Mathematical ananlysis of toluene biodegradation by rhodococcus erythropolis in bioreactor using new approach to homotopy perturbation method

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Abstract

The mathematical model for toluene removal and CO_2 production by rhodococcus erythropolis has been discussed. This paper presents an analytical method (Homotopy perturbation method) to solve the nonlinear differential equations that describe the biomass formation, toluene mineralization, and CO_2 production in liquid and gas phase with respect to time. Approximate analytical expressions for the concentration of biomass formation, toluene mineralization, and CO_2 production in liquid and gas have been derived for various values of the relevant parameters. Our analytical results are compared with the experimental data. In addition, the sensitivity of the kinetic parameters was also analyzed.

Keywords: *Toluene; CO_2 production; Rhodococcus erythropolis; Modeling; Homotopy perturbation method;*

Introduction

Pollution in the atmosphere has become one of the major cause of premature death in many countries [1]. It is due to the volatile organic compounds (VOCs), which are introduced into the atmosphere through anthropogenic or biogenic activities [2]. Nowadays several steps are taken to reduce the emission of volatile organic compounds (VOC) like toluene, nitric oxide, ethanol etc., because of its harmfulness towards to human. Among these VOCs, toluene occur in the commonly used consumer products such as paints, glues and nail polish removers.

Toluene is a clear, colorless liquid solvent with a distinctive smell. It occurs naturally in crude oil and in the tolu tree. It can be released into the air, water, and soil at places where it is produced or used and particularly in heavy vehicular traffic. Toluene can enter into the body by breathing outdoor or indoor air containing this substance. It can affect your nervous system (brain and nerves) such as headaches, dizziness, or unconsciousness. However, effects such as incoordination, cognitive impairment, and vision and hearing loss may become permanent. High levels of toluene exposure during pregnancy, such as those associated with solvent abuse, may lead to retardation of mental abilities and growth in children. Other health effects of potential concern may include immune, kidney, liver, and reproductive effects. To control the release of VOC's like nitrous oxide, nitric oxide, toluene etc. from industries, biofilters are being used instead of the chemical complex absorption method [3].

Biofilters have dual role: one is reducing the turbidity and pathogen particles like the conventional filters, and the other is removing the biodegradable organic matter (BOM) and other bioavailable materials through the microbial metabolism of the biofilm attached to the media.[4]. Many researchers have conducted experimental studies for removal of VOC's (toluene) using biofiltration [5,6]. Biotrickling filtration is a potential and cost effective alternative for the treatment of VOC emission in air, so it is necessary to deepen into the key aspects of design and operation for the optimization of this technology [7].

Mathematical modeling is widely used for optimize and investigate in order to reduce the number of physical experiments required during the removal of volatile organic compounds. Recently, Malhautier et al. [8] developed a mathematical model for the characterization of kinetic parameters in the biodegradation of toluene by Rhodococcus erythropolis in a bioreactor. To the best of our knowledge, there are no rigorous approximate analytical solutions presented for the concentrations of substrate, biomass and CO_2 in liquid and gas phase. The main aim of this article is to find the approximate analytical expressions for the concentrations of substrate, biomass and CO_2 in liquid and gas phase.

Mathematical model

The system of nonlinear ordinary differential equations under consideration is as follows [8] :

$$\frac{dCO_{2L}(t)}{dt} = \alpha \frac{dX(t)}{dt} + \beta X(t) \quad (1)$$

$$\frac{dCO_{2G}(t)}{dt} = \frac{dCO_{2L}(t)}{dt} H_{CO_2} \quad (2)$$

$$\frac{dS(t)}{dt} = -\frac{\mu(S)}{Y_{X/S}} X(t) \quad (3)$$

$$\frac{dX(t)}{dt} = \mu(S)X(t) \quad (4)$$

Where $\mu(S) = \frac{\mu_{max} S}{K_S + S + \frac{S^2}{K_I}}$ (5)

is the specific growth rate. The initial conditions for Eqs. (1) – (4) are represented as follows:

At $t = 0, CO_{2L}(t) = CO_{2L_0}, \quad CO_{2G}(t) = CO_{2G_0}, \quad S(t) = S_0, \quad X(t) = X_0$ (6) Using Eq. (3) and (4), the following linear differential equation can be obtained.

$$\frac{d}{dt}\left[Y_{X/S} S(t) + X(t)\right] = 0 \quad (7)$$

The exact solution of equation (7) is

$$S(t) = S_0 + \frac{X_0}{Y_{X/S}} - \frac{X(t)}{Y_{X/S}} \quad (8)$$

Eqn. (8) provides the relationship between the substrate and the biomass concentration. The plot of $S(t)$ versus $X(t)$ gives the intercept $S_0 + \frac{X_0}{Y_{X/S}}$ and slope $-\frac{1}{Y_{X/S}}$. The yield coefficient of substrate utilization Y_{xS} can be calculated from these parameters. The other parameters μ_{max} and K_S can be estimated from the linear plot of $\frac{1}{\mu(S)}$ versus $\frac{1}{S}$ using the equation $\mu(S) = \mu_{max} S/(K_S + S + S^2/K_I)$ [9].

