J Ind Microbiol Biotechnol (2008) 35:495–500
DOI 10.1007/s10295-008-0307-z

ORIGINAL PAPER

Modeling of microorganisms transport in a cylindrical pore

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Received: 4 April 2007 / Accepted: 19 December 2007 / Published online: 22 January 2008

Abstract A mathematical model accounting for key parameters as microbial propagation, metabolite formation, dispersion, microbial chemotaxis and water flooding has been proposed to simulate the transport of microorganisms and their metabolites in a cylindrical pore with oil adhered to its inside surface. The model focuses on the transport and the concentration distributions of microorganisms and their metabolites in the cylindrical pore, especially the concentrations that on the oil–water interface. Results from the present model indicate that microorganisms and their metabolites assembled on the oil–water interface during the water flooding process, and the concentration gradients of microorganisms and their metabolites from the pore center region up to the oil–water interface in radial direction of the cylindrical pore were consequently formed. Equilibrium concentrations of microorganisms and their metabolites in the cylindrical pore were obtained when water flow rate within a certain scope, and there existed a critical water flow rate at which the maximum equilibrium concentration of microorganisms on the oil–water interface was developed. Investigations carried out in this study may provide better understanding on the transport mechanism of microorganisms in porous media.

Keywords Microorganism · Transport · Cylindrical pore · Mathematical model · Water flooding

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Introduction

Much attention has been paid to the application of microorganisms over the recent decades due to their potential application in engineering, such as microbial enhanced oil recovery, bioremediation of polluted soils and groundwater. Investigations in laboratories [8, 18] and field trials [12] have showed that microorganisms in oil reservoirs have the capacity to release residual oil, which adheres to the pore surfaces and is trapped inside pores of reservoirs. Since most of microorganisms inhabit porous media of petroleum reservoirs during water flooding process, the transport of microorganisms and microbial activities in porous media were crucial to understand the mechanism of microbial enhanced oil recovery.

The transport of microorganisms in porous media involves both physicochemical and biological processes such as microbial propagation and decay, dispersion, metabolite formation and substrate consumption etc. Recent works have showed that the transport of microorganisms in porous media depends on the bacterial slug size, flow rate of water, porosity, permeability, and the wettability of porous media [17]. Strains, which can adapt themselves in shape to pores have been experimentally proved to have stronger transport ability in porous media [9]. Numerical simulations [3, 15, 19] demonstrated that the pore surface retention and microbial plugging in the porous media were important to microbial transport processes. Microbial chemotaxis, which was neglected in many works, also plays a significant role in microbial transport, especially under the lower water flow rate [16].

As for the transport of microorganisms in a single pore, particularly, in the pore with the inside surface rich in nutrients, little work has been reported, and the transport mechanism in such a pore is not well understood yet. Any of the porous media consists of numerous single pores, and therefore, the transport of microorganisms in a pore plays a primary role in the investigation of the transport mechanism of microorganisms in porous media. The present paper focuses on the transport of microorganisms in a cylindrical pore with its inside surface covered by a thin layer of crude oil served as the carbon source of microorganisms. The influence of microbial propagation, dispersion and microbial chemotaxis on the concentration profiles of microorganisms and metabolites in the pore was taken into account, and particularly, the impact of the water flow rate on the concentrations of microorganisms and metabolites on the oil–water interface was investigated.

Model development

Physical model of cylindrical pore

The cylindrical pore to describe the transport of microorganisms and their metabolites is considered as a straight and symmetrical pore. Two incompressible and isothermal fluids of oil and water are presented in the cylindrical pore. Oil adheres to the inside surface of the pore in the form of a thin layer and serves as the carbon source of microorganisms. Water flows through the pore and contains abundant nutrients. Metabolites formatted during microbial propagation are supposed to have inhibition on microbial propagation. It is assumed that microorganisms and their metabolites exist only in aqueous phase.

