



# Numerical modelling of biophysicochemical effects on multispecies reactive transport in porous media involving *Pseudomonas putida* for potential microbial enhanced oil recovery application

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## HIGHLIGHTS

- Developed kinetic and reactive transport model for *Pseudomonas putida* in porous media.
- Parametric values for kinetic model are determined from experimental observations.
- pH affects sucrose and biosurfactant concentration than microbe during its transport.
- At pH 7.5, biosurfactant concentration is higher and it favours more oil recovery.
- Higher resident time of slug and lesser  $S_w$  within reservoir improves oil recovery.

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## ABSTRACT

pH and resident time of injected slug plays a critical role in characterizing the reservoir for potential microbial enhanced oil recovery (MEOR) application. To investigate MEOR processes, a multispecies (microbes–nutrients) reactive transport model in porous media was developed by coupling kinetic and transport model. The present work differs from earlier works by explicitly determining parametric values required for kinetic model by experimental investigations using *Pseudomonas putida* at different pH conditions and subsequently performing sensitivity analysis of pH, resident time and water saturation on concentrations of microbes, nutrients and biosurfactant within reservoir. The results suggest that nutrient utilization and biosurfactant production are found to be maximum at pH 8 and 7.5 respectively. It is also found that the sucrose and biosurfactant concentrations are highly sensitive to pH rather than reservoir microbial concentration, while at larger resident time and water saturation, the microbial and nutrient concentrations were lesser due to enhanced dispersion.

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## 1. Introduction

Microbial enhanced oil recovery (MEOR) is an economical, environment friendly and easy to implement technique applied to improve the oil recovery from hydrocarbon reservoirs either by using microbes or microbial products (Sen, 2008). The fundamental and key processes that governs the performance of *in-situ* MEOR technique are transport of injected microbes and nutrients within porous reservoir (Nielsen et al., 2014), biosurfactant production by microbes (Sen, 2008) and reduction of interfacial tension (IFT)

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between oil and water by produced biosurfactant (Bryant and Lockhart, 2002). These fundamental processes of MEOR are influenced by; *in-situ* geo-environmental factors such as pH, temperature and salinity (Bryant and Lockhart, 2002); and operational factors that includes resident time of injected fluid, injection velocity and duration of injection process (Bryant and Lockhart, 2002). Even though MEOR has several advantages, it is practised remotely at the global level because of the following reasons: (i) lack in understanding on *in-situ* geo-environmental aspects of microbes and (ii) the sensitivity of critical factors such as pH, resident time and water saturation on fundamental processes of MEOR technique which leads to uncertainty in the prediction of oil recovery (Bryant and Lockhart, 2002; Brown, 2010). Hence, it is necessary to quantify the sensitivity of these factors on MEOR processes by developing a suitable kinetic and reactive transport model in order

to predict MEOR performance for a specific micro-organism (Brown, 2010; Xiao et al., 2013).

Researchers performed experimental and modelling studies in order to understand the effect of pH and temperature on different microbes for potential MEOR application. Sun et al. (2011) had experimentally characterized the biosurfactant produced by *Geobacillus* strain at different pH and temperature conditions. Vaz et al. (2012) produced and characterized the biosurfactant from *Bacillus subtilis* different pH and temperature conditions. Arora et al. (2014) experimentally studied the use of *Clostridium* sp. for potential MEOR application at reservoir temperature conditions. Sivasankar and Suresh Kumar (2014) modelled the effect of reservoir temperature on MEOR processes and predicted its performance under non-isothermal conditions using *Bacillus* sp. They also performed numerical investigation on the combined effect of pH and temperature on MEOR processes using *Bacillus licheniformis*. Kanna et al. (2014) reported that the biosurfactant produced by *P. putida* can reduce the IFT between hydrocarbon and water at various pH conditions. Such reduction of IFT by rhamnolipids, a biosurfactant produced by *Pseudomonas aeruginosa* (Gudiña et al., 2015) would enhance the recovery of residual oil from hydrocarbon reservoir during MEOR application. However, the study made on *P. putida* for potential MEOR application is relatively less compared to *Bacillus* sp. microbes. Among several physicochemical parameters, pH is one of the main parameters that affects the microbial metabolism (Rousk et al., 2009). Hence, the prevalence of different pH conditions within the reservoir affects: (i) the growth of microbes, (ii) consumption of nutrients and (iii) the stability of produced biosurfactant within the reservoir during MEOR application. However, to the best of the author's knowledge, no modelling study has been carried out on *P. putida* that quantifies the effect of pH and the other critical operational factors that includes resident time and water saturation on fundamental MEOR processes which considers transport of microbes and nutrients, production of biosurfactant, and its consecutive IFT reduction. Thus, in order to better characterize the suitability of MEOR process in a typical petroleum reservoir, in the present work, an attempt has been made to analyse the sensitivity of pH, resident time and water saturation on fundamental MEOR processes through development of experimentally verified kinetic and transport models for *P. putida*, nutrients and produced biosurfactant.

The objectives of the present study are: (a) to determine the kinetic parametric values from experimental investigations, and subsequently to develop a kinetic model that simulates the effect of pH on growth of *P. putida*, nutrient utilization, production of biosurfactant, and IFT reduction; (b) to develop a multispecies reactive transport model in porous media for *P. putida* and nutrients by coupling the kinetic model with the corresponding transport model; and (c) to perform sensitivity analysis of pH, resident time and water saturation on concentrations of microbes, nutrients and biosurfactant within reservoir using the developed multispecies reactive transport model.

