Describing Terephthalic Acid biodegradation with double Haldane model

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Introduction. The Haldane model is frequently used to model the substrate inhibition in a biological process[1]. In this study the original Haldane model was modified to a double Haldane Model according to Chung et al[2]. The double Haldane model was used to give a better adjustment of the model to the experimental data during the adaptation phase (lag phase) and the exponential growth phase (log phase), commonly observed in Terephthalic Acid (TA) biodegradation processes.

Methods. Biodegradation experiments were carried out in shaking flasks with a mixed culture of *Comamonas* sp. and *Rhodococcus* sp. The medium added to the shaking flasks was prepared by adding (g L-1); KH2PO4, 0.15; MgSO4•7H2O, 0.075; NaCl, 0.075, and different quantities of TA as required, to a 50 mM phosphate buffer. pH was adjusted to 7.1 with 0.1 N H3PO4. TA and biomass concentration during the biodegradation experiments were determined by TOC, with a Shimadzu TOC-Vcsn equipped with a TNM-1 module (Shimadzu, Japan). The adjustment of the model (Equation 1) to the experimental data was done with a fitting procedure based on Runge-Kutta method and a Marquardt optimization with 20 convergence steps, using commercial software (Model Maker, Cherwell Scientific Publishing, UK).

$$\frac{dS}{dt} = -\frac{R_{\max,i}.S}{K_{S,i} + S + \frac{S^2}{K_{I,i}}}; \quad \frac{dX}{dt} = -Y_{X/S,i}\frac{dS}{dt} \quad (1)$$

i = *lag* or *log* phase

Results. Fig. 3C shows an example of model best fitting to the experimental TA and biomass concentrations obtained with initial 2.65 g TOC L^{-1} of TA. In this example, the goodness of fit was 0.979, similarly as observed during all the experiments. Also it is observed a clear Lag phase at the beginning of the degradation of TA. In all cases, a clear Lag phase from 10 to 17 hours followed by a complete TA degradation phase was observed. Table 3 presents the results obtained from the model adjustment for each one of the kinetic and parameters during both Lag and Log phases. $Y_{X/S}$, estimated directly from substrate and biomass concentration, was not significantly different during the Lag and the Log phase. On the contrary, K_S, K_I, and R_{max} values were statistically lower during the Lag phase than during the Log phase, which means that the cultures were less inhibited during the Log phase, probably due to an adaptation to the culture conditions.

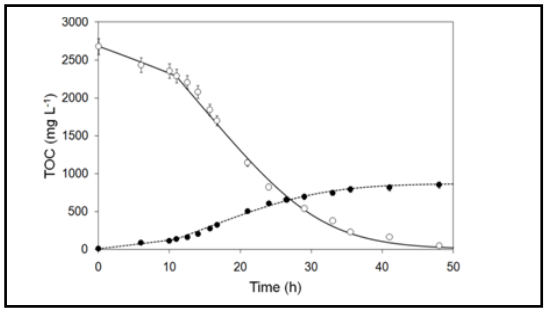

Fig.1 Example of model adjustment (solid line) to experimental data obtained with 2.65 g TOC L^{-1} of TA, biomass (●) and TA (○).

Table 1. Kinetic and stoichiometric parameters observed during Lag and Log phase with the mixed culture

	K_S gTOC/L	K_I gTOC/L	R_{max} gTOC/Lh	$Y_{X/S}$ gTOC/gTOC
Lag Phase	0.01±0.01	0.80±0.07	0.15±0.03	0.28±0.07
Log Phase	1.67±0.04	2.57±0.31	0.29±0.02	0.32±0.08

Conclusions. The degradation process of TA observed when Lag and Log phase are present was adequately fitted by a double Haldane model, with a relatively high inhibition constant.

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