



Short communication

An explicit expression for determining cometabolism kinetics using progress curve analysis

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ABSTRACT

We present an explicit expression for describing the kinetics of cometabolic biotransformation of environmental pollutants. This expression is based on the Lambert W function and explicitly relates the substrate concentration, S , to time, t , the two experimentally measured variables. This explicit relationship simplifies kinetic parameter estimation as differential equation solution and iterative estimation of the substrate concentration are eliminated. The applicability of this new expression for nonlinear kinetic parameter estimation was first demonstrated using noise containing synthetic data where final estimates of the kinetic parameters were very close to their actual values. Subsequently 1,1,1-trichloroethane degradation data at initial concentrations of 750 and 375 μM were described using the explicit expression resulting in r and K_s estimates of 0.26 $\mu\text{M}/\text{mg d}$ and 28.08 μM and 0.30 $\mu\text{M}/\text{mg d}$ and 28.70 μM , respectively, very similar to 0.276 $\mu\text{M}/\text{mg d}$ and 31.2 μM , respectively, that were reported in the original study. The new explicit expression presented in this study simplifies estimation of cometabolic kinetic parameters and can be easily used across all computational platforms thereby providing an attractive alternative for progress curve analysis.

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1. Introduction

Cometabolism describes the microbial transformation of a non-growth compound in the presence of a growth substrate or alternatively by resting cells in the absence of a growth substrate (Criddle, 1993; Hovarth, 1972). This phenomenon is especially important because some of the most recalcitrant environmental contaminants such as chlorinated alkenes, polyaromatic hydrocarbons, halogenated aliphatic and aromatic hydrocarbons, methyl tertiary butyl ether, dioxane, and polychlorinated biphenyls can be degraded by cometabolism (Alvarez-Cohen and Speitel, 2001). As a result, cometabolic biotransformation of environmental contaminants, both under aerobic and anaerobic conditions, continues to be extensively studied (Barret et al., 2010; Conrad et al., 2010; Delgadillo-Mirquez et al., 2011; Elango et al., 2011; House and Hyman, 2010).

The importance of quantitatively describing cometabolism has been long recognized and multiple kinetic modeling approaches have been proposed to describe contaminant biotransformation (Alvarez-Cohen and McCarty, 1991; Chang and Alvarez-Cohen, 1995; Chang et al., 1993; Criddle, 1993). The resulting kinetic expressions are more complex than the classical Michaelis–Menten

or Monod type models given the duality of substrates and the loss of biotransformation activity because of the absence of growth substrate and/or product toxicity. One such modeling approach couples the Monod equation for substrate depletion with a first order decay of cometabolizing biomass (Galli and McCarty, 1989) and was successfully used to describe the degradation of 1,1,1-trichloroethane (TCA) by *Clostridium* sp.

$$\frac{dS}{dt} = -\frac{rS}{K_s + S} \quad (1)$$

where S is the substrate concentration, t is time, r the maximum rate of substrate degradation, K_s is the half velocity coefficient, and X is the biomass concentration. The decrease in the active cometabolizing biomass was described by a first order relationship

$$\frac{dX}{dt} = -bX \quad (2)$$

where b is the decay constant. From Eq. (2), the time course of biomass concentration is $X = X_0 e^{-bt}$ which on substituting in Eq. (1) results in the following integral expression which is implicit in the substrate concentration

$$K_s \ln \left(\frac{S}{S_0} \right) + S - S_0 = \frac{rX_0}{b} (e^{-bt} - 1) \quad (3)$$

Because an explicit kinetic expression for the substrate concentration was not available, a multi-step approach was used for kinetic parameter estimation (Galli and McCarty, 1989) and

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experimental TCA degradation data were well described by the above modeling approach. However, implicit expressions like Eq. (3) are not best suited for kinetic parameter estimation from experimental S versus t data because iterative estimation of S is needed at each combination of r and K_s values. While Eq. (3) can be rewritten such that t is an explicit function of S , the resulting expression violates two basic assumptions of nonlinear parameter estimation. The first requires that variability be associated with only the dependent variable while the independent variable is error free and second requires that error in the dependent variable is normally distributed. It is thus desirable to explicitly relate S with t to simplify r and K_s estimation in cometabolism experiments.

In this study, we derive an explicit expression for the above cometabolism model and illustrate its application for nonlinear kinetic parameter estimation using a combination of synthetic and experimental data. Specifically, progress curve analysis was performed using the explicit kinetic expression that resulted in rapid and robust kinetic parameter estimates and the values obtained in this study were comparable to those previously published.

