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THREE DIMENSIONAL SIMULATION OF THERMO-SOLUTAL CONVECTION IN POROUS MEDIA

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ABSTRACT

A 3D simulation model has been developed to investigate the compositional variation in porous media as a result of thermo-solutal convection. The function of thermal diffusion, pressure diffusion, and convection in the compositional separation process is discussed, and a criterion to predict the dominant driving force between thermal diffusion and pressure diffusion can be estimated based on diffusion coefficients and both temperature and pressure gradients. The thermo-solutal convection has strong effect on compositional separation results and causes a vertical compositional distribution against the vertical thermal diffusion in the combined heating case, and this is verified in diffusion flux components analysis.

INTRODUCTION

Riley and Firoozabadi [1] studied the thermal diffusion process in an oil reservoir cavity with an aspect ratio of 0.05 and focused on the horizontal compositional variation. They stated that the horizontal composition gradient would increase until a maximum is reached as permeability increases. Jiang et al. [2] conducted numerical simulations to investigate the thermo-solutal convection in a two dimensional porous cavity with an aspect ratio of 10, and predicted both horizontal and vertical compositional variations due to different values of permeability in the porous medium. When the aspect ratio is as high as 100, the vertical compositional variation is significant, however, when the aspect ratio is small as low as 0.05, the horizontal compositional variation is profound. Ghorayeb and Firoozabadi [3] discussed which of the two diffusion processes (thermal and pressure) is the dominant force in establishing compositional variations. However, they only investigated the case when thermal diffusion and pressure diffusion occurred in the same direction.

In this work, the three dimensional compositional variation inside a porous cavity containing a binary mixture of methane/n-butane with a mole fraction of 20% methane is investigated numerically in terms of diffusion fluxes. The main focus of this work is on the features of thermal diffusion, molecular diffusion, and pressure diffusion fluxes at the central point and their distributions along the x , y , and z centerlines, or in central x - z and x - y planes inside the porous cavity. The calculation of all the diffusion coefficients was based on the Firoozabadi's model [4, 5]. Other researchers have discussed the importance of diffusion in Porous media[6-9].

MODELLING AND SOLUTION SCHEME

Figure 1 shows the three dimensional model considered with the boundary conditions. The dimensions are $L = 0.5\text{m}$, $W = 0.5\text{m}$, and $H = 5.0\text{m}$.

The mass continuity equations solved in the present simulation model are:

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \vec{V}_f) = 0 \quad (1)$$

$$\frac{\partial x_1 \rho_m}{\partial t} + \nabla \cdot (x_1 \rho_m \vec{V}_f) = -\nabla \cdot \vec{J}_1 \quad (2)$$

where ρ_m is the molar density of the mixture; $\vec{V}_f = u\vec{i} + v\vec{j} + w\vec{k}$ is the average velocity vector of the

mixture; x_1 is the mole fraction of methane; and \vec{J}_1 is the molar diffusion flux of methane:

$$\vec{J}_1 = -\rho_m (D_m \nabla x_1 + D_T \nabla T + D_p \nabla P) \quad (3)$$

where T is temperature, P is pressure, and D_m , D_T , and D_p are molecular, thermal, and pressure diffusion coefficients, respectively.

The intrinsic velocity of the fluid inside the porous medium is calculated using Darcy's law:

$$\vec{V}_f = -\frac{\kappa}{\phi\mu}(\nabla P - \rho\vec{g}) \quad (4)$$

where κ and ϕ are the permeability and porosity of the porous medium, respectively; μ is the viscosity of the fluid mixture, ρ is the mass density of the fluid mixture, and \vec{g} is the gravitational acceleration.

The energy transfer is described by the equation,

$$(\rho C_p)_e \frac{\partial T}{\partial t} + \phi \vec{V}_f \cdot \nabla \left\{ (\rho C_p)_f T \right\} = k_e \nabla^2 T \quad (5)$$

where $(\rho C_p)_e = (1 - \phi)(\rho C_p)_p + \phi(\rho C_p)_f$ and

$k_e = (1 - \phi)k_p + \phi k_f$ are the effective heat capacity and thermal conductivity of the porous medium filled with the fluid mixture, respectively.