Approximate analytical solution for Eqs. (1) – (4) using a new approach to the Homotopy perturbation method.

In recent years, solving system of nonlinear ordinary differential equations have gained importance due to the need of the analytical solutions various fields of science and engineering. Most researchers have contributed to the study of solutions

of nonlinear ordinary differential equations by applying various analytical techniques like variational iteration method [10], Homotopy analysis method [11], Homotopy perturbation method [12], Laplace Adomian decomposition method [13], a new approach to Homotopy perturbation method [14] etc. Among these a new approach to the Homotopy perturbation method was applied to solve the nonlinear ordinary differential equations Eqs. (1) – (4). The advantage of this method is that it provided a simple approximate solution in the zeroth iteration itself [15]. Using this method the concentration of biomass $X(t)$ is obtained as follows (Appendix A):

$$X(t) = \frac{X_0 X_{SS}}{X_0 + S_0 Y_{X/S} e^{-At}}$$

(9)

Substituting Eq. (9) in the Eq. (8), the concentration of substrate $S(t)$ can be obtained as follows:

$$S(t) = S_0 + \frac{X_0}{Y_{X/S}} - \frac{X_0 X_{SS}}{Y_{X/S}(X_0 + S_0 Y_{X/S} e^{-At})}$$

(10)

The concentration of CO_2 in liquid $CO_{2L}(t)$ and gas phase $CO_{2G}(t)$ can be obtained using Eq. (1), (2) and (9).

$$CO_{2L}(t) = CO_{2L_0} + \left[\alpha + \frac{\beta}{\mu_{max}}\left(\frac{K_S}{S_0} + \frac{S_0}{K_I} + 1\right)\right]\left[\frac{(X_0 + S_0 Y_{X/S})X_0}{X_0 + S_0 Y_{X/S} e^{-At}} - X_0\right]$$

(11)

$$CO_{2G}(t) = CO_{2G_0} + H\left(CO_{2L}(t) - CO_{2L_0}\right)$$

(12)

where the parameter

$$A = X_{SS}\mu_{max}/Y_{X/S}(K_S + S_0 + S_0^2/K_I)$$

(13)

and

$$X_{SS} = X_0 + S_0 Y_{X/S}$$

(14)

$$S_{SS} = 0$$

(15)

$$CO_{2L_{SS}} = CO_{2L_0} + \left[\alpha + \frac{\beta}{\mu_{max}}\left(\frac{K_S}{S_0} + \frac{S_0}{K_I} + 1\right)\right] S_0 Y_{X/S}$$

(16)

$$CO_{2G_{SS}} = CO_{2G_0} + H\left[\alpha + \frac{\beta}{\mu_{max}}\left(\frac{K_S}{S_0} + \frac{S_0}{K_I} + 1\right)\right] S_0 Y_{X/S}$$

(17)

are the steady state solution of biomass, substrate and CO_2 in liquid and gas phase respectively.

Discussion

Eqs. (9) – (12) represents the simple analytical expression for the concentration of biomass, liquid toluene, CO_2 concentration in liquid phase and CO_2 concentration in gas phase respectively in terms of the kinetic parameters μ_{max}, K_S, K_I, $Y_{X/S}$, α and β. Fig. 1 shows the comparison of analytical results with numerical simulation for the concentration of liquid toulene and Gaseous CO_2 for experimental values of kinetic parameters.

*****(Figure 1)*****

To analyze and predict the influence of kinetic parameters for decreasing the emission of toluene, a sensitivity analysis was calculated for experimental values of the parameters in Fig. 2(a) and 2(b). From the figure, it is evident that the parameters like to μ_{max}, K_S , K_I and $Y_{X/S}$ has the same level of influence over the concentration of biomass, liquid CO_2 and gaseous CO_2. But for liquid toluene, they have different percentage level. The percentage of change in biomass, liquid CO_2 and gaseous CO_2 with respect to μ_{max}, K_S , K_I and $Y_{X/S}$ is 87%, -3%, 0.02% and 15.98% respectively. The negative sign indicates that the concentration increases when the toluene half saturation constant decreases. The percentage of change in concentration of liquid toluene (substrate) with respect to μ_{max},K_S and K_I is 103%, -3.03% and 0.03% respectively. The main variable of interest in this study is μ_{max}, because of its high level of impact on the concentration of biomass, substrate, liquid CO_2 and gaseous CO_2.