2. Theory

Substituting $\phi = S/K_s$ and rearranging, Eq. (3) can be rewritten as

$$K_s \ln(\phi K_s) + \phi K_s = K_s \ln(S_0) + S_0 + \frac{rX_0}{b}(e^{-bt} - 1) \tag{4}$$

Dividing by K_s and rearranging results in

$$\ln(\phi) + \phi = \ln\left(\frac{S_0}{K_s}\right) + \frac{S_0}{K_s} + \frac{rX_0}{K_s b}(e^{-bt} - 1) \tag{5}$$

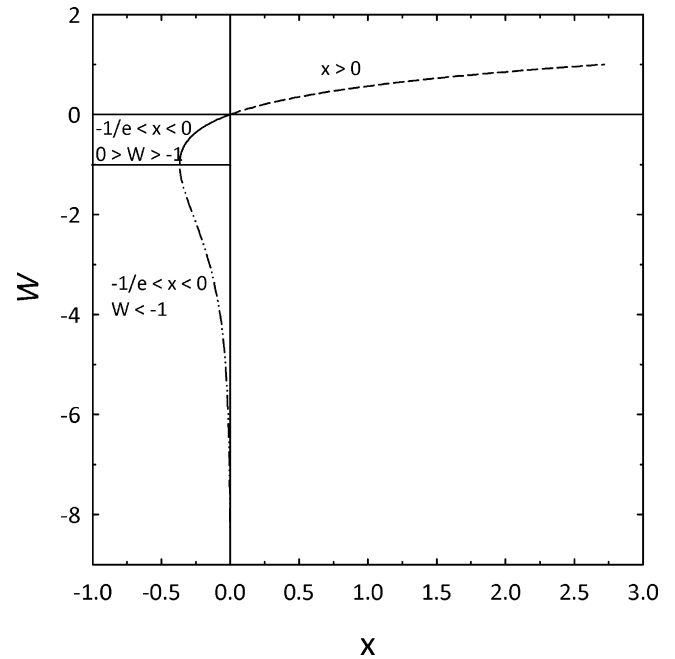


Fig. 1. The Lambert W function as a function of x {(---) $x > 0$; (—) $-1/e < x < 0$ and $0 > W > -1$; (.....) $-1/e < x < 0$ and $W < -1$ }.

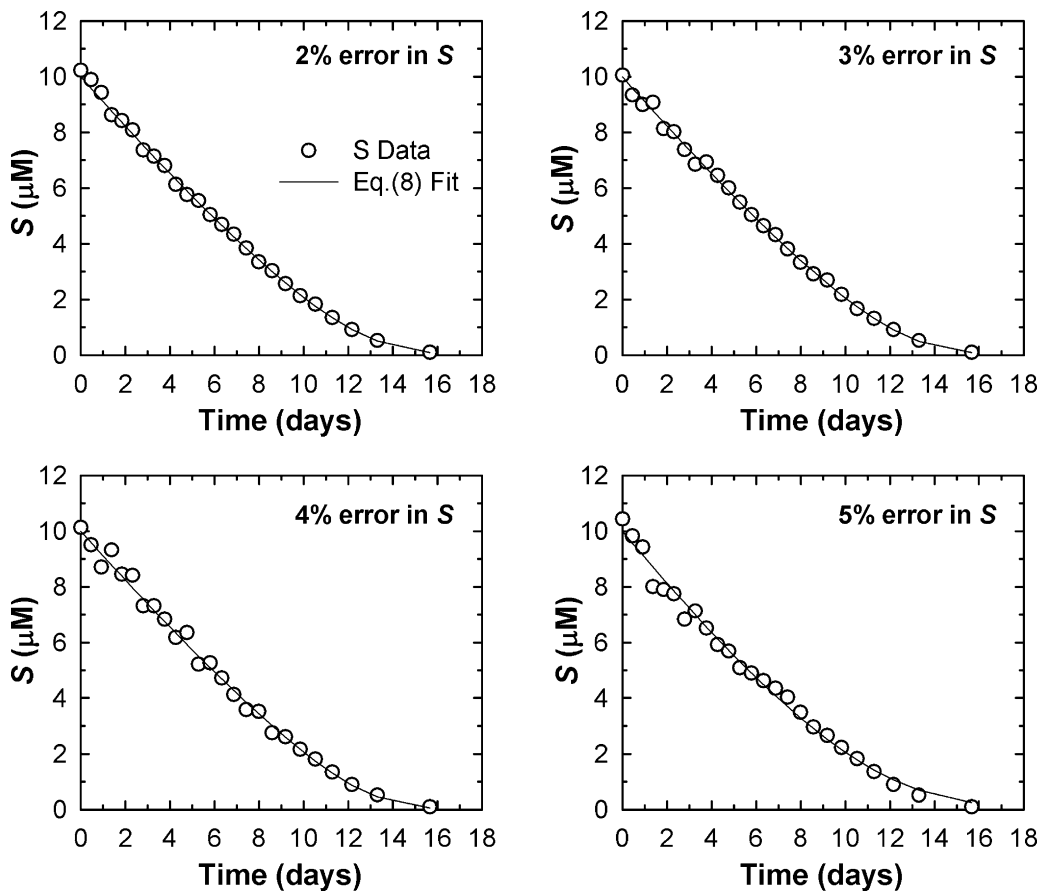


Fig. 2. Synthetic substrate depletion data at varying error levels along with best fit lines from Eq. (9). Final estimates of r and K_s and the associated standard errors and parameter correlation are shown in Table 1. Actual values of r and K_s were $1 \mu\text{M}/\text{mg d}$ and $1 \mu\text{M}$, respectively.

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