Model conformation

The transport equations of microorganisms and their metabolites in the cylindrical pore are in the forms of

$$\frac{\partial C_M}{\partial t} = \nabla(D_M \cdot \nabla C_M) - \nabla(u_W C_M) - \nabla(u_C C_M) + \mu_M C_M \tag{1}$$

and

$$\frac{\partial C_P}{\partial t} = \nabla(D_P \cdot \nabla C_P) - \nabla(u_W C_P) + r_P \tag{2}$$

where C_M and C_P are the concentrations of microorganisms and their metabolites in the cylindrical pore, respectively. The four terms on the right hand side of Eq. (1) corresponds to the microbial dispersion, water flooding, chemotaxis and microbial propagation, respectively. The three terms on the right hand side of Eq. (2) corresponds to the metabolite dispersion, water flooding and metabolic yield, respectively.

Parameter description

The actively propagation of microorganisms in porous media is the foundation of application of microorganisms in microbial enhanced oil recovery and remediation of polluted soils and groundwater. It has been proved that the growth rate of microorganisms is influenced by concentrations of both limiting substrate and metabolites, and here we use a modified Monod equation [10] to simulate the microbial propagation

$$\mu_M = \mu_{MAX} \frac{C_S}{K_D + C_S} \cdot \left(1 - \frac{C_P}{C_P^*}\right)^n \tag{3}$$

where μ_M is the specific growth rate of microorganisms, μ_{MAX} the maximum specific growth rate achievable when $C_S >> K_D$, C_S the concentration of carbon source oil, K_D the saturate constant, C_P the concentration of inhibitory metabolites, C_P^* the critical concentration of inhibitory metabolites above which microorganisms cease to propagate, and n is a constant.

The metabolites considered here are the secondary metabolites of microorganisms, and its formation rate relates to the concentration of microorganisms, which can be expressed as [14]

$$r_P = K_P C_M \tag{4}$$

where K_P is the specific formation rate of metabolites.

Chemotaxis refers to the ability of microorganisms to sense the gradient concentration of chemicals in water and the direct motion towards chemoattractant and/or away chemorepellent [20]. It was studied in laboratory that the swimming speed of microorganisms was greater than the typical groundwater flow rate, particularly, in the present of chemical gradient. Therefore, microbial chemotaxis plays a critical role in the transport process of microorganisms in porous media at a lower water flow rate. The chemotactic velocity of microorganisms, u_C, is assumed to be proportional to an exponential change in carbon source concentration [5, 7]

$$u_C = K_C \nabla(\ln C_S) \tag{5}$$

where K_C is the chemotactic coefficient of microorganisms. In this model the concentration of the carbon source, oil, in water is far lower than that on the oil–water interface for the low solubility of hydrocarbons in aqueous phase. Thus we set the distribution of oil in radial direction of the pore as an exponential expression

$$C_S = C_{Si} \exp\left[K_S(r - R)\right] \tag{6}$$

where C_{Si} is the concentration of carbon source on the oil–water interface, K_S the distribution coefficient of carbon source.

The influence of water flooding on the transport of microorganisms and their metabolites is considered in this study, and the water flow rate in the cylindrical pore is given by laminar flow [1]

$$u_W(r) = \frac{\Delta P}{4\eta L}\left(R^2 - r^2\right) \tag{7}$$

where η is the viscosity of aqueous phase and $\Delta P/L$ is the pressure drop per pore length, which depends on the inject rate of water.

The cylindrical pore was initially saturated by water, and then the suspension of microorganisms (tenth pore volume) with original concentration, C_M^0, was applied onto the cylindrical pore followed by flushing with water. The initial and boundary conditions were given by

$$C_M(r,x) = C_M^0 \quad x \le 0.1X,\ t = 0 \tag{8}$$

$$C_M(r,x) = 0 \quad x > 0.1X, t = 0 \tag{9}$$

$$C_P(r,x) = 0 \quad t = 0 \tag{10}$$

$$\frac{\partial C_M(r,x)}{\partial r} = 0 \quad r = 0 \,\text{or}\, r = R, t > 0 \tag{11}$$

$$\frac{\partial C_P(r,x)}{\partial r} = 0 \quad r = 0 \,\text{or}\, r = R, t > 0 \tag{12}$$

$$C_M(r,x) = 0 \quad x = 0,\ t > 0 \tag{13}$$

$$C_P(r,x) = 0 \quad x = 0,\ t > 0 \tag{14}$$

$$\frac{\partial C_M(r,x)}{\partial x} = 0 \quad x = X, t > 0 \tag{15}$$

$$\frac{\partial C_P(r,x)}{\partial x} = 0 \quad x = X, t > 0 \tag{16}$$

where R, X, r and x are the radius, length, radial coordinate and axial coordinate of the cylindrical pore, respectively. Parameters used in the model are list in Table 1.