*****(Figure 2)*****

Fig. 3(a) – (d) shows the concentration of biomass $X(t)$ versus time t for various values of maximum specific biomass growth rate μ_{max}, toluene half saturation constant K_S, toulene inhibition constant K_I and biomass to toluene yield coefficient $Y_{X/S}$ respectively. From Fig. 3(a), it is evident that when the maximum specific growth rate increases, the concentration of biomass increases and reaches its steady state value for short interval of time. From Fig. 3(b)-3(d), it is inferred that the parameter K_S is inversely proportional to the concentration of biomass where as K_I and $Y_{X/S}$ is directly proportional to biomass. And variation in K_S doesn't show much deviation in biomass concentration compared to other parameters μ_{max} , K_I and Y_{xS}. Fig. 3(d) shows that different value of biomass is obtained for different of substrate utilization yield $Y_{X/S}$. This is because the steady state value of biomass X_{SS} depends upon the value of Y_{xS}, i.e. $X_{SS} = X_0 + S_0 Y_{X/S}$.

*****(Figure 3)*****

The influence of kinetic parameters over substrate concentration with respect to time t for are illustrated in Fig. 4(a) – (c) respectively. From Fig. 4(a) and 4(c), it is evident that the degradation of the substrate increases for increase in biomass growth rate μ_{max}, toulene inhibition constant K_I and decrease in toluene half saturation constant K_S.

*****(Figure 4)*****

The impact of kinetic parameters on CO_2 production in liquid phase and gas phase was illustrated in Fig. 5 and 6. From these figures, it is true that the kinetic parameters shows same level of influence on CO_2 in both liquid and gaseous phase.

*****(Figure 5 and 6)*****

Conclusion

A nonlinear mathematical model comprising a set of ordinary differential equation describing toulene degradation by rhodococcus erythropolis has been solved analytical in a rigorous mathemtical approach using new approach to the Homotopy perturbation method. Approximate analytical expressions for biomass, liquid toluene, liquid CO_2 and gaseous CO_2 production were obtained. The obtained analytical results were compared with numerical simulation and it shows satisfactory agreement. Also the steady state solution of each concentration and the analytical relation between biomass and substrate are reported. The sensitivity analysis of the parameters is also presented in order to provide necessary information for parameter analyzation, control, model simplification and experimental design.

Appendix A: Approximate analytical solutions for Eq. (1) using HPM.

Using the relation Eq. (6), Eq. (1) can be written as

$$\frac{dX(t)}{dt} = \frac{\mu_{max}X(t)[S_0Y_{xS}+X_0-X(t)]}{K_S+S(t)+S(t)^2/K_I} \quad \text{(A.1)}$$

In order to solve Eq. (1), construct the homotopy as follows:

$$(1-p)\left\{\frac{dX(t)}{dt} - B[S_0Y_{xS}+X_0-X(t)]X(t)\right\} + p\left[\frac{dX}{dt}(K_S+S(t)+\frac{S(t)^2}{K_I}) - \mu_{max}S(t)X(t))\right] = 0 \quad \text{(A.2)}$$

Where

$$B = \frac{\mu_{max}}{K_S+S(0)+S(0)^2/K_I} \quad \text{(A.3)}$$

The approximate solution of (A.2) is as follows:

$$X = X_{zeroth} + pX_{first} + p^2X_{second}+\ldots \quad \text{(A.4)}$$

Substituting (A.4) in Eq. (A.2) and equating the like powers of p

$p^0 : \frac{dX_{zeroth}(t)}{dt} - B[S_0 Y_{xS} + X_0 - X_{zeroth}(t)]X_{zeroth}(t) = 0$

(A.5)

The initial condition for the above equation is

At $t = 0, X_{zeroth}(0) = X_0$

(A.6)

Solving Eq. (A.5), $X_{zeroth}(t)$ can be obtained as follows

$X_{zeroth}(t) = \frac{X_0 X_{SS}}{X_0 + S_0 Y_{xS} e^{-At}}$

(A.7)

Where $A = X_{SS}\mu_{max}/Y_{X/S}(K_S + S_0 + S_0^2/K_I)$ and $X_{SS} = X_0 + S_0 Y_{xS}$

(A.8)

Substituting (A.7) in Eq. (A.2), $X(t) \approx X_{zeroth}(t)$ which is the Eq. (7) in the text.

