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Modeling aerobic biotransformation of vinyl chloride by vinyl chloride-assimilating bacteria, methanotrophs and ethenotrophs

Yiwen Liu [a], Huu Hao Ngo [a,*], Wenshan Guo [a], Jing Sun [b], Dongbo Wang [c,d], Lai Peng [b], Bing-Jie Ni [b,*]

[a] Centre for Technology in Water and Wastewater, School of Civil and Environmental Engineering, University of Technology Sydney, Sydney, NSW 2007, Australia
[b] State Key Laboratory of Pollution Control and Resources Reuse, College of Environmental Science and Engineering, Tongji University, Shanghai 200092, China
[c] College of Environmental Science and Engineering, Hunan University, Changsha 410082, China
[d] Key Laboratory of Environmental Biology and Pollution Control (Hunan University), Ministry of Education, Changsha 410082, China

HIGHLIGHTS

- A novel model was developed to describe aerobic groundwater VC biotransformation.
- This model considers both aerobic metabolism and cometabolism of VC.
- The model well describes VC, methane and ethene dynamics in all microcosms tested.
- Interactions between methanotrophs and etheneotrophs enhance aerobic VC degradation.
- This model will be a useful tool to support process optimization for VC remediation.

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ABSTRACT

Recent studies have investigated the potential of enhanced groundwater Vinyl Chloride (VC) remediation in the presence of methane and ethene through the interactions of VC-assimilating bacteria, methanotrophs and ethenotrophs. In this study, a mathematical model was developed to describe aerobic biotransformation of VC in the presence of methane and ethene for the first time. It examines the metabolism of VC by VC-assimilating bacteria as well as cometabolism of VC by both methanotrophs and ethenotrophs, using methane and ethene respectively, under aerobic conditions. The developed model was successfully calibrated and validated using experimental data from microcosms with different experimental conditions. The model satisfactorily describes VC, methane and ethene dynamics in all microcosms tested. Modeling results describe that methanotrophic cometabolism of ethene promotes ethenotrophic VC cometabolism, which significantly enhances aerobic VC degradation in the presence of methane and ethene. This model is expected to be a useful tool to support effective and efficient processes for groundwater VC remediation.

1. Introduction

Groundwater is a critically important water source world-wide, and it accounts a large amount of drinking water supplies [1]. Due to tetrachloroethene (PCE) and trichloroethene (TCE) being dumped into the environment as a consequence of intensive industrial use of chloroethene-based solvents and degreasing agents, chloroethene contamination of groundwater has been recognized as a significant environmental problem world-wide [2–4]. PCE and TCE are persistent toxic chemicals and can cause serious health problems in people [5]. However, under favorable anaerobic conditions, dechlorinating bacteria can utilize organic matter/hydrogen as electron donors to reduce PCE and TCE to ethene sequentially. They can do this via intermediates such as *cis*-dichloroethene (cDCE) and vinyl chloride (VC) [6].

However, anaerobic reductive dechlorination of VC to ethene is the slowest process of all the reductive dechlorination steps due

* Corresponding authors.
E-mail addresses: ngohuuhao121@gmail.com (H.H. Ngo), bjni@tongji.edu.cn (B.-J. Ni).

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to the possible absence or inactivation of capable microorganisms, thus leading to incomplete dechlorination of chloroethenes and the accumulation of VC [7]. VC is a well-known human carcinogen and its contamination of groundwater is of great concern [8,9]. For this reason, a maximum VC contaminant level of 2 μg/L in drinking water has been set by the US Environmental Protection Agency (US EPA), which is lower than that of any other volatile organic compound [10].

Alternatively, a following post aerobic polishing process, where VC is generally accepted to be more readily biodegradable [11], is a possible solution to address the slow and incomplete anaerobic reductive dechlorination of VC. Some aerobic bacteria that can grow using VC as the primary substrate (i.e., VC-assimilating bacteria) have been isolated from environmental samples such as soil, groundwater and activated sludge [12–16]. Other aerobic bacteria which can grow on methane and ethene as primary substrates and produce monooxygenase enzymes, can also degrade VC to nonchlorinated products through cometabolism [17,18]. Besides VC-assimilating bacteria, methanotrophs and ethenotrophs (ethene-assimilating bacteria) are both good candidates for aerobic VC remediation applications [6], since significant levels of methane and ethene can be generated in the anaerobic zone and further migrate with VC into the aerobic zone [19].

