-changed pores, it is not. These findings provide a fundamental observation for an understanding of gas transport in a nanopore structure.

KEYWORDS:gas transport, nanopore structure, simulation.

I. INTRODUCTION

Gas transport plays a key role in various processes, especially in porous materials [1], where gases transfer under the natural convection and diffusion, classified in the laminar flow [2]. There are significant differences in gases transport in the nano and the macro-scale structure [3] that can be investigated on theoretical [4], semi-empirical [5], and experimental [6] approaches or their combination. Several processes in porous materials i.e. adsorption, chemical reaction, catalysis, filtration, storage, etc., are controlled by fluid transport.

The porous structure of real materials is often non-unique and complex [7]. As consequently, the average values of parameters for gases transfer in the real porous structure need to found out from experimental performances. However, to understand the gases transport in real porous structures, the basic characters for this process through the single pore, throat, and branch, which is difficult to empirically determine, need to be explored. These processes can be revealed by applying the recent achievements of computational science. In this study, the effects of pore geometries on to transport of gas, particularly for CO_2, were simulated.

II. GAS TRANSPORT MODELS AND NUMERICAL SOLUTION

Gases transport in nanoporous structure is in laminar flow that expressed by steady-continuous equation (1).

$$\rho(u\cdot\nabla)u = 0 \quad (1)$$

where ρ is gas density, μ is gas dynamic viscosity and u is gas velocity.

Consideration for non-compressible gas, the density of gas relates to its pressure p as (2).

$$\rho = \frac{pM}{RT} \quad (2)$$

where M is the molar mass, R is the universal gas constant, and T is temperature.

Initial pressure for gas in pores was assumed to be 1 atm $\left(p_0 = p_{ref} = 1\right)$. We suppose that the pressure of the gas at the outer boundary is in the proportional gradient. Equation (3) described the outer condition.

$$\frac{\partial p}{\partial n} = 0 \quad (3)$$

with n is the outward unit vector of the boundary.

The finite element method in COMSOL® was used for solving (1) for CO_2 gas with an inlet gas velocity of 0.01 m/s.

III. RESULTS AND DISCUSSION

For cylindrical pore, the simplest geometry, effects of pore dimension on velocity profile of CO_2 at 293 K are shown in Fig. 1. It can see for larger pores that CO_2 transfers deeper into the pore. CO_2 only transfers into short length ca. 2 nm from the inlet of pore in 1 nm of diameter (Fig. 1a)). However, with pores in 2 nm and 3 nm of diameter, CO_2 can transport under the contribution of the molecular diffusion, resulting in widespread distribution of CO_2 in pores as presented in Fig. 1b), 1c). The effect of different geometries of pore on CO_2 transport can be compared from Fig. 1 to Fig. 3. In Fig. 1a) and 2a), CO_2 can transfer deeper onto

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a)

b)

c)

