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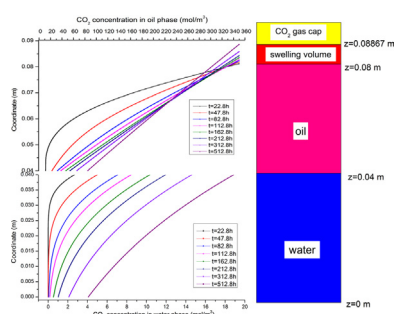
Numerical modeling of CO₂ diffusion into water-oil liquid system using moving mesh technique

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GRAPHICAL ABSTRACT



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ABSTRACT

A new diffusion model is developed to study the mass diffusion of CO₂ in the water-oil liquid system. The diffusion stages are divided by the position of diffused CO₂ front in the liquid system. The 1st and 2nd diffusion stages are performed to characterize the CO₂ diffusion in individual oil phase and in water-oil liquid system, respectively. The Peng-Robinson equation of state combined with the diffusion model of two stages are developed to describe the diffusion process of CO₂ in the water-oil liquid system. The developed model is validated by matching the pressure changes results of model calculation with an experimental acquisition. Besides, a moving mesh technique is applied to determine the oil swelling effect caused by the CO₂ diffusion. The results indicate that both CO₂ concentration profiles and oil swelling effect exhibit distinct characteristics at different stages. The CO₂ distributes only in the oil phase at the 1st diffusion stage but presents simultaneously in both water and oil phases at the 2nd diffusion stage. The oil swelling factors are 0.90% and 10.84% at the end of the 1st (t = 12.8 h) and 2nd (t = 512.8 h) diffusion stages, respectively.

1. Introduction

In CO₂ injection enhanced oil recovery (EOR) methods, gaseous CO₂ is injected into the oil reservoirs to enhance oil recovery through the mechanism of oil swelling, viscosity reduction, and interfacial tension reduction [1–3]. Diffusion of CO₂ into the oil is governed by the principal driving force caused by a concentration difference of CO₂ in

aqueous and liquid phases [4,5]. The injected CO₂ gas may diffuse into the oil phase or both water and oil phases, which depends on the existence of bound water or injected water possessing a water saturation ranging from 5% to 50% [6–8]. Meanwhile, during the process of CO₂ storage and capture (CSC), CO₂ is injected into abandoned crude oil reservoirs with a high water saturation; the dominant mechanism of CSC is the diffusion of CO₂ in the liquid phase [9]. CO₂ diffuses

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Nomenclature			
$c_o(z,t)$	CO ₂ concentration in oil phase, mol/m ³	D_w	CO ₂ diffusion coefficient in the water phase, m ² /s
D_o	CO ₂ diffusion coefficient in the oil phase, m ² /s	k_{pc}	partition coefficient
z	position variable, m	h	mesh step
t	time variable, s	N	the number of total nodes
$L_{o1}(t)$	time-dependent oil-gas position at the 1st diffusion stage, m	P	pressure, Pa
t_0	time of front of diffused CO ₂ reaches the oil-water interface, s	V	molar volume, m ³
c_{eq}	equilibrium concentration, mol/m ³	R	universal gas constant, KPa·m ³ /(K·mol)
T	time variable at the 2nd diffusion stage, s	T	temperature, K
$L_{o2}(t)$	time-dependent oil-gas position at the 2nd diffusion stage, m	a	attraction parameter
$f(z)$	CO ₂ concentration distribution in the oil phase of time $t = t_0$, mol/m ³	b	van der Waals volume, m ³ /mol
c_z	CO ₂ concentration at the oil-CO ₂ gas interface, mol/m ³	α	alpha function
ρ_{CO2}	CO ₂ density, kg/m ³	a_c	constant
M_{CO2}	molar mass of CO ₂ , kg/mol	P_c	critical pressure, Pa
		T_c	critical temperature, K
		T_r	reduced temperature, K
		ω	acentric factor
		RTh_o	oil swelling factor
		Th	the oil thickness at time t , m
		Th_i	the oil thickness at time 0, m

simultaneously into the water phase and oil phase when both oil and water are presenting in the liquid phases. However, the simultaneous diffusion of CO₂ in the water and oil phases are neglected in previous studies [4,10–21].