Symbols used

Symbols	Unit	Meaning
CO_{2G}	(g m^{-3})	CO_2 concentration in gas phase
CO_{2G_0}	(g m^{-3})	initial CO_2 concentration in liquid phase
CO_{2L}	(g m^{-3})	CO_2 concentration in liquid phase
CO_{2L_0}	(g m^{-3})	initial CO_2 concentration in liquid phase
H_{CO2}	(g m^{-3})	dimensionless Henry's law constant for CO_2
K_I	(g m^{-3})	toluene inhibition constant
K_S	(g m^{-3})	toluene half saturation constant
S	(g m^{-3})	Concentration of substrate
S_0	(g m^{-3})	Initial concentration of substrate
t	(h)	Time
X	(g m^{-3})	Concentration of biomass (Bacteria)
X_0	(g m^{-3})	Initial concentration of biomass (Bacteria)
$Y_{X/S}$	(gX gS^{-1})	biomass to toluene yield
Greek symbols		
μ	(h^{-1})	specific biomass growth rate
μ_{max}	(h^{-1})	maximum specific biomass growth rate
α	(gCO_2 gX^{-1})	constant of the Luedeking-Piret model
β	(gCO_2 gX^{-1})	constant of the Luedeking-Piret model
Subscripts		
0	Initial concentration	
max	Maximum	
S	Substrate	
SS	Steady state	
X/S	Substrate utilization yield	

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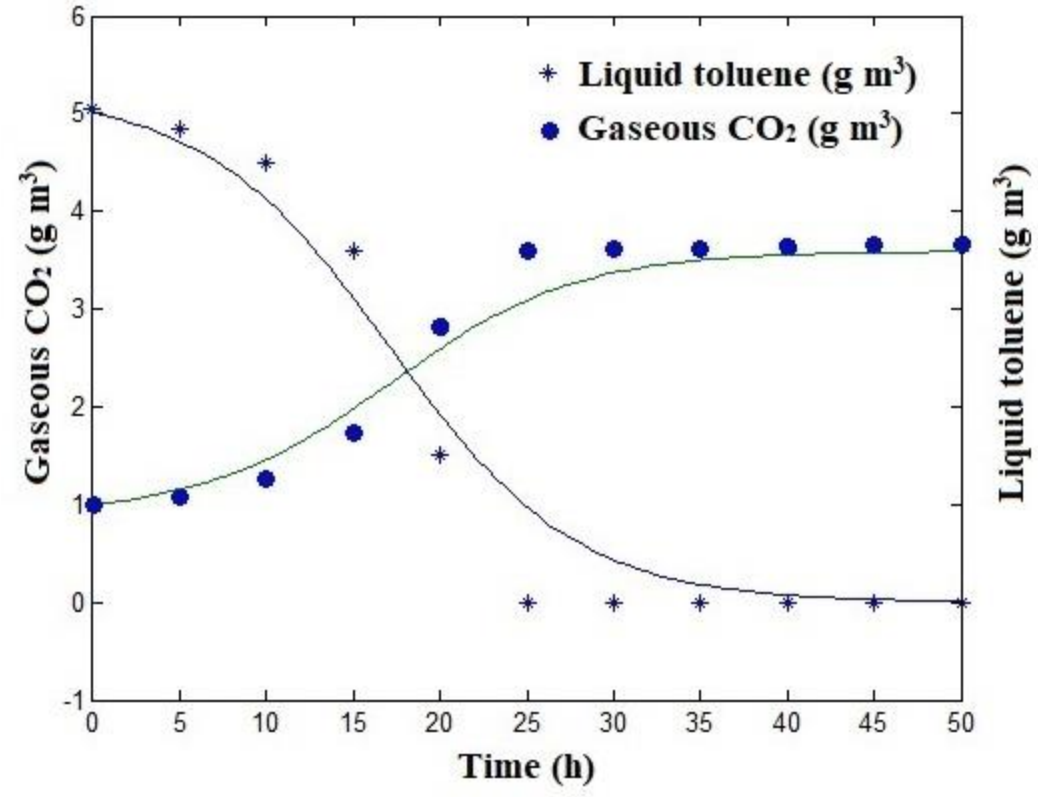

Fig. 1 Comparison of numerical simulstion (symbols) and analytical expression (solid line) [Eq. (10) and (12)] for the concentration of liquid toluene $S(t)$ and carbondioxie in gas phase $CO_{2G}(t)$ respectively.