Table 1 Base values of the parameters used in simulation

Parameter	Value
D_M[a]	2.78×10^{-6} cm^2 s^{-1}
K_C[a]	5.56×10^{-5} cm^2 s^{-1}
K_P	0.05 kg metabolites (kg microorganisms h)$^{-1}$
R	1.0×10^{-3} m
X	1.0 m
μ_{MAX}[b]	1.0 h^{-1}
η	1.0×10^{-3} Pa s

[a] Lewus et al. [11]

[b] Dinopoulou et al. [4]

Results

In the present model, the original concentration of microorganisms, C_M^0, is set as a baseline when dealing with the dates, and the ratio of C_M/C_M^0 is calculated. The water flow rate used in model prediction is represented by the average velocity of laminar flow, $\bar{u}_W$, which is written as

$$\bar{u}_W = \frac{\int_A u_W(r)dA}{A} = \frac{\Delta P}{8\eta L}R^2 \tag{17}$$

where A is the cross section area of the cylindrical pore.

Concentrations of microorganisms and their metabolites in the cylindrical pore

Microbial concentration on the oil–water interface increases for the propagation of microorganisms by consuming carbon source oil, and the concentration of metabolites simultaneously increases in metabolism (Fig. 1). Concentrations of microorganisms and their metabolites on the oil–water interface can reach a set of equilibrium concentrations, and never change with water flooding time when the water flow rate is lower than a critical rate, unless microorganisms and their metabolites are washed out of the cylindrical pore by water.

Microorganisms tend to assemble on the oil–water interfacial region, thus in radial direction, equilibrium concentrations of microorganisms and metabolites near the oil–water interface are higher than that in the pore center region after the equilibrium is obtained. Equilibrium concentrations of microorganisms are almost the same in axial direction of the pore, but equilibrium concentrations of metabolites increase from the upstream to the downstream of the cylindrical pore (Fig. 2a, b).

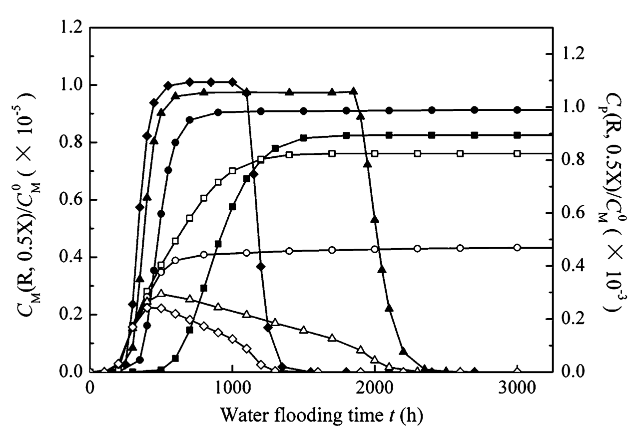

Fig. 1 Concentration profiles of microorganisms (*solid*) and metabolites (*open*) on the oil–water interface: (*filled square*) $\bar{u}_W = 1.0$ cm h^{-1}; (*filled circle*) $\bar{u}_W = 1.8$ cm h^{-1}; (*filled triangle*) $\bar{u}_W = 2.25$ cm h^{-1}; (*filled diamond*) $\bar{u}_W = 2.5$ cm h^{-1}

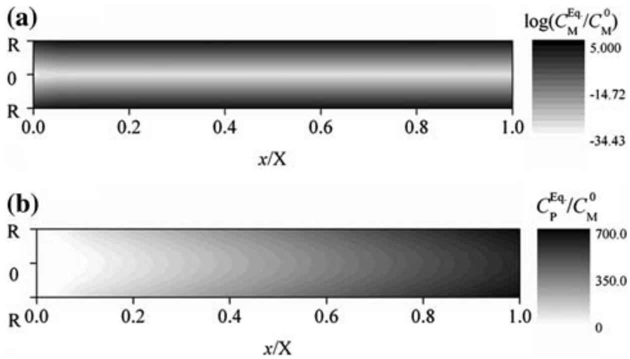

Fig. 2 Equilibrium concentrations of microorganisms (**a**) and metabolites (**b**) in the cylindrical pore, $\bar{u}_W = 1.25$ cm h^{-1}

