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ECT imaging and CFD simulation of different cyclic modulation strategies for the catalytic abatement of hazardous liquid pollutants in trickle-bed reactors

Rodrigo J.G. Lopes [a,*], Rosa M. Quinta-Ferreira [a], F. Larachi [b]

[a] Centro de Investigação em Engenharia dos Processos Químicos e Produtos da Floresta (CIEPQPF), GERSE – Group on Environmental, Reaction and Separation Engineering, Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Polo II – Pinhal de Marrocos, 3030-790 Coimbra, Portugal

[b] Department of Chemical Engineering, Laval University, Québec, QC, Canada G1V 0A6

HIGHLIGHTS

- ▶ Various cyclic-based modes in TBR were investigated for liquid pollutant removal.
- ▶ ON–OFF liquid, ON–OFF gas, and gas/liquid alternating promoted TOC conversion.
- ▶ ECT flow patterns underlined the liquid pulsation intensity and cycle frequency.
- ▶ CFD mappings of interstitial flow replicated accordingly the ECT measurements.

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ABSTRACT

Aiming to accomplish stringent regulations for the secure disposal of hazardous compounds, trickle beds have been envisaged from a process intensification point of view to adhere to environmental guidelines. In this work, several experimental and computational runs were performed under reacting flow conditions and cyclic (flow rate) modulations for the mineralization of liquid pollutants through electrical capacitance tomography (ECT) and computational fluid dynamics (CFD) techniques, respectively. First, we have investigated the hydrodynamics of propagating liquid pulsations generated via ON–OFF liquid, ON–OFF gas, and gas/liquid alternating cyclic operations. Here, the liquid pulsation intensity generated in ON–OFF gas mode indicated a negligible dependence with respect to cycle frequency apart from being qualitatively analogous with respect to ON–OFF liquid mode. Second, the effect of oxidation temperature and the gas and liquid flow rates unveiled the gas/liquid alternating mode as being able to generate sizable liquid payloads interrupted by gas and liquid streams. Correspondingly, we found higher detoxification rates due to the periodic pulsations sustained down to the reactor outlet by conferring improved catalyst wetting efficiencies. Finally, two-dimensional mappings of different cross-sections allowed inferring by means of ECT and CFD how the liquid payloads were morphologically in disposition to preserve or dissipate their original structure.

1. Introduction

Aiming to realize the maximum benefit and the highest volumetric productivity for a target value-added product, process intensification has been tackled with innovative experimental and theoretical techniques. The contemporary methodology encompasses the minimization of raw material and energy resources utilization and waste production. In the realm of multiphase reaction engineering, this fact is partly ascribed to the novel operating windows that can be attained within fluidized beds, bubble columns, and trickle-bed reactors (TBRs). The ubiquitous applications of trickle beds can vary from high throughput production as in raw materials' conversions in the petroleum industry and hydroprocessing to the environmental detoxification in biochemical and agro-processing manufacturing industries [1].

Pulsing flow in trickle beds has been ascertained to improve heat and mass transfer rates, thereby increasing the overall conversion and throughput. According to the open literature, the growing number of publications devoted to biochemical processes as well as advanced oxidation processes has foreseen TBRs for the sustainable catalytic mineralization of wastewaters and gas streams polluted with hazardous organic compounds [2]. Bearing in mind the multitude of potential hydrodynamic states, literature studies have predominantly addressed trickle and pulse flow regimes in view of the fact that these contacting patterns are typically accomplished in commercial-scale trickle beds. Our case study aligns with the

* Corresponding author. Tel.: +351 239798758.
E-mail address: rodrigo@eq.uc.pt (R.J.G. Lopes).

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