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Modeling of VOC mass transfer in two-liquid phase stirred tank, biotrickling filter and airlift reactors

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ABSTRACT

A modeling framework based on general mass balances and transfer equations was here developed in order to compare the hexane mass transfer performance of two-liquid phase stirred tank reactor (STR), airlift (ALR) and biotrickling filter (BTF) using silicone oil as model non-aqueous phase under abiotic conditions. This modeling approach resulted in an isomorphous expression for all configurations consisting of a parameter β_s^* (characterizing the maximum fraction of VOC transferable from the gas to the aqueous phase) and the gradient established between the gas and the aqueous phase. The models were validated against experimental data (at empty bed residence times, EBRT, of 120, 60 and 40 s) exhibiting an overall goodness of fit of 0.98, 0.98 and 0.70 for the two-liquid phase STR, BTF and ALR, respectively. The two-liquid phase BTF exhibited the maximum value of β_s^* (0.87–0.58), followed by the STR (0.77–0.49) and the ALR (0.23–0.19). Finally, a sensitivity analysis conducted in the two-liquid phase BTF showed that β_s^* was more sensitive to changes in recirculating liquid flow rate than in the EBRT, confirming that the liquid flow rate is a key operational variable in BTF systems.

1. Introduction

Two-phase partitioning bioreactors (TPPBs) are based on the addition of a non-aqueous phase (NAP) to a biological process in order to overcome a limited transfer of gaseous substrates to the aqueous phase [1]. Hence, TPPBs have been widely used for the treatment of hydrophobic volatile organic compounds (VOCs) like hexane, methane, styrene, sulfides, and ethene [2–6]. TPPBs also constitute a robust and reliable technology in wastewater and soil treatment applications [7]. In addition, TPPBs appear to have a great potential for enhancing the productivity in fermentation technology [8]. This NAP exhibits a high affinity for the target VOC and creates a new transfer pathway from the gas phase to the NAP, and then from the NAP to the aqueous phase [9]. A higher overall concentration gradient is thus established, which increases the driving force for VOC transfer to the aqueous phase [10]. The presence of a NAP can also improve the transfer of VOCs by increasing the gaseous interfacial area, which leads to a higher mass transfer coefficient [11].

TPPBs devoted to the biodegradation of hydrophobic VOCs have been implemented with a wide number of NAPs and in several bioreactor configurations [2,12,13]. Studies comparing the performance of several NAPs in the same TPPB configuration can be found in literature and allow for an optimized selection of the NAP. For instance, Muñoz et al. [14] compared the performance of heptamethylnonane and the perfluorocarbon FC40 for the degradation of α-pinene in a stirred tank reactor (STR), while Aldric et al. [15] studied the performance of silicone oils of diverse viscosity in the transfer of isopropylbenzene and oxygen in a STR. However, despite the fact that TPPBs have been implemented in configurations such as STR, biofilters, biotrickling filters (BTFs) and airlifts (ALRs), there are no systematic studies comparing their mass transfer capacity under similar operating conditions. These studies are of paramount importance since the reactor configuration directly impacts on the energy requirements of the process [13,16], which has been identified as a major limitation for TPPBs scale-up [16].

The aim of this work was to systematically compare the VOC transfer performance of a two-phase STR, ALR and BTF using hexane and silicone oil (liquid NAP) as model hydrophobic VOC and NAP, respectively, under abiotic conditions. When a liquid NAP is used, TPPBs are specifically called two-liquid phase systems (TLPSs). A mathematical model capable of accurately describing the hexane mass transfer from the gas phase was developed for each reactor configuration. A parameter characterizing the maximum fraction of VOC transferred from the contaminated gas stream to the aqueous phase (β_s^*) was obtained and used to assess the mass transfer capacity of the reactors evaluated.