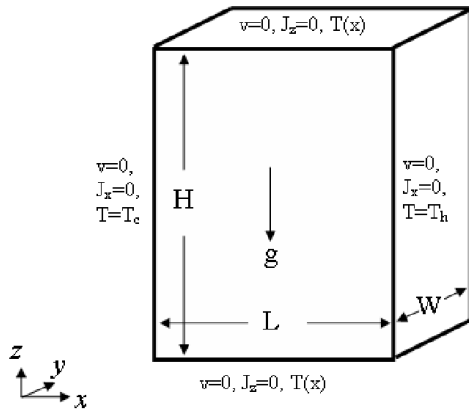


Figure 1 3D porous cavity with lateral heating

In the solution procedure, the velocity from Eq. (4) is substituted into Eq. (1) to solve for pressure. Note that both molar density and mass density of the fluid mixture appear in these equations, and the relation between them is $\rho = \rho_m M$, where M is the molecular weight of the mixture ($M = M_1 x_1 + M_2 x_2$).

A control volume method is used, as well as the second-order central differencing scheme and power-law scheme. The resulting discrete linear algebraic system is solved with the conjugate gradient iteration method, NSPCG. A mesh sensitivity analysis was performed under lateral heating boundary condition to select proper mesh density.

RESULTS AND DISCUSSION

In oil reservoirs, the geothermal gradient is usually three dimensional. In some cases, it can be simplified to lateral heating with top and bottom rock layers providing linear temperature profiles. Therefore, two cases of lateral heating and combined heating have been analyzed in this work to investigate the competition and coupling of thermal diffusion, pressure diffusion, molecular diffusion, and thermo-solutal convection in terms of flux components.

Lateral heating case: A lateral heating condition is applied in the x dimension with the left wall kept at 334 K and the right wall at 344 K. On both the front and rear walls, reflective boundary conditions are applied, that is, all fluxes are zero, and in the z direction, a linear temperature distribution as function of x is applied at the top and bottom walls as shown in Fig. 1. The permeability and porosity are respectively 10 md and 0.2, and the porous cavity is filled with a binary mixture of C_1/nC_4 with 20% mole fraction of methane. The pressure at the central reference point, (0.25, 0.25, 2.5) is 11.1463 MPa. A $71 \times 11 \times 71$ mesh was used.

Because of the reflective boundary condition applied in the y direction, any property distribution in the y direction will be flat. Therefore, the temperature, pressure, methane mole fraction, and Soret coefficient distributions in the x - z plane will give the most important information about the compositional variation inside the porous cavity under the lateral heating boundary condition. Distributions in the x - z plane at the center of the cavity are shown in Fig. 2. The temperature varies only in the x direction, and pressure only in the z direction (Figs. 2(a) and 2(b)). Therefore, the linear temperature and pressure distributions are not distorted by the convection flow in the porous cavity with a permeability of 10 md. However, the compositional variation appears in both x and z directions, which is a consequence of thermal diffusion, pressure diffusion, molecular diffusion, and thermo-solutal convection (Fig. 2(c)), and the Soret coefficient varies in both x and z directions (Fig. 2(d)). Methane moves towards the hot wall and the top under thermal diffusion, pressure diffusion, and convection flow, thus the top-hot wall corner has the highest mole fraction of methane, whereas normal-butane moves towards the cold wall and the bottom, so, the bottom-cold wall corner has the highest mole fraction of n-butane. The Soret coefficient at the center point has a value of about -5.0×10^{-3} 1/K, and the variation over the entire cavity is about 5%. Towards the hot wall and the top boundary, the absolute value of the Soret coefficient increases, but towards the cold wall and the bottom, it decreases.