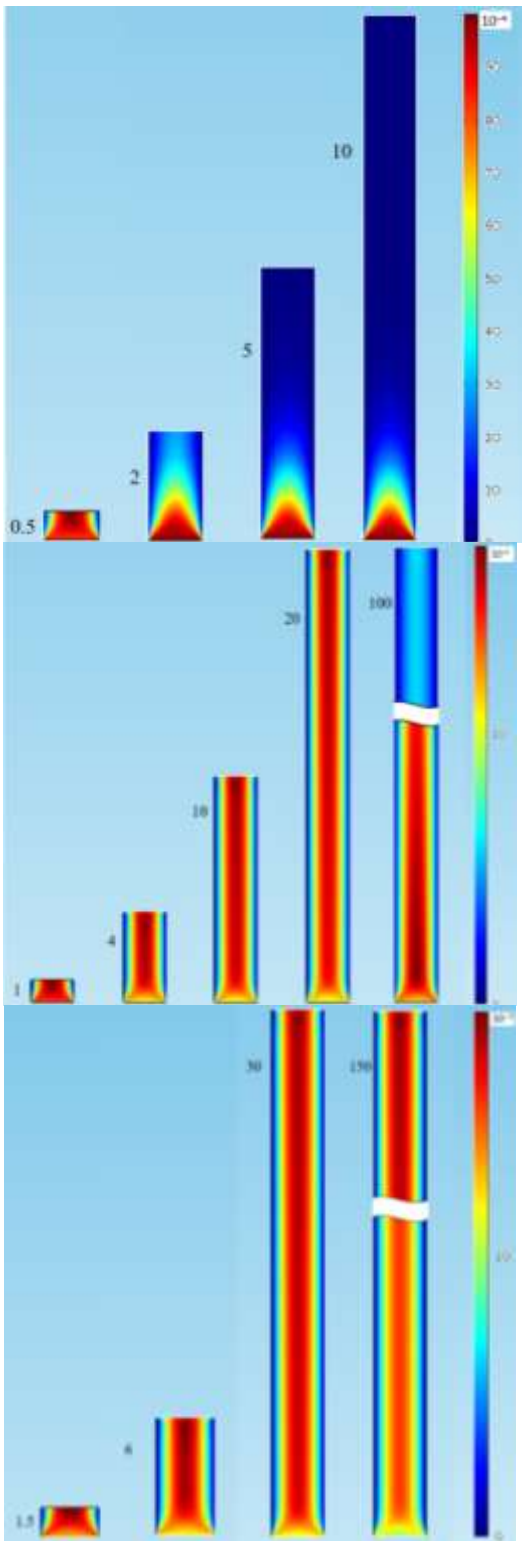

Figure 1. Effect of cylindrical pore length to CO_2 transport in different pore radii a) 1 nm, b) 2 nm and c) 3 nm

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the expanded pore with 0.5 nm of inlet width due to the lower pressure at the outlet in comparison to that at the inlet for expanded trapezoid-pores [8]. The larger of expanding angle, the space for CO_2 transport is wider, causing the dense CO_2 at the inlet but CO_2 is then rapidly diluted at a deeper location as shown in Fig. 2a). The same behavior was reported earlier [9]. For reduced trapezoid-pores, as expected, CO_2 concentrated at the throat, where CO_2 concentrations are similar for the different reducing angles.

Pore geometry affects significantly the penetration of gases in porous media [10]. Figure 3 shows results of simulated CO_2 transport into hourglass-pore with different throat widths. It can be observed that CO_2 transferred along the symmetrical axis of the pore and accumulated at the throat. It is difficult to transfer CO_2 through the hourglass-pore although the pore width was enlarged to 2 nm (w = 2). This is in contrast to the cylindrical pore (Fig. 2a)), maybe due to minor head loss, and is known as the "shooting" mechanism [11].

Figure 4 shows the CO_2 distribution for traveling in the 90^o elbowed tubular pores (2 nm of diameter). It can be seen that CO_2 molecules traveled parallel to the pore walls, leading to the outer boundary. The bended pores did not almost affect the CO_2 concentration profile which is similar to what for CO_2 transport in the cylindrical pore (Fig. 1b)). As some previous groups worked on methane [12] and water [13], the bending nanopore contributed to promoting the fluid flux due to reducing the Lennard-Jones potential at the middle point [12].

In the last consideration for the branched pore, different CO_2 distributions in the symmetrical and asymmetrical branches were observed as in Fig. 5. As expected, the total inlet CO_2 flow was equally divided into each branch for the symmetrical branch (Fig. 5a)). This behavior was also reported in previous work [14], where the fractal structure, generated from the simple three-direction branches, was modeled. However, head loss of the sub-branch depends on its angle [15]. Consequently, the CO_2 concentration in the branch decreased with increasing angle of branch as shown in Fig. 5b). This result indicates the complex profiles of fluid in real porous media, which are structured by numerous branches with different angles.

