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Study of thermodiffusion of carbon dioxide in binary mixtures of n-butane & carbon dioxide and n-dodecane & carbon dioxide in porous media

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ABSTRACT

Convection due to a thermodiffusion phenomenon has an important effect on component separation of hydrocarbon mixtures in a porous medium. A numerical study of carbon dioxide diffusion in porous medium is investigated in the presence of different fluid mixtures such as n-butane & carbon dioxide and n-dodecane & carbon dioxide single phase. In this paper, all physical properties with an exception of the mixture conductivity are assumed as varying with temperature and concentration. The fluid is maintained at a pressure of 150 bar and remains in the liquid state. Constant temperature gradients in horizontal and vertical directions are applied on the three-dimensional porous domain. Thermodiffusion coefficients applied in simulation were calculated by using Abbasi et al.'s [J. Non-Equilib. Thermodyn. 35 (2010) 1] thermodiffusion model. Results reveal that for a certain concentration of carbon dioxide, the thermodiffusion coefficient reaches a maximum leading to large separation. In the presence of the Soret effect, the vertical density distribution tends closer to the one without the Soret effect. With an increase in the permeability, the convection becomes dominant and contributes to a decrease in the vertical and horizontal component separation considerably.

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1. Introduction

Thermodiffusion as well as molecular diffusion is one way in mass flux in multicomponent systems in which is driven by temperature gradients. Thermodiffusion along the effect of natural convection has a great effect in concentration distribution in hydrocarbon reservoirs, and it can either lessen or weaken the separation in mixtures. A variety of researches have studied the effect of thermodiffusion in porous medium [1-3]. It was found that convection has an important role on the accuracy of Soret measurement. Costeseque et al. [4] carried out diffusion experiments in both free and porous medium Soret cells. It was found that the molecular diffusion and thermodiffusion coefficients in porous medium were related to those ones in clear fluid via the tortuosity. However, the ratio of the molecular diffusion coefficient to the thermodiffusion coefficient, known as Soret coefficient for binary mixtures, is identical for both configurations. Riley and Firoozabadi [5] presented a model to investigate the effects of natural convection and thermodiffusion along with molecular and pressure diffusions on a single-phase binary hydrocarbon mixture in a horizontal cross-sectional reservoir in the presence of a prescribed linear temperature field. It was found that the permeability has a great effect on the horizontal compositional variation. Delware et al. [6] studied these phenomena for a binary system in a square cavity. Their results showed that in the lateral heating case, the Soret effect is found to be weak; whereas in the bottom heating case the Soret effect is more prominent. Nasrabadi et al. [7] presented a numerical simulation of two-phase muticomponent diffusion and natural convection in porous medium. Thermodiffusion, pressure diffusion, and molecular diffusion were included in the diffusion expression from the thermodynamics of irreversible process. Results showed that the natural convection has an important role on the phase distribution in the gas and oil non-isothermal medium. Jaber et al. [8] simulated Soret effect for a ternary mixture in porous cavity considering variable viscosity and diffusion coefficients. It was found that for a permeability below 200 md, the thermodiffusion has a dominant effect: and above this level, buoyancy convection becomes the dominant mechanism. In addition, it was noted that the variation of viscosity has an important effect on the molecular and thermodiffusion.

Among different thermodiffusion models [9–20], the kinetic theory and non-equilibrium thermodynamics have more reliable results. In the kinetic approach, thermodiffusion coefficients are considered in terms of the specific heat of transport of the two

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