If there is no convection in the cavity, the diffusion process will reach steady state when the diffusion flux is zero, that is,

$$\vec{J}_1 = -\rho_m (D_m \nabla x_1 + D_T \nabla T + D_p \nabla P) = 0 \quad (8)$$

Since there is only a horizontal temperature gradient and the vertical pressure gradient is non-zero, the composition gradients in horizontal and vertical directions can be estimated by:

$$\frac{\partial x_1}{\partial x} = -\frac{D_T}{D_m} \frac{\partial T}{\partial x} \quad \text{and} \quad \frac{\partial x_1}{\partial z} = -\frac{D_p}{D_m} \frac{\partial P}{\partial z} \quad (10)$$

Using the data at the center of the cavity, we can obtain approximately the value of compositional gradients as

$$\frac{\partial x_1}{\partial x} \sim 0.016 \text{ (m}^{-1}\text{)} \quad \text{and} \quad \frac{\partial x_1}{\partial z} \sim 2.4 \times 10^{-5} \text{ (m}^{-1}\text{)}. \text{ Therefore,}$$

under a convection free condition, the thermal diffusion and pressure diffusion effects are completely balanced by the molecular diffusion. However, in the presence of

7.0×10^{-10} mol/m²/sec. This is because the pressure gradient is non-zero in z direction, but zero in both x and y directions. The pressure diffusion flux component J_z is positive in this case, which means that methane as the lighter component moves up and n-butane as the heavier component moves down under the driving force of gravity inside the porous cavity.

Comparing the magnitudes of thermal diffusion and pressure diffusion fluxes one observes that thermal diffusion dominates in the x direction and pressure diffusion in the z direction. However, the convection caused by thermal-solutal expansion is so strong for 10md permeability that pressure diffusion is negligible in terms of compositional variation, because the vertical compositional gradient of 0.007 (m⁻¹) is two orders of magnitude higher than the gradient of 2.4×10^{-5} (m⁻¹) by pressure diffusion alone.

Figure 2 Distributions in the x - z central plane inside the porous cavity (lateral heating case)

convection, the compositional distribution in the porous cavity has approximately a 0.4% methane mole fraction difference in the horizontal direction and a 3.4% difference in the vertical direction. Although these are about 9 times different in mole fraction, the average compositional gradient in the horizontal direction is about 0.008 (m⁻¹), close to the vertical average compositional gradient 0.007 (m⁻¹). Thermal diffusion and pressure diffusion separation effects at steady state are not balanced by molecular diffusion alone, but by the mass balance equation involving convection.

$$\nabla \cdot (\rho_{mi} \vec{V}_f + \vec{J}_1) = 0 \quad (11)$$

This balance depends on the momentum and energy transport phenomena inside the porous cavity due to thermo-solutal convection.

The thermal diffusion flux is significant only in the x direction in the lateral heating case, and the x component of thermal diffusion flux, J_x , is of the magnitude 5.0×10^{-7} mol/m²/sec. The values of y and z components of thermal diffusion fluxes, J_y and J_z , are actually zero because the temperature gradients are zero in both y and z directions.

The molecular diffusion flux has no y component in the lateral heating case, that is $J_y = 0$. The magnitudes of x and z components of molecular diffusion fluxes are about -1.0×10^{-7} and -2.0×10^{-7} mol/m²/sec, respectively, and both are negative in this case.

The pressure diffusion in x and y directions has zero flux components J_x and J_y , but J_z is of the magnitude

Combined heating case: the different walls are kept at different temperatures. In the x dimension, the left wall is kept at 334 K and the right wall at 344 K; in the y dimension, the front wall is kept at 334 K and the rear wall at 344 K; in the z dimension, the bottom wall is kept at 344 K and the top wall at 334 K. Thus, the temperature gradients are positive in both x and y directions, but negative in the z direction. The other parameters are the same as in the lateral heating case. There is a physical problem at the adjoining edge/corner of two/three walls with different temperatures. However, in numerical treatment, only the average surface temperatures were used.

When steady state is reached, the distributions of temperature, pressure, methane mole fraction, and Soret coefficient along the x , y , and z centerlines are obtained. It is obvious that the temperature distributions in all three directions are approximately linear along the centerlines of the cavity with a slight variation near the boundary. There is no pressure variation along horizontal directions and the vertical distribution of pressure is linear. Therefore, the thermo-solutal convection does not distort linear temperature and pressure distributions in the porous cavity, since the convection flow with 10 md permeability is mild and contributes most to the separation of methane [2].