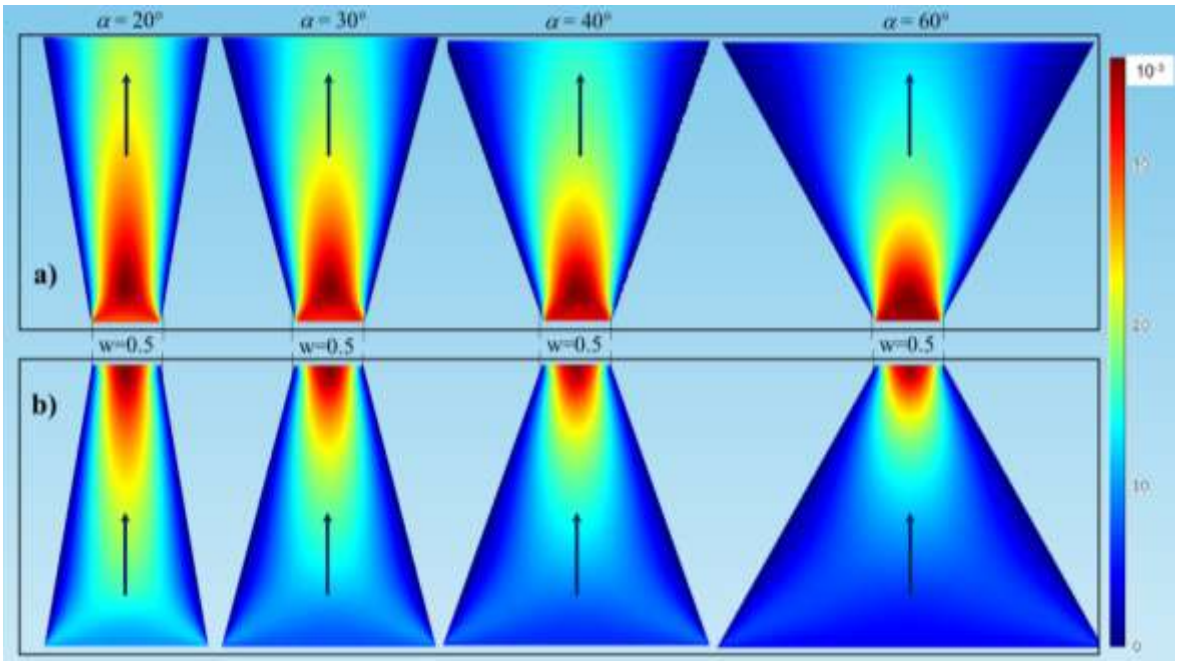

Figure 2. CO_2 transport into a) expanded and b) reduced trapezoid-pores with different opening angles

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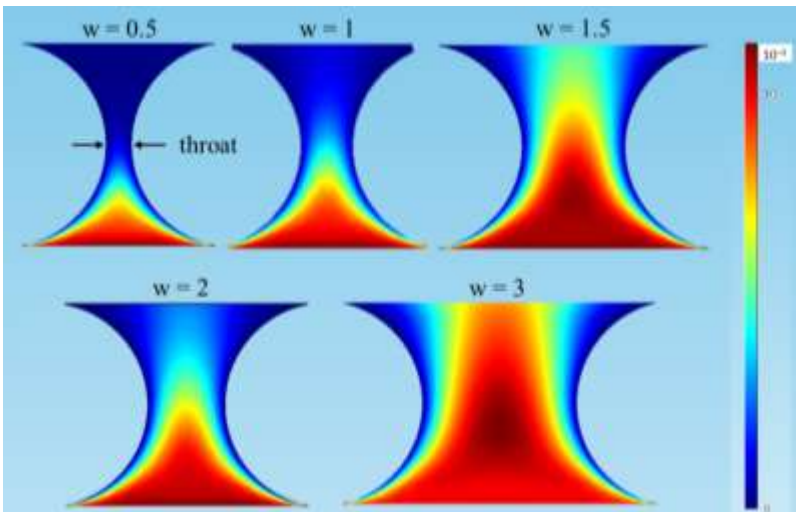

Figure 3. CO_2 transport through hourglass-pore with different throat widths

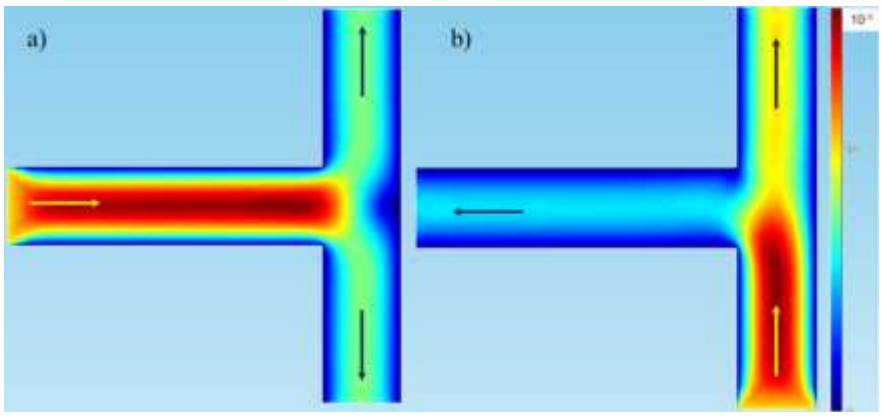

Figure 5. CO_2 transport in branched pores

IV. CONCLUSION

Behaviors of the CO_2 transport in different geometrical nanopores were studied by COMSOL® software. It found that CO_2 could only transfer in a short distance from the inlet for 1 nm of the cylindrical pore, but CO_2 could travel through the pores with a diameter larger than 2 nm. It is advantageous to the CO_2 transport in the expanded pores; but in the hourglass-shaped pores, it is contrast. The CO_2 distribution profile in the bended and branched pore was also presented. This work provides the primary observation of the CO_2 transport in individual nanopores that useful for understanding gas transport in complex porous structures.

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