In a tertiary CO₂ displacing process, after the water-flooding or in water-wet reservoirs, a significant volume of water may exist in reservoirs in the form of free water or bound water [22–24]. CO₂ may not directly contact with the oil phase, hindering the recovery performance, especially for the tertiary CO₂ flooding process in the water flooded reservoirs [25,26]. Also, the injected CO₂ and water phase are separated by the oil phase (i.e., water film on the rock), in water-wet reservoirs [27,28]. In this study, the diffusion process of CO₂ in the water and oil phases is considered in a scenario that the CO₂ and water phase are separated by the oil phase, which can be found in the CO₂ flooding in water-wet reservoirs or CSC processes.

During the CO₂ diffusion in the water and oil phases, the CO₂ concentration and mass of diffused CO₂ increase with time, which also inevitably leads to the swelling of water and oil phases. Whereas, the swelling of water and oil phases is critical factor to evaluate the oil recovery performance and CO₂ storage capacity. The oil swelling effect caused by CO₂ diffusion increases the elastic energy of hydrocarbon chains of oil, thus forcing the remaining oil turn into movable oil and contributing to enhance oil recovery. The oil swelling effect also allows CO₂ to essentially expand oil, which pushes the oil out of the dead pores [29–31]. However, the CO₂ diffusion in the water phase is always ignored and only the CO₂ diffusion in the oil phase was considered in various workers [7,32–37]. With the co-existence of water and oil phases in the reservoir, the CO₂ diffusion process in the water phase has a great impact on the mass of injected CO₂ mass and oil recovery. Therefore, it is of fundamental and practical importance to investigate the CO₂ diffusion in oil and water phases.

Do and Pinczewski [38] studied the oil swelling deduced by the diffusion process when it directly contacted with the injection gas. The gas concentration in the oil phase was assumed to be in the form of variable power profile to solve the diffusion problem with moving boundary condition. Riazi [39] proposed a pressure decline method to measure the CO₂ diffusion coefficient in reservoir fluids. He demonstrated that the oil swelling, measured by the pressure and the position of the oil-gas interface changed with time. However, the proposed model only focused on the calculation of diffusion coefficients rather than oil swelling factors caused by the diffusion. Yang et al. [40] investigated the oil swelling effect resulted from the CO₂ diffusion in the heavy oil sample through the dynamic pendant drop volume analysis (DPDVA) method. The CO₂ diffusion coefficient in the oil phase was

calculated by monitoring the interface movement of oil pendant drop sample in the gas cell. Li et al. [41] studied the diffusion of CO₂ in a porous media saturated by oil under reservoir conditions. In their study, the radial diffusion process was used to describe both convection and diffusion induced by the swelling of the oil phase. Besides, the mathematical models were derived to calculate the diffusion coefficient and interface mass transfer coefficient. Vali et al. [42] introduced a moving mesh method to study the oil swelling in the diffusion process. The accuracy of the model was validated by comparing the results with 2D glass micromodel experimental results. Li et al. [19] investigated the diffusion coefficients of supercritical CO₂ in the oil-saturated cores and the oil swelling effect in low permeability reservoirs. They used the radial diffusion model to study the supercritical CO₂ diffusion process in the oil-saturated cores. The oil swelling factor was considered by introducing the oil saturation into the diffusion equation. However, the diffusion of CO₂ in the water phase is ignored in their research. Rezk et al. [43] determined the diffusion coefficient and the mass transfer coefficient of oil-CO₂ systems. The swelling factor was considered by analyzing the experimental results. Fayazi et al. [44] investigated the diffusion coefficient and oil swelling of oil-propane system utilizing Magnetic Resonance Imaging (MRI) technique. The propane concentration profile was obtained by using MRI and the swelling process was modeled by using the moving mesh technique and tracking the interface movement. However, the dilution diffusivity was treated as one in the infinite diffusion process. In those studies mentioned above, the oil swelling factor caused by the diffusion of CO₂ in the oil phase was taken into consideration in the process of determining the diffusion coefficients, regardless of whether the oil phase was bulk phase or in porous media. However, only a single oil phase was considered in those works, instead of the liquid system which composed of both oil and water phases. The single oil phase in the liquid assumption fails to describe the real diffusion situation in reservoirs. In this paper, the oil swelling effect and the movement of the interface between oil and gas was determined by using the moving mesh technique in the process of CO₂ diffusion in the oil–water liquid system. The swelling of water phase was ignored due to the much smaller diffusion coefficient value of water phase than that of oil phase [25,45,46].

In addition, some scholars studied the mass transfer of CO₂ in oil–water system to solve particular engineering problems such as water blocking and carbonated water injection (CWI). Do and Pinczewski [47] investigated the CO₂ concentration distribution in oil and water phases by using a system of ordinary partial equations; besides, they concluded that the major diffusion resistance was the water blocking phase. However, the volume variation and oil swelling were ignored.

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