The compositional variation is significant in the vertical direction as shown in Fig. 3. Because of symmetry, compositional variations along the x and y centerlines are matched but much less than the compositional variation along the z centerline. It is remarkable that the composition at the top of the cavity is higher than at the bottom, which is opposite to the thermal driving force due to bottom heating in the z direction. Because of the higher temperature at the bottom, methane should migrate toward the bottom under the negative temperature gradient in the z -direction. But, the thermo-solutal convection dominates the mass transfer in the z -direction and results in an approximately linear

distribution with a higher methane mole fraction at the top.

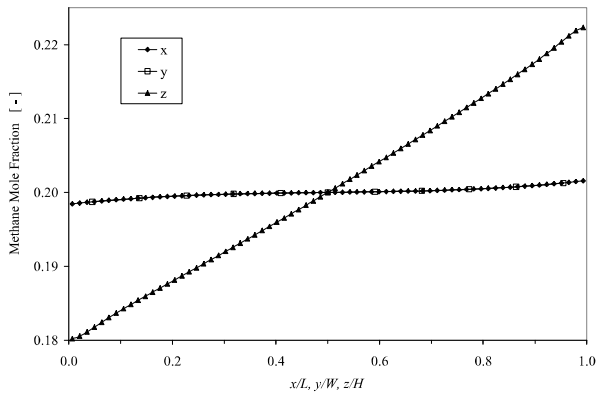


Figure 3 Composition distributions along x , y , and z centerlines in the cavity (combined heating case)

In Fig. 4, the thermal diffusion flux is significant in all three directions. The horizontal components of thermal diffusion flux, J_x and J_y , are of the magnitude 5.0×10^{-7} mol/m²/sec along all three x , y , and z centerlines. The value of J_z is much lower with the magnitude of 0.5×10^{-7} mol/m²/sec along all three centerlines. The difference between horizontal flux components and the vertical flux component comes from the temperature gradient difference in different directions: $\frac{\partial T}{\partial x} = \frac{\partial T}{\partial y} \sim 20.0$ K/m, but $\frac{\partial T}{\partial z} \sim$

2.0 K/m. There is a 10 times difference, which is the same order as the difference between the horizontal and vertical components of the thermal diffusion flux. Their distributions are all linear, which depend on the approximately constant temperature gradient and linear distributions of the Soret coefficient both horizontally and vertically.

The molecular diffusion flux distributions along the x , y , and z centerlines are shown in Fig. 5. The x component of molecular diffusion flux, J_x , along the x centerline, J_{x-x} in the figure, matches the y component J_y along the y centerline, J_{y-y} . So do J_{y-x} and J_{x-y} , and J_{z-x} and J_{z-y} . This is because of the symmetrical boundary conditions in both x and y directions inside the porous cavity. Along the x centerline, components J_y and J_z of molecular diffusion flux are linear, but the component J_x is quadratic. The same is true for the molecular diffusion flux along the y centerline.

The drastic variations of molecular diffusion fluxes along the vertical z centerline appear near the wall boundaries but the central part is quite linear. The magnitude of molecular diffusion flux, in all three directions, is of the order of 10^{-7} mol/m²/sec.

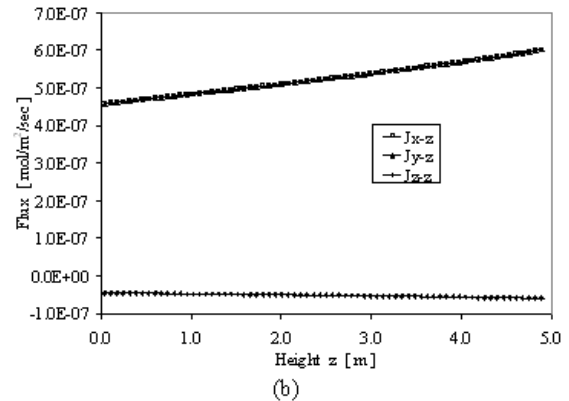
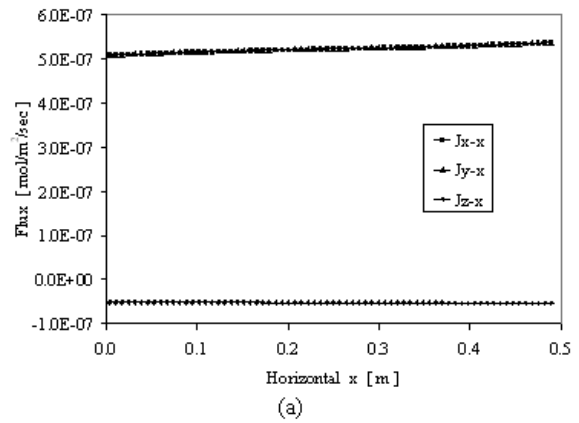


