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A novel mathematical approach for the understanding and optimization of two-phase partitioning bioreactors devoted to air pollution control

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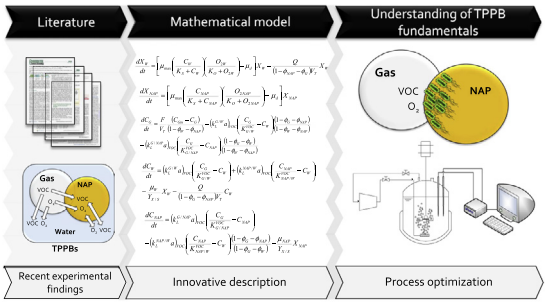
HIGHLIGHTS

- An innovative mathematical description of TPPBs was developed.
- Potential VOC uptake from the NAP and aqueous phase renewal were considered.
- The model was validated with experimental data from literature.
- No parameter fitting was carried out for model validation.

GRAPHICAL ABSTRACT



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ABSTRACT

Two-phase partitioning bioreactors (TPPBs) support the removal of volatile organic compounds (VOCs) from contaminated gaseous emissions at unprecedented rates and concentrations. TPPBs are biological multiphase systems provided with a non-aqueous phase (NAP) with high affinity for the target VOC. Although modeling of TPPBs is a research field that has rapidly evolved, recent experimental findings such as the direct VOC uptake from liquid NAPs and the quantification of simultaneous partial mass transfer coefficients have not been incorporated yet in a comprehensive mathematical description. In this work, a mathematical description of TPPBs, including continuous aqueous phase renewal and potential VOC uptake directly from the NAP, was developed. Model simulations indicated that TPPB performance can be enhanced by improving the partial mass transfer coefficient between the gas and the NAP (by increasing the contact between the gas and the NAP). The model also showed that microorganisms with half-saturation constants <5 g m^{-3} and ability to take up VOC directly from the NAP can boost significantly TPPB performance. The present modeling platform was tested against experimental data from literature for methane, hexane and dichloromethane and no parameter fitting was carried out.

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1. Introduction

Two-phase partitioning bioreactors (TPPBs) devoted to air pollution control are multiphase systems based on the addition into a biological process of a non-aqueous phase (NAP) with high affinity for target gaseous pollutants [1]. TPPBs support the biological removal of volatile organic compounds (VOCs) from contaminated gaseous streams at unprecedented rates and concentrations [2,3]. The presence of the NAP improves the transfer of hydrophobic VOCs from the gas to the microorganisms and overcomes operational issues induced by the toxicity of some hydrophilic VOCs [4]. Moreover, most NAPs used for TPPB implementation show a high affinity for O_2 and consequently, the

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increase in the VOC mass transfer in TPPBs is concomitant with an increase in the O_2 transfer rate, enhancing the opportunities for complete VOC mineralization [5,6]. Thus, the VOC biodegradation performance in TPPBs is often superior to that recorded in conventional biological gas treatment systems [7,8].

Modeling of TPPBs is a research field that has rapidly evolved, bringing key insights on the mechanisms underlying VOC biodegradation and identifying relevant experimental research niches for the optimization of this technology platform. For instance, Cruickshank et al. [9] described the strong impact of O_2 limitation on the performance of TPPBs by means of a comprehensive mathematical model. The key role of the biological kinetic parameters (particularly the VOC half-saturation constant K_S) on the performance of TPPBs was anticipated by the mathematical description proposed by Fazaelipoor [10]. Likewise, the occurrence of a direct VOC uptake in the NAP was early proposed in the mathematical description of the benzene vapor removal in TPPBs by Nielsen et al. [11,12]. The impact of the NAP addition on the VOC absorption in TPPBs has been better understood from the modeling approach of Dumont et al. [13,14]. Mechanistic models for TPPBs using solid NAPs are also available in the literature [15]. However, although such models can give useful information they cannot be directly applied to TPPBs using liquid NAPs.

The increased pace of experimental studies in TPPBs conducted in the past 10 years has significantly expanded our understanding of the complex mass transfer phenomena and substrate uptake mechanisms, which constitute the fundamental processes governing the performance of these multiphase systems [5,8]. Recent experimental findings confirmed the direct VOC uptake from liquid NAPs in some instances, opening new possibilities for the development of high-performance TPPBs [16,17]. Moreover, the quantification of simultaneous mass transfer pathways established in TPPBs has been recently reported for O_2 by determining partial mass transfer coefficients [18]. However, this fundamental knowledge recently gained in microbiology and mass transfer aspects has not been incorporated yet in a comprehensive mathematical description of TPPBs.