Extensive studies on VC degradation in groundwater have been carried out with either ethene or methane being present [6,13,18,20]. Recent studies have examined enhanced VC remediation linked to methane and ethene oxidation, through the interactions among methanotrophs, ethenotrophs and VC-assimilating bacteria [10]. In the presence of all three substrates and microorganisms, the VC degradation rate was significantly higher than those with the presence of either methane or ethene only. This is likely due to the fact that methanotrophs promoted ethenotrophic VC degradation [10], since methanotrophs can produce epoxyethane, a compound known to stimulate ethene and VC degradation by ethenotrophs, in methane enrichment cultures that are fed ethene [21]. Therefore, advancing our understanding of such a system is of great significance to future strategies for remediating VC.

Mathematical modeling is particularly important toward a full understanding of mechanisms involved in biological VC removal systems, which has been applied to describe metabolic VC degradation [12] and VC cometabolism associated with either methane or ethene presence [11,13,17,21]. However, little effort to date has been dedicated to modeling the VC dynamics associated with the presence of both methane and ethene, as well as the possible interactions among methanotrophs, ethenotrophs and VC-assimilating bacteria. Thus it is difficult to predict the rate and extent of VC degradation under such conditions.

This study aims to develop a new and generalized model for the prediction of VC remediation under the conditions of each substrate alone (VC, methane and ethene) and combinations of these substrates (mixtures of each two substrates or all three substrates). The model is calibrated and validated using experimental data from a comprehensive study report.

2. Model development

2.1. Existing aerobic VC degradation models

Metabolic VC degradation has been widely modeled with the Michaelis–Menten kinetics where the concentrations of VC are considered [12]. It was also adapted in our current study to describe the metabolism of VC using VC-assimilating bacteria.

With respect to the cometabolic VC degradation through methane oxidation by methanotrophs, a previous study modeled this process as simultaneous pollutant and growth substrate binding, where the pollutant competed for binding with growth substrate. This links the net rate of methane turnover to the VC turnover rate [21]. However, both methane and VC transformation rates were modeled with the Michaelis–Menten kinetics, which unnecessarily brought in more parameters (i.e., maximum reaction rate of methane oxidation, methane affinity constant for methane oxidation, maximum reaction rate of cometabolic VC degradation, VC affinity constant for cometabolic VC degradation and cometabolic transformation capacity).

Similarly, the cometabolic VC degradation through ethene oxidation by ethenotrophs that has been described in previous studies was also modeled with complicated differential equations for substrate and pollutant transformation. These considered the competitive inhibition and inactivation of primary substrate and pollutant [11,13]. Such a model structure would increase the model complexity and the current available dataset may not be enough to calibrate this kind of model. Instead, keeping the model simple can limit the number of model parameters, and consequently make the model's implementation and application easier. Therefore, model simplifications are required for model calibration and actual application purposes. Additionally, previous models only considered metabolic VC degradation and VC cometabolism associated with either methane or ethene, which may not actually work in the presence of both methane and ethene, considering the interaction between methanotrophs and ethenotrophs.

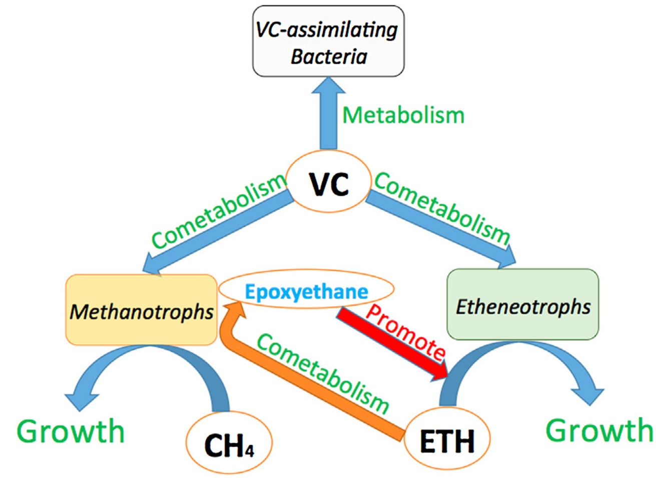

Fig. 1. Schematic representation of the proposed aerobic VC biodegradation model concept in the presence of VC-assimilating bacteria, methanotrophs and ethenotrophs.

2.2. Development of a generalized aerobic VC biotransformation model

VC is usually generated in groundwater during incomplete anaerobic reductive dechlorination of chloroethenes to ethene [7]. Meanwhile, the strong reducing conditions induce significant methane production in groundwater [19]. Thus, all three substrates (i.e., VC, methane and ethene) can prevail in the following aerobic conditions. The model developed in this work considered the metabolism of VC by VC-assimilating bacteria, and cometabolism of VC by both methanotrophs and ethenotrophs using methane and ethene respectively, under aerobic conditions (Fig. 1). One previous experimental study revealed that cometabolic methanotrophic oxidation of ethene to epoxyethane stimulated the activity of ethenotrophs and thus further enhanced ethenotrophic VC removal [10]. This scenario was also included in the generalized model. These biological reaction kinetics were integrated with the pre-