## 2. Materials and methods

The experimental procedure for the present study was adopted from Kanna et al. (2014).

### 2.1. Microorganism and maintenance

Strain *P. putida* MTCC 2467 was procured from Microbial Type Culture Collection (MTCC), India for this present work. The culture was maintained in nutrient agar plates with composition as follows (g/L): peptone, 5.0; beef extract, 1.0; yeast extract, 2.0;

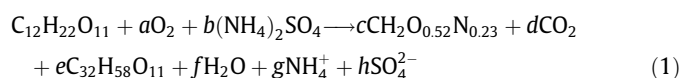
NaCl, 5.0; agar, 20.0; pH  $7.0 \pm 0.3$ , storage temperature  $-2^\circ\text{C}$  to  $-8^\circ\text{C}$ .

### 2.2. Media and cultivation conditions

Nutrient broth preparation was similar to that of nutrient agar composition as described in Section 2.1 with the exclusion of agar. *P. putida* (MTCC 2467) was grown in nutrient broth for 10–12 h at  $30^\circ\text{C}$  ( $A_{600\text{nm}}$  0.7–0.9) and 2% (v/v) of the inoculum was used for production of bio-surfactant using mineral salt medium with the following composition (g/L)  $\text{KNO}_3$ , 0.3;  $\text{Na}_2\text{HPO}_4$ , 0.2;  $\text{KH}_2\text{PO}_4$ , 0.014; NaCl, 0.001;  $\text{MgSO}_4$ , 0.06;  $\text{CaCl}_2$ , 0.004;  $\text{FeSO}_4$ , 0.002; 0.1 ml of trace element solution containing (g/L)  $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ , 2.32;  $\text{H}_3\text{BO}_3$ , 0.56;  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ , 1.0;  $\text{MnSO}_4 \cdot 4\text{H}_2\text{O}$ , 1.78;  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$ , 0.39;  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ , 0.42;  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ , 0.004; KI, 0.66; EDTA, 0.5;  $\text{K}_2\text{SO}_4$ , 3.0. Sucrose (2% w/v) and ammonium sulphate (0.3% w/v) was used as carbon and nitrogen sources because of its higher microbial yield compared to other carbon and nitrogen sources (Kanna et al., 2014).

### 2.3. Development of material balance equation

Based on experimental observations, the values of biomass yield with respect to sucrose [ $Y_{XS}$ ], yield of biosurfactant with respect to sucrose [ $Y_{PS}$ ], maximum microbial growth rate [ $\mu_{\text{max}}$  ( $\text{h}^{-1}$ )] and half saturation constant of sucrose [ $K_{XS}$  ( $\text{gl}^{-1}$ )] are computed at different pH conditions between 5 and 8. The value of  $Y_{XS}$  is computed from the slope of the line drawn between microbial concentration and sucrose concentration, while, the value of  $Y_{PS}$  is computed from the slope of the line drawn between biosurfactant and sucrose concentration. Subsequently, for varying pH conditions, the material balance equation for microbe (*P. putida*), nutrients (sucrose, ammonium sulphate) and biosurfactant (rhamnolipid) is developed [Eqs. (1)–(8)] in order to determine the value of other critical parameters namely yield of microbes with respect to ammonium sulphate [ $Y_{XN}$ ] and stoichiometric values of reactants and products involved in the reaction as given in Eq. (1)



Eq. (1) represents the material balance equation for present reaction, in which the term  $a$ ,  $b$ ,  $c$ ,  $d$ ,  $e$ ,  $f$ ,  $g$  and  $h$  corresponds to the number of moles of oxygen ( $\text{O}_2$ ), ammonium sulphate ( $(\text{NH}_4)_2\text{SO}_4$ ), *P. putida* ( $\text{CH}_2\text{O}_{0.52}\text{N}_{0.23}$ ) (Libner et al., 2009), carbon di oxide ( $\text{CO}_2$ ), rhamnolipid ( $\text{C}_{32}\text{H}_{58}\text{O}_{11}$ ), water ( $\text{H}_2\text{O}$ ), ammonium ion ( $\text{NH}_4^+$ ), and sulphate ion ( $\text{SO}_4^{2-}$ ) respectively. The values of  $b$ ,  $c$  and  $e$  are determined from experimental observations and they are reported through Eq. (2)–(4)

$$b = \frac{\text{Concentration of } (\text{NH}_4)_2\text{SO}_4 \text{ utilised}}{\text{Concentration of sucrose utilized}} \times \frac{\text{Molecular weight of sucrose}}{\text{Molecular weight of } (\text{NH}_4)_2\text{SO}_4} \text{ mole} \quad (2)$$

In Eq. (2), the utilized concentration of ammonium sulphate and sucrose are determined from experimental observations by computing the difference between the initial and final concentrations of ammonium sulphate and sucrose. The utilized concentration of ammonium sulphate and sucrose varies depending on the respective pH values

$$c = Y_{XS} \cdot \frac{\text{Molecular weight of sucrose}}{\text{Molecular weight of } Pseudomonas putida} \quad (3)$$

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