In this work, a novel mathematical description of TPPBs accounting for the last experimental findings reported in the literature was proposed. A comprehensive description of the complex mass transfer phenomena occurring simultaneously in TPPBs was done by means of partial mass transfer coefficients for both VOC and O_2. The model also features potential VOC/O_2 uptake in the NAP and continuous aqueous phase renewal (usually done to avoid nutrients limitations and remove inhibitory metabolites). Finally, the results obtained from a sensitivity analysis and model simulations were compared with recent experimental data, critical research niches being identified and discussed.

2. Mathematical model

2.1. Two-phase partitioning bioreactor

The TPPB considered in this work was a standard stirred tank reactor operated with silicone oil as a NAP. Silicone oil was selected since it is the most investigated NAP in TPPBs devoted to air pollution control [1,5]. In addition, silicone oil is, to the best of our knowledge, the only liquid NAP so far reported that is fully biocompatible, water immiscible and non-biodegradable [19,20]. The gas phase consisted of an air stream laden with a single VOC continuously introduced to the reactor, while the aqueous phase consisted of a diluted nutrients solution renewed at a constant flow rate. The mathematical model was based on the following parameters: liquid phase composition, gas and water flow rates, VOC and O_2 concentrations (in gas, NAP and water), VOC and O_2 partition between phases, mass transfer coefficients between phases and kinetics of microbial growth. A constant temperature of 25 °C was considered for model simulations (the kinetic, mass transfer and partition coefficients used were obtained at this temperature).

2.2. Model assumptions

The following key assumptions were made in order to provide a standardized modeling framework: (i) the TPPB was operated under complete mixing conditions; (ii) the microbial kinetic parameters remained the same regardless of the liquid phase the microorganisms grow; (iii) the specific microbial decay rate accounted for 10% of the maximum specific growth rate [21]; (iv) the gas holdup was assumed to remain at 10% relative to the total working volume regardless of the NAP percentage [22,23]; and (v) the TPPB performance was not affected by the dynamic viscosity of the NAP at oil percentages ranging 10–20% (the hydrodynamic conditions were not taken into account in the model).

2.3. Model equations

The mathematical model was based on mass balances for biomass in both NAP and aqueous phase as well as on mass balances for VOC and O_2 in the gas, NAP and aqueous phase. A double Monod-type equation was used to describe the specific microbial growth rate in both the aqueous phase (μ_W) and the NAP (μ_{NAP}) in order to account for the effect of O_2 limitations:

$$\mu_W = \mu_{max}\left(\frac{C_W}{K_S + C_W}\right)\left(\frac{O_{2W}}{K_O + O_{2W}}\right) - \mu_d \quad (1)$$

$$\mu_{NAP} = \mu_{max}\left(\frac{C_{NAP}}{K_S + C_{NAP}}\right)\left(\frac{O_{2NAP}}{K_O + O_{2NAP}}\right) - \mu_d \quad (2)$$

Substrate inhibition was not considered in the present work since TPPBs are mainly used for the removal of very hydrophobic VOCs at low loading rates (conditions commonly resulting in mass transfer limitations). However, inhibition can be easily incorporated in the model by using a Haldane–Andrews type kinetics.

The balance for biomass in the aqueous phase was described by:

$$\frac{dX_W}{dt} = \left[\mu_{max}\left(\frac{C_W}{K_S + C_W}\right)\left(\frac{O_{2W}}{K_O + O_{2W}}\right) - \mu_d\right]X_W - \frac{Q}{(1 - \phi_{NAP} - \phi_G)V_T}X_W \quad (3)$$

Likewise, the balance for biomass in the NAP was described as:

$$\frac{dX_{NAP}}{dt} = \left[\mu_{max}\left(\frac{C_{NAP}}{K_S + C_{NAP}}\right)\left(\frac{O_{2NAP}}{K_O + O_{2NAP}}\right) - \mu_d\right]X_{NAP} - \frac{Q_N}{(1 - \phi_W - \phi_G)V_T}X_{NAP} \quad (4)$$

The aqueous phase and the NAP can be continuously renewed to provide nutrients, remove potentially inhibitory metabolites and avoid excessive biomass accumulation. However, in the studies used for validating the model of the present work any author indicates NAP renovation due to the relative short length of the experiments (shorter than 3 months). To the best of our knowledge, none of the TPPBs operated as stirred tanks reported planned or uncontrolled losses of NAP. Accordingly, the purge term for the NAP was simplified ($Q_N = 0$) for these specific cases.

The need for water renewal during VOC removal in TPPBs has been consistently pointed out by several authors [16,17,24]. On the other hand, the mass balance for VOC in the gas phase was described as follows:

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