Influence of key factors on the equilibrium concentrations of microorganisms and their metabolites on the oil–water interface

Concentrations of microorganisms and metabolites on the oil–water interface play an important role in the application of microorganisms in engineering projects, and it is also the key parameter we concerned in this model. Here we discuss the equilibrium concentrations of microorganisms and metabolites on the oil–water interface obtained during the water flooding process. In order to invest the effect of key parameters on the equilibrium concentrations of microorganisms and metabolites, all the numerical simulations in this work were conducted by varying one of the parameters and all the other parameters held constant.

Microorganisms with higher specific growth rate propagate more quickly, and the equilibrium concentration of microorganisms on the oil–water interface can reach to a higher value (Fig. 3). Dispersion of microorganisms with higher diffusivity causes more microorganisms move to the pore center region from the oil–water interface, and the equilibrium concentration of microorganisms on the oil–water interface decreases (Fig. 4). Microbial chemotaxis results in the migration of microorganisms from the pore center region to the carbon source oil, so higher chemotactic velocity enhanced the enrichment of microorganisms on the oil–water interface (Fig. 5). Within a certain scope of water flow rate, equilibrium concentrations of microorganisms on the oil–water interface increase with water flow rate (Fig. 6).

Concentrations of microorganisms in the cylindrical pore are influenced by parameters mentioned above. For a given species of microorganisms inhabiting in a specific environment, parameters as microbial propagation, microbial chemotaxis, metabolite inhibition and dispersion may be determined accordingly. While for the parameter of water flow rate, it is practically variable, and an expected concentration profile of microorganisms in pores may be achieved by controlling the water flow rate, which is valuable in industrial application of microbial enhanced oil recovery. For this reason, we investigated the influence of water flow rate, $\bar{u}_W$, on the equilibrium concentrations of microorganisms and their metabolites on the oil–water interface in a wide scope. As can be seen in Fig. 7 that the equilibrium concentration of microorganisms on the oil–water interface increases efficiently with the increase of the water flow rate up to about 0.55 cm h^{-1}, and a relaxative trend of the equilibrium concentration is achieved with a further increase of the water flow rate up to 1.80 cm h^{-1}. A maximum equilibrium concentration of microorganisms and a minimum equilibrium concentration of metabolites on the oil–water interface are obtained at 1.80 cm h^{-1}. When the water flow rate exceeded this critical rate, 1.80 cm h^{-1}, microorganisms may be completely washed out of the cylindrical pore by water.

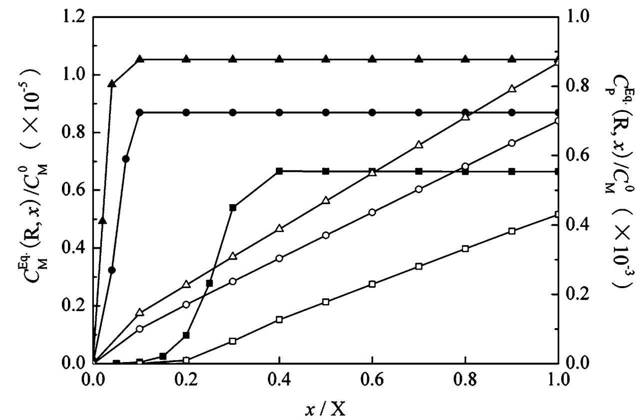

Fig. 3 Equilibrium concentrations of microorganisms (*solid*) and metabolites (*open*) on the oil–water interface with different maximum specific growth rates: (*filled square*) $\mu_{MAX} = 0.5$ h^{-1}; (*filled circle*) $\mu_{MAX} = 1.0$ h^{-1}; (*filled triangle*) $\mu_{MAX} = 2.0$ h^{-1}