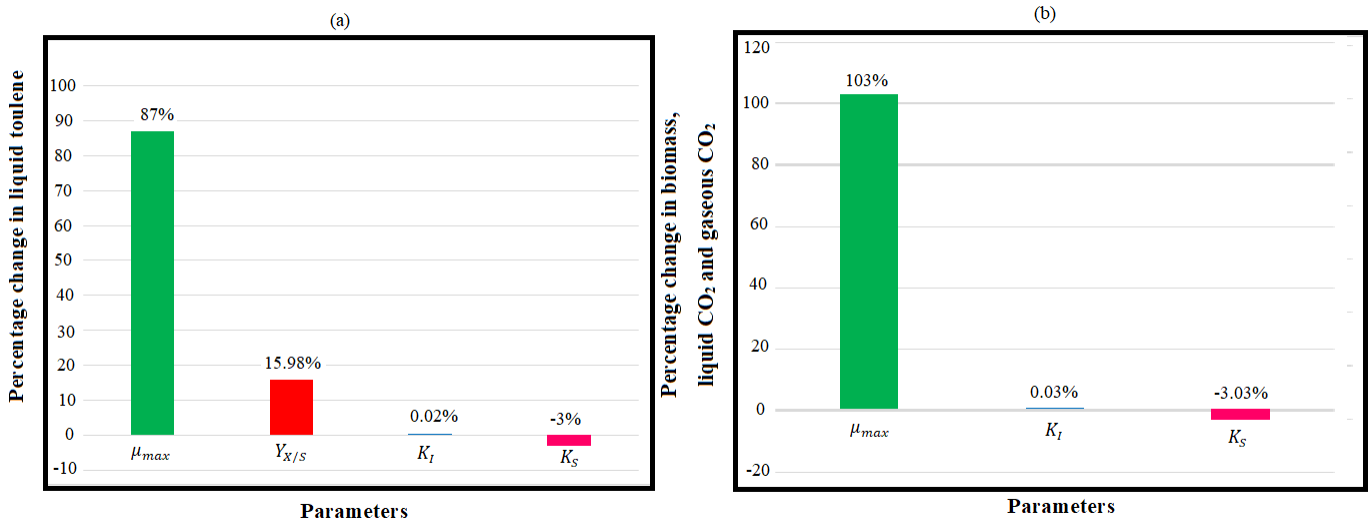

Fig. 2 Percentage change in (a) liqiuid toluene (b) biomass, liquid CO_2 and gaseous CO_2 versus kinetic parameters.