Figure 4 Thermal diffusion flux along centerlines

Finally, distributions of pressure diffusion fluxes are shown in Fig.6. The horizontal components, J_x and J_y , are zero along all three centerlines. This is consistent with the pressure distribution inside the porous cavity. But, the pressure gradient in the vertical direction is not zero, and J_z has a magnitude of 7×10^{-10} mol/m²/sec along all three centerlines.

All three components, J_x , J_y , and J_z , of the molecular diffusion and thermal diffusion fluxes approximately have the same order of magnitude equal to 10^{-7} mol/m²/sec, but the non-zero component of the pressure diffusion flux in the z direction is of the order of 10^{-10} mol/m²/sec, much smaller than the thermal diffusion fluxes. Therefore, in this case, thermal diffusion dominates in all directions, and pressure diffusion is very weak.

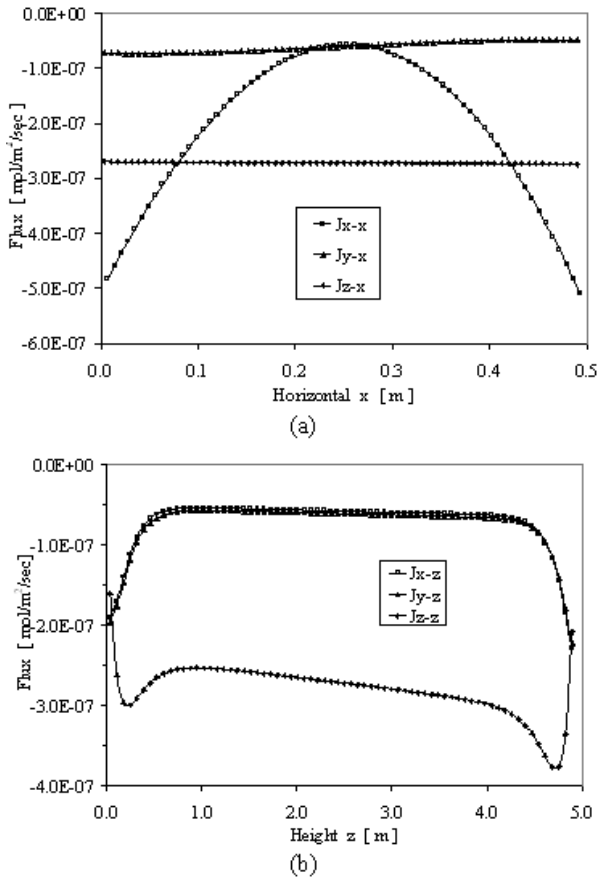


Figure 5 Molecular diffusion flux along centerlines

Dominant driving force: Both thermal diffusion and pressure diffusion are important driving forces for the compositional variation in porous media. In order to have a clear vision of each diffusion effect, quantitative analyses in three dimensions have been performed.

The pressure diffusion was evaluated under isothermal and convection-free conditions. Since there is no pressure gradient in horizontal directions, only vertical diffusion fluxes should be considered. Therefore, at steady state, there will be balanced diffusion fluxes between molecular diffusion and pressure diffusion. That is,

$$D_m \frac{\partial x_1}{\partial z} = D_p \frac{\partial P}{\partial z}$$

For this C₁/nC₄ binary mixture case, $D_m = 3.16 \times 10^{-9} \text{ m}^2/\text{s}$, $D_p = 1.5 \times 10^{-17} \text{ m}^2/\text{Pa}/\text{sec}$, and $\frac{\partial P}{\partial z}$ is approximately equal to ρg . Therefore, the induced vertical gradient $\frac{\partial x_1}{\partial z}$ is about $2.4 \times 10^{-5} \text{ m}^{-1}$. As the cavity has a height of 5.0 meters, the methane composition variation is predicted to be 0.012%.