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Nomenclature

a	interfacial area between the gas bubbles and the liquid phase (water or NAP + water) per unit of volume (m^{-1})
A_b	bubble surface (m^2)
C_g	VOC concentration in the gas phase ($kg\,m^{-3}$)
C_{NAP}	Bulk VOC concentration in the non-aqueous phase ($kg\,m^{-3}$)
C_{gb}^{in}	VOC concentration in the bubble at $z = 0$ in the stirred tank reactor ($kg\,m^{-3}$)
C_g^{in}	VOC concentration in the gas phase at the inlet of the reactor ($kg\,m^{-3}$)
C_{gb}^{out}	VOC concentration in the bubble at $z = Z$ in the stirred tank reactor ($kg\,m^{-3}$)
C_g^{out}	VOC concentration in the gas phase at the outlet of the reactor ($kg\,m^{-3}$)
C_w	bulk VOC concentration in the aqueous phase ($kg\,m^{-3}$)
C_w^{in}	VOC concentration in the aqueous phase at the inlet of the ALR ($z = 0$) and BTF ($z = Z$) ($kg\,m^{-3}$)
C_w^{out}	VOC concentration in the aqueous phase at the outlet of the BTF ($z = 0$) ($kg\,m^{-3}$)
EBRT	empty bed residence time
H	gas hold-up in the stirred tank reactor (dimensionless)
k_{lNAP}	individual VOC mass transfer coefficient at the NAP through the gas–NAP interphase ($m\,s^{-1}$)
k_{lw}	individual VOC mass transfer coefficient at the water phase through the gas–water interphase ($m\,s^{-1}$)
m_{ef}	effective Henry constant for de VOC in the aqueous phase (dimensionless)
m_{NAP}	Henry constant for the VOC in the NAP (dimensionless)
m_w	Henry constant for the VOC in water (dimensionless)
Q_g	gas flow rate ($m^3\,s^{-1}$)
Q_L	total liquid flow rate in the BTF ($m^3\,s^{-1}$)
R	volumetric VOC transfer rate ($kg\,m^{-3}\,s^{-1}$)
R_{max}	maximum volumetric VOC transfer rate ($kg\,m^{-3}\,s^{-1}$)
R_β^2	correlation coefficient of β_s^* determination (dimensionless)
R_M^2	goodness of fit of the models (dimensionless)
S	packed column section of the BTF (m^2)
t	time (s)
t_b	bubble residence time (s)
u_g	superficial gas velocity in the riser ($m\,s^{-1}$)
u_L	superficial total liquid velocity in the riser ($m\,s^{-1}$)
V_b	bubble volume (m^3)
V_c	packed column volume of the BTF (m^3)
V_g	total gas volume (m^3)
V_L	total liquid volume (m^3)
V_r	total reactor volume (m^3)
Z	height of the gas–liquid dispersion of the STR, the riser of the ALR and the packed column of the BTF (m)
β_s^*	maximum VOC fraction transferred from the gas to the aqueous phase including the VOC transferred through the organic phase (dimensionless)
β_s'	maximum VOC fraction transferred from the gas to both liquid phases (NAP + water) (dimensionless)
ξ	lumped parameter with units of concentration ($kg\,m^{-3}$)
η	lumped parameter with units of an individual mass transfer coefficient ($m\,s^{-1}$)
ϕ_o	volumetric fraction of the organic phase (dimensionless)
ϕ_w	volumetric fraction of the water phase (dimensionless)
E	dimensionless parameter
ω	dimensionless parameter
ν	dimensionless parameter
Σ	dimensionless coefficient
Ω	dimensionless coefficient
Γ	dimensionless coefficient

2. Theoretical framework

In this section, the equations describing the VOC transfer from the gas to the liquid phase in each reactor configuration operated with a single water phase are developed. Then, the equations are adapted to TLPSs.

2.1. Single-phase systems

2.1.1. Single-phase stirred tank reactor

A stirred tank reactor contains a well mixed liquid phase with gas bubbles rising (Fig. 1a). These bubbles have a constant volume (V_b) and surface (A_b) when the transferred compound has a low gas molar fraction (as it is the case for VOC-laden air streams) and the pressure difference between the top and the bottom of the tank is negligible. The VOC mass flow from a bubble to the liquid phase is proportional to the bubble's area and the concentration gradient:

$$V_b \frac{dC_g}{dt} = -k_{lw} A_b \left(\frac{C_g}{m_w} - C_w \right) \quad (1)$$

where m_w and k_{lw} are the dimensionless Henry's constant in water and the liquid mass transfer coefficient, respectively; while C_g and C_w represent the VOC concentration in the gas and the water phase, respectively. The ratio A_b/V_b (contact area per unit of gas volume) can be expressed as the ratio between the specific area (a, contact area per reactor volume) and the gas hold-up in the stirred tank ($H = V_g/V_r$), where the volume of reactor, V_r, equals the sum of the total volume of gas phase in contact with the liquid phase, V_g, and liquid phase, V_L. The previous mass balance can be thus rewritten as follows:

$$\frac{dC_g}{dt} = -k_{lw} \frac{a}{H} \left(\frac{C_g}{m_w} - C_w \right) \quad (2)$$

The previous equation can be integrated between $t = 0$ and the residence time of the bubbles in the reactor (t_b).

$$\ln \left(\frac{C_{gb}^{out} - m_w C_w}{C_{gb}^{in} - m_w C_w} \right) = -k_{lw} \frac{a}{m_w H} t_b \quad (3)$$

where C_{gb}^{in} and C_{gb}^{out} are the initial and the final VOC concentration in the rising gas bubbles, respectively.

On the other hand, t_b can also be defined as the ratio between V_g and the total gas flow (Q_g), and based on the fact that V_g is equal to HV_r, t_b can be expressed as:

$$t_b = \frac{HV_r}{Q_g} \quad (4)$$