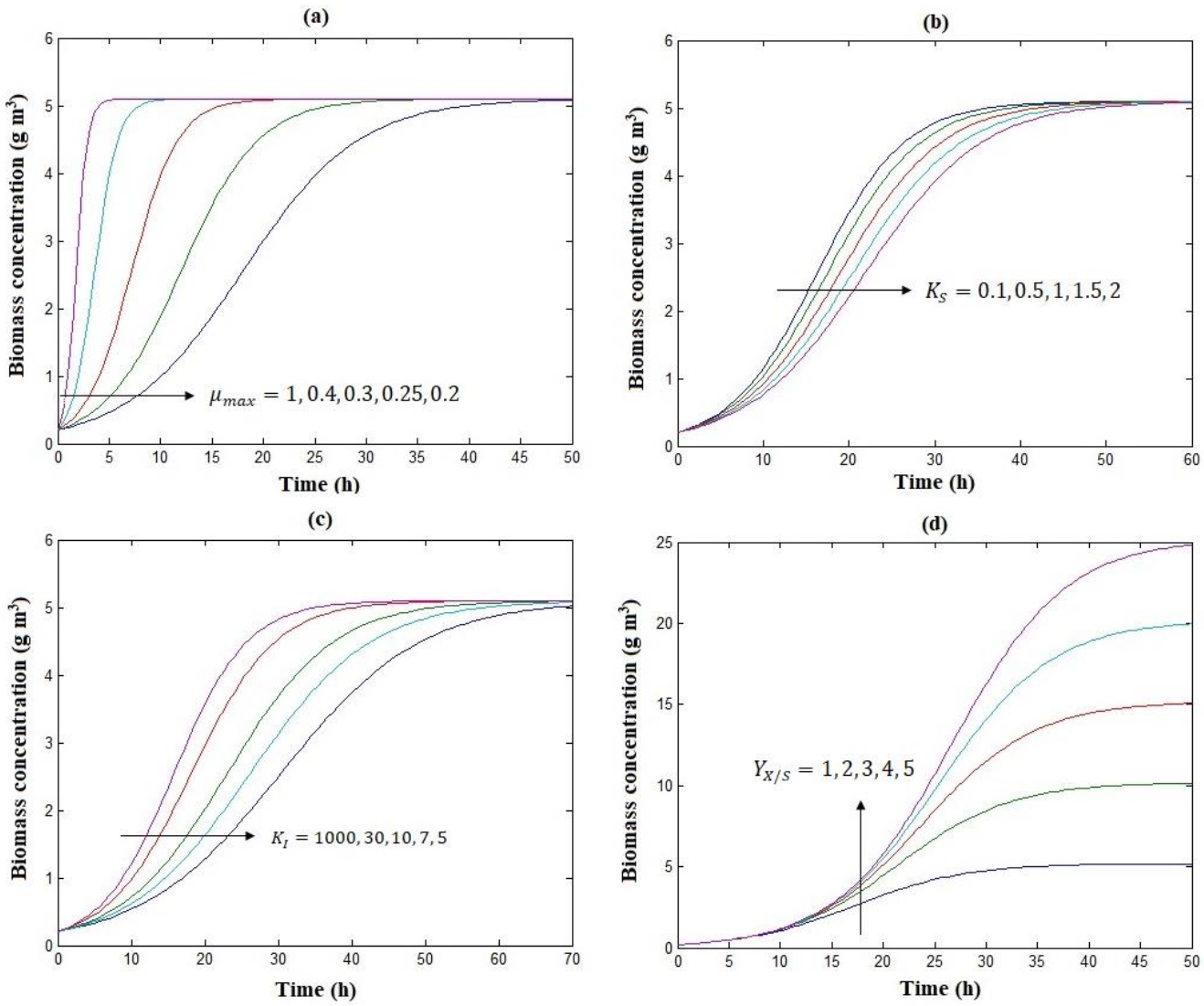

Fig. 3 Concentration profile of biomass $X(t)$ (Eq. (9)) versus time t for some experimental values of the parameters and for various values of (a) maximum specific growth rate μ_{max} (b) toluene half saturation constant K_S (c) toluene inhibition constant K_I and (d) biomass to toluene yield $Y_{X/S}$ respectively.

