

## Equilibrium Modeling

### *Models of sorption isotherm*

The mechanism of As sorption on the biosorbent surface was described by applying isotherm equilibrium models of Langmuir and Freundlich, which are based on two parameters. Multi-layer sorption or sorption on heterogeneous surfaces was described by Freundlich model with the equation described below (Eq. 3):

$$Q_e = Q_F C_e^n \quad (3)$$

In the equation linearity related parameter was mentioned with  $n$  and capacity of Adsorption with units  $\text{mg}^{1-n} \text{g}^{-1} \text{L}^n$  was shown with  $Q_F$ .

Langmuir model was used to describe the monolayer adsorption and sorption on planar surfaces with the Eq. 4 given below:

$$Q_e = Q_L K_L C_e (1 + K_L C_e)^{-1} \quad (4)$$

In the equation mentioned above,  $K_L$  is representing the constant of sorption equilibrium with unit ( $\text{L mg}^{-1}$ ) and maximum As sorbed amount ( $\text{mg g}^{-1}$ ) was described by  $Q_L$ .

### *Kinetic modeling of sorption*

On biosorbents mass, the sorption rate of As was examined by applying pseudo-first order and pseudo-second order. Following equations 1 and 2 were used for pseudo-first order which is grounded on the capacity of solid biosorbent.

$$\log(q_e - q_t) = \frac{\log q_e - k_1 t}{2.303} \quad (1)$$

In the above equation As sorbed amount at any time  $t$  ( $\text{mg g}^{-1}$ ) is mentioned with  $q_t$ , equation constant rate with unit  $\text{min}^{-1}$  is mentioned as  $k_1$  and sorbed As amount at equilibrium with unit  $\text{mg g}^{-1}$  is named as  $q_e$ . Plotting  $\log (q_e - q_t)$  vs  $t$  was used to determine  $k_1$  which is the constant rate of biosorption.

The kinetic model, pseudo-second order was utilized which suggest that sorption rate is proportional to the square of the number of remaining free sorption active sites. Following is the equation (Eq 2) to describe the pseudo-second order.

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \quad (2)$$

In the above equation of pseudo-second order. equilibrium constant rate with unit ( $\text{g mg}^{-1} \text{min}^{-1}$ ) is mentioned with  $k_2$ . The intercept of  $1/(k_2 q_e^2)$  and slope of  $1/q_e$  are linear between the relationship of  $t$  and  $t/q_t$ .