Thermal diffusion in the horizontal direction can be estimated in convection free condition, too. There is no

pressure diffusion in the horizontal direction, so, at steady state, $D_m \frac{\partial x_1}{\partial x} = D_T \frac{\partial T}{\partial x}$. In this study case, $D_m =$

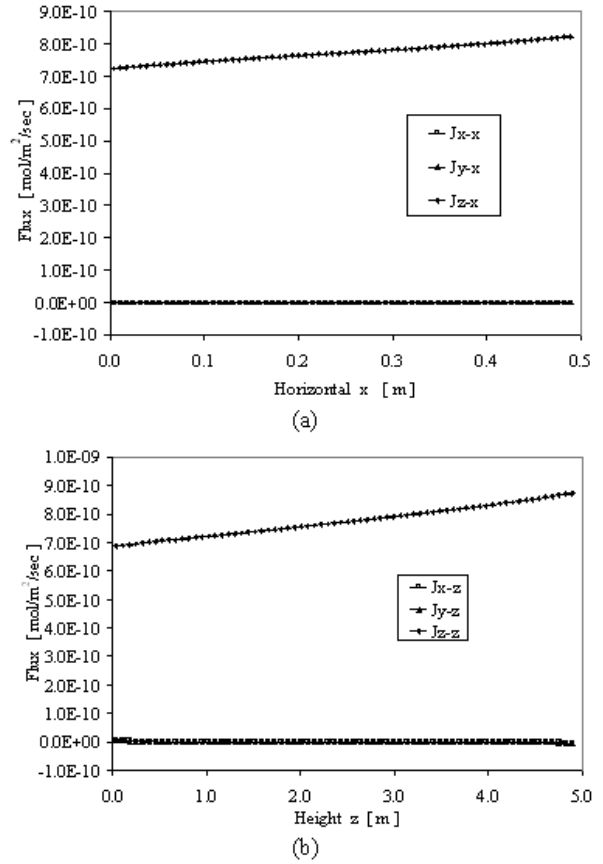


Figure 6 Pressure diffusion flux along centerlines

$3.16 \times 10^{-9} \text{ m}^2/\text{s}$, and $D_T = 2.52 \times 10^{-12} \text{ m}^2/\text{K}/\text{sec}$. Therefore, the induced horizontal methane gradient is $\frac{\partial x_1}{\partial x} = 0.0008 \frac{\partial T}{\partial x}$. With a temperature gradient equal to 20.0 K/m, the composition gradient will be 0.016 m^{-1} . This is a much larger value compared to the pressure diffusion case.

If a temperature gradient is applied in the vertical direction, the thermal diffusion and pressure diffusion will compete with each other if these diffusion fluxes are in opposite directions. In this case, we can estimate that if $\frac{\partial T}{\partial z} > 0.03 \text{ K/m}$, thermal diffusion dominates, and if $\frac{\partial T}{\partial z} < 0.03 \text{ K/m}$, pressure diffusion dominates in the molecular transport process. In the lateral heating case examined, the thermal diffusion was found to dominate over the pressure diffusion.

CONCLUSIONS

Three dimensional numerical simulations of thermo-solutal convection in a porous cavity have been conducted to investigate the compositional variations that

can occur inside the cavity. The magnitudes of thermal, molecular, and pressure diffusion fluxes were analyzed and compared to identify the most dominant factor in the component separation.

The numerical simulation results indicate that compositional variations can occur in both horizontal and vertical directions for both lateral heating and combined heating cases due to thermal, molecular, and pressure diffusion. The dominant driving force in the separation process, thermal diffusion or pressure diffusion, could be determined based on the values of the temperature gradient, gravitational acceleration, and the diffusion coefficients. The thermo-solutal convection was found to have a strong effect on the compositional variation, and cause a compositional distribution against the thermal driving force, as shown in the combined heating case.

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