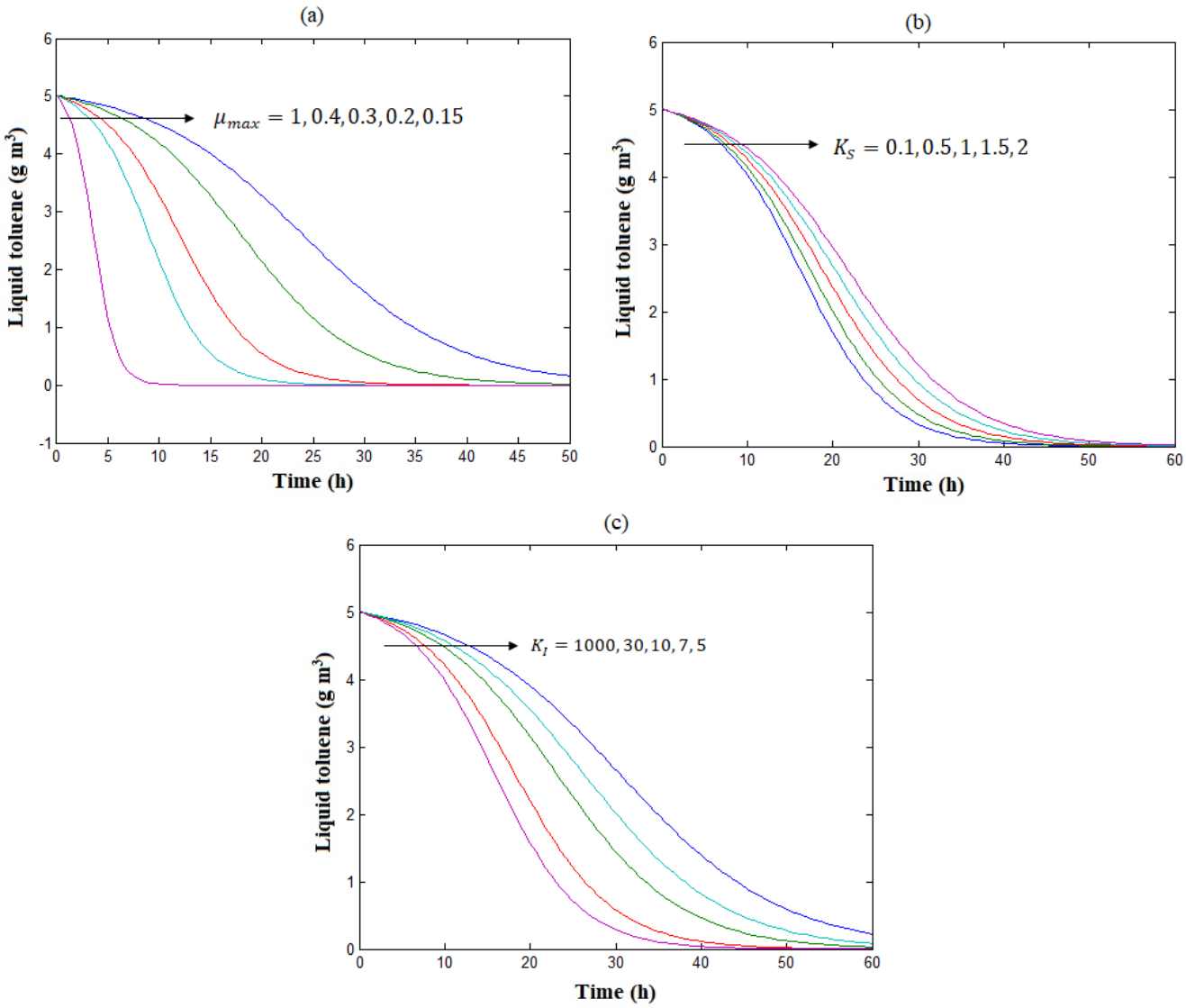

Fig. 4 Concentration profile of substrate (liquid toulene) $S(t)$ [Eq. (10)] versus time t for some experimental values of the parameters and for various values of (a) maximum specific growth rate μ_{max} (b) toluene half saturation constant K_S and (c) toluene inhibition constant K_I respectively.

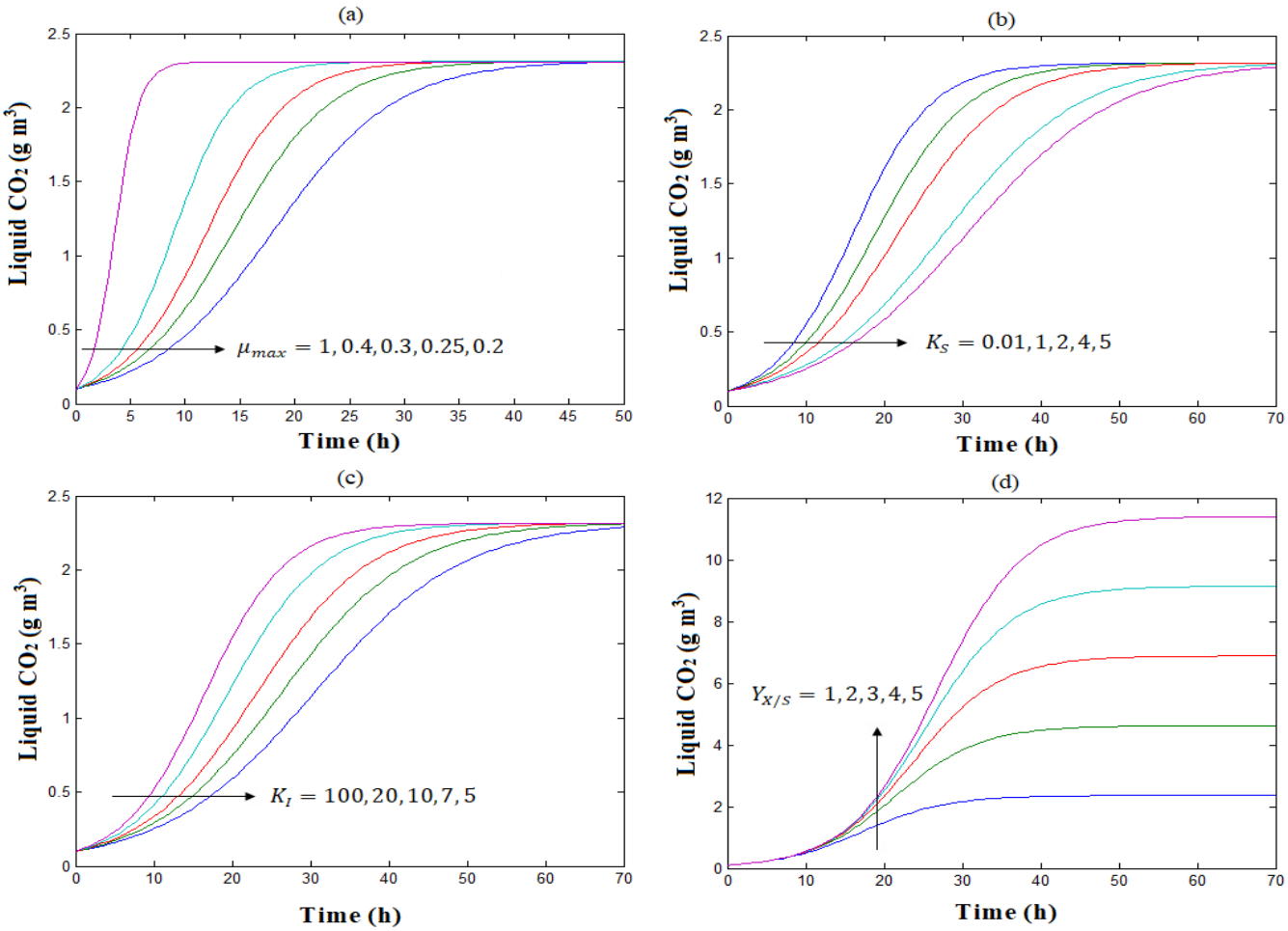

Fig. 5 Concentration profile of liquid carbondioxide $CO_{2L}(t)$ [Eq. (11)] versus time t for some experimental values of the parameters and for various values of (a) maximum specific growth rate μ_{max} (b) toluene half saturation constant K_S (c) toluene inhibition constant K_I and (d) biomass to toluene yield $Y_{X/S}$ respectively.