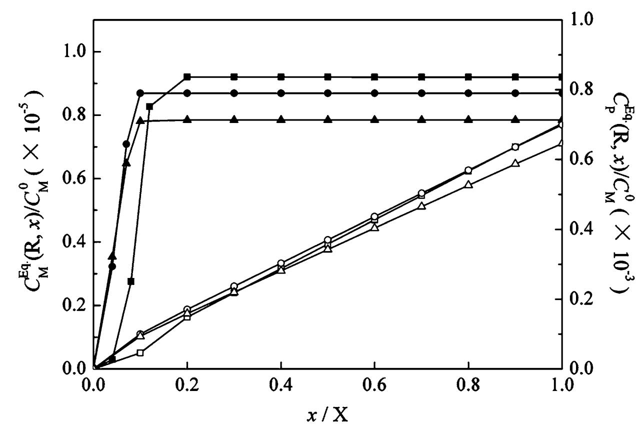

Fig. 4 Equilibrium concentrations of microorganisms (*solid*) and metabolites (*open*) on the oil–water interface with different microbial diffusivities: (*filled square*) $D_M = 1.39 \times 10^{-6}$ cm^2 s^{-1}; (*filled circle*) $D_M = 2.78 \times 10^{-6}$ cm^2 s^{-1}; (*filled triangle*) $D_M = 5.56 \times 10^{-6}$ cm^2 s^{-1}

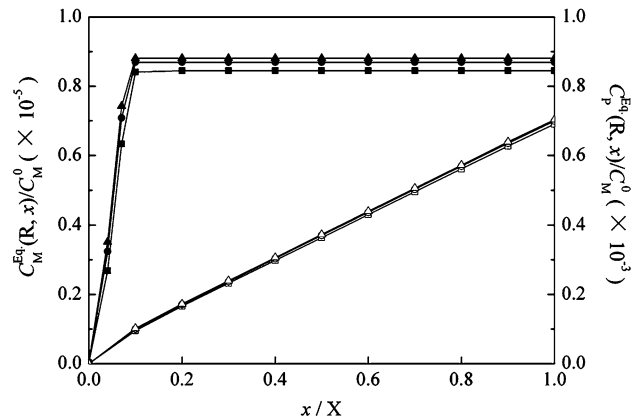

Fig. 5 Equilibrium concentrations of microorganisms (*solid*) and metabolites (*open*) on the oil–water interface with different microbial chemotactic coefficients: (*filled square*) $K_C = 2.78 \times 10^{-5}$ cm^2 s^{-1}; (*filled crcle*) $K_C = 5.56 \times 10^{-5}$ cm^2 s^{-1}; (*filled triangle*) $K_C = 1.11 \times 10^{-4}$ cm^2 s^{-1}

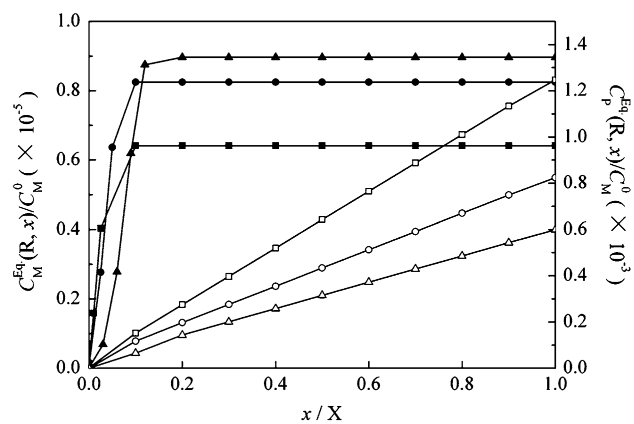

Fig. 6 Equilibrium concentrations of microorganisms (*solid*) and metabolites (*open*) on the oil–water interface with different water flow rates: (*filled square*) $\bar{u}_W = 0.5$ cm h^{-1}; (*filled circle*) $\bar{u}_W = 1.0$ cm h^{-1}; (*filled triangle*) $\bar{u}_W = 2.0$ cm h^{-1}

Discussion

Metabolites present in aqueous phase inhibit the propagation of microorganisms according to Eq. (3), especially for the condition that metabolites concentration exceeds the critical inhibitory concentration C_P^*. Till the effects of microbial propagation, metabolite inhibition, chemotaxis, dispersion and water flooding keep balance, the concentration of microorganisms will not change with water flooding time, and the equilibrium concentrations of microorganisms and metabolites in the cylindrical pore are consequently obtained.

Microorganisms, which are capable of using oil as their carbon source are likely to migrate to the substrate due to microbial chemotaxis, such as *Pseudomonas aeruginosa* [13], and in the present model microorganisms aggregated

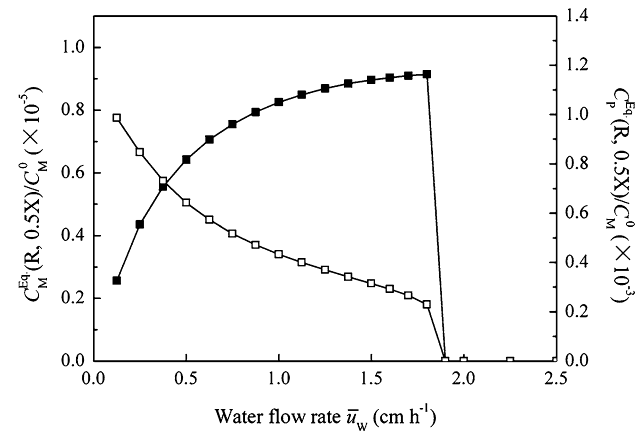

Fig. 7 Effect of water flow rate $\bar{u}_W$ on equilibrium concentrations of microorganisms (*solid*) and metabolites (*open*) on the oil–water interface

on the oil–water interface in radial direction of the cylindrical pore. Microorganisms on the oil–water interface propagated rapidly for the abundant carbon source and consequently enriched in the interfacial region, however, in the pore center region microorganisms propagated slowly and were largely flushed by water flooding, thus the equilibrium concentrations of microorganisms in radial direction of the pore presented an acute distribution. The equilibrium concentration gradient of metabolites was shallow compared to that of microorganisms for there was no radial motion of metabolites to the interface as chemotaxis. These results were supported by works of Jing et al. [6]. In their experimental work, they found that microbial concentration could reach to $10^7 \sim 10^8$ cells ml^{-1} within 10 μm away from the oil–water interface, but it reduced rapidly to $10^3 \sim 10^4$ cells ml^{-1} farther away. Metabolites were drove from the inlet to the outlet of the pore by water, so the equilibrium concentration of metabolites in the downstream was higher than that in the upstream of the pore.

Higher microbial chemotactic velocity caused more microorganisms migrated to the oil–water interface in a certain period, higher specific growth rate resulted in higher growth rate, so the concentration of microorganisms on the oil–water interface increased rapidly, and the equilibrium concentration was accordingly higher. In contrast, microorganisms moved from the oil–water interface to the pore center region under the effect of microbial dispersion, so microorganisms with higher diffusivity resulted in lower equilibrium concentration on the oil–water interface. Magnifying the water flow rate resulted in more loss of metabolites, and the inhibition of metabolites on microbial propagation was weakened, therefore, the equilibrium concentration of microorganisms on the oil–water interface increased. But microorganisms and metabolites may be completely washed out of the cylindrical pore by water with a higher water flow rate (1.80 cm h^{-1}). A similar behavior was obtained in the experimentally microbial water flooding tests by Behlulgil et al. [2], their observed dates showed that the efficiency of microbial water flooding diminished at the highest flow rate.

Conclusions

In summary, a mathematical model incorporated with the microbial propagation, metabolite formation, chemotaxis, dispersion and water flooding has been developed to characterize the transport of microorganisms and metabolites in a cylindrical pore, oil adhered to the inside surface of the pore as a form of thin layer and served as carbon source. The transport of microorganisms is fundamentally important to understand the mechanism of microbial enhanced oil recovery and bioremediation of polluted soils, since the residual oil and organic pollutions adhered to the surfaces and/or trapped in the pores of subsurface. Results by this model show that the propagation and chemotaxis of microorganisms contribute to enhance the enrichment of microorganisms on and near to the oil–water interface; for a given species of microorganisms, different equilibrium concentrations of microorganisms and metabolites were obtained under different water flow rates, and there existed a critical water flow rate at which a maximum equilibrium concentration of microorganisms and a minimum equilibrium concentration of metabolites on the oil–water interface were developed.

Acknowledgments This work was supported by the National Natural Science Foundation of China (Grant No. 50374038) and the Ministry of Education of China (Grant Nos. 20030251002, 03071).

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