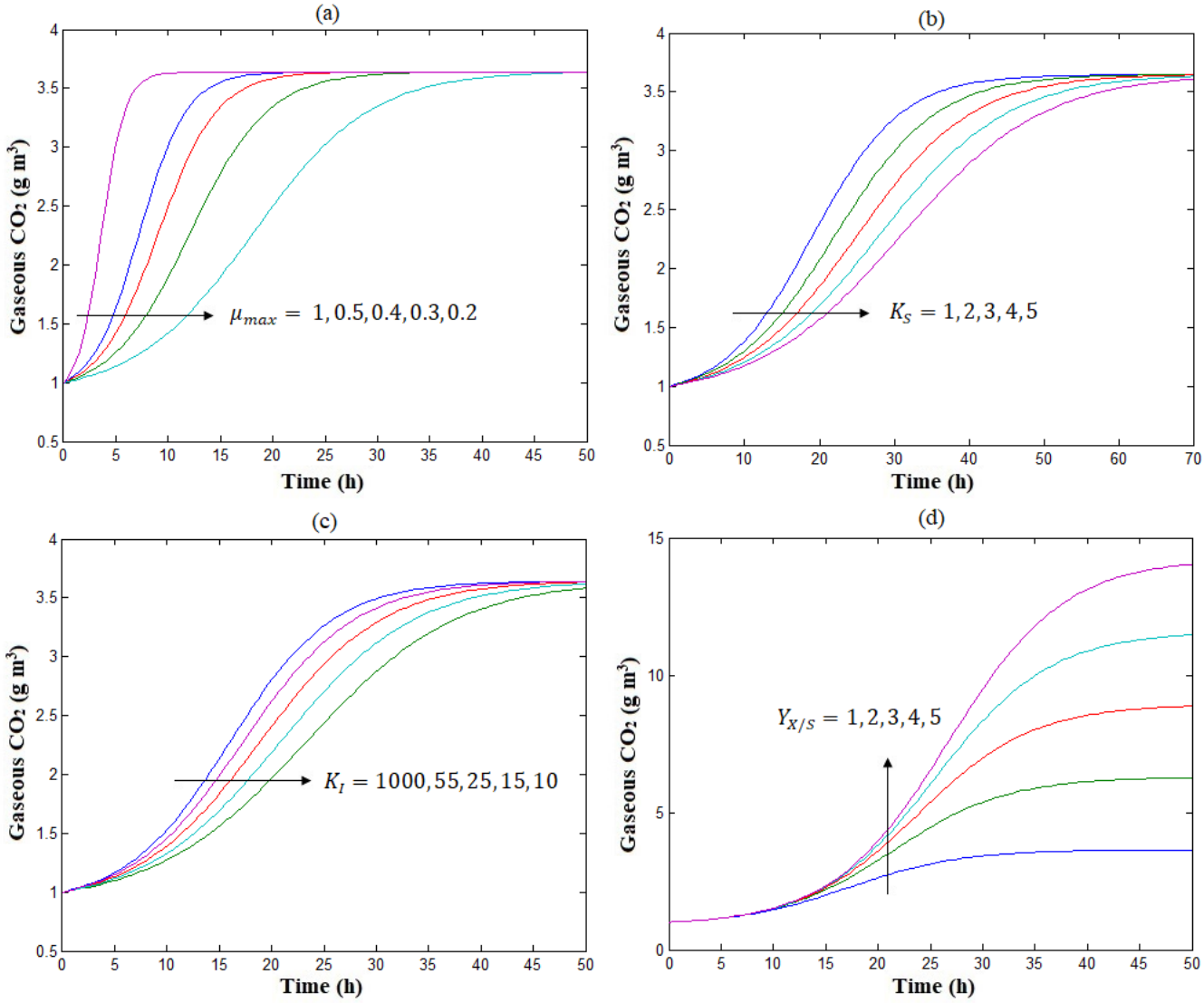

Fig. 6 Concentration profile of liquid carbondioxide $CO_{2G}(t)$ [Eq. (12)] versus time t for some experimental values of the parameters and for various values of (a) maximum specific growth rate μ_{max} (b) toluene half saturation constant K_S (c) toluene inhibition constant K_I and (d) biomass to toluene yield $Y_{X/S}$ respectively.