



## Removal of chlorinated organic volatile compounds by gas phase adsorption with activated carbon

Jesus Lemus, M. Martin-Martinez, Jose Palomar<sup>\*</sup>, Luisa Gomez-Sainero, Miguel Angel Gilarranz, Juan J. Rodriguez

Sección de Ingeniería Química, Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain

### HIGHLIGHTS

- ▶ Chloromethanes were removed from gas streams by adsorption with commercial activated carbons (ACs).
- ▶ Fixed-bed experiments were performed to obtain thermodynamic and kinetic parameters.
- ▶ Efficient regeneration of exhausted adsorbent was achieved at mild conditions.
- ▶ The influence of AC chemical surface on the process was theoretically and experimentally analyzed.

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### ABSTRACT

This paper discusses the removal of chlorinated volatile organic compounds (Cl-VOCs) from gas streams by means of fixed-bed adsorption with a commercial activated carbon (AC). Column experiments were performed at different conditions (inlet concentration, temperature, pressure, gas flow rate and bed length). A two-parameter model introduced by Yoon and Nelson was applied to predict the entire breakthrough curves for chloromethane adsorption. Complete regeneration of the exhausted AC was performed at mild conditions (atmospheric pressure and room temperature). In order to gain a better knowledge on the effect of the surface chemistry of AC on the adsorption of Cl-VOCs, the quantum-chemical COSMO-RS method was used to simulate the interactions between AC surface groups and different Cl-VOCs as monochloromethane, dichloromethane and trichloromethane. This information can be useful for tailoring the ACs with the objective of improving their adsorption capacities by further functionalization. To confirm this, the commercial AC tested was modified by means of different thermal and oxidative treatments (nitric acid and ammonium persulfate), being the surface chemistry and textural properties of the resulting materials characterized by different techniques. The modified ACs were then tested in column adsorption experiment with different Cl-VOCs. The uptake of these compounds increased with the basic character of the AC surface.

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### 1. Introduction

Chlorinated volatile organic compounds (Cl-VOCs) play an important role in the chemical and pharmaceutical industries, where they are used as solvents and reagents. They are also employed in aerosols, adhesives, dry cleaning, etc. [1] Cl-VOCs are mainly regarded as xenobiotics, resistant to biodegradation and, hence, persistent in the environment. Most of them are toxic or carcinogenic and present potential hazard under exposure [2]. Therefore, Cl-VOCs are classified nowadays as hazardous gas pollutants and were included in the list of the seventeen highly harmful chemicals targeted in the emissions reduction effort of the U.S.

Environmental Protection Agency [3,4]. Emissions of these compounds to the atmosphere contribute to the destruction of the ozone layer, to the formation of photochemical smog and to global warming. Hence, they are restricted by strong legal regulations. This enforces the need of developing effective technologies for the treatment of residual streams contaminated with Cl-VOCs. This paper will focus in three of the most common chlorinated compounds in off gases: monochloromethane (MCM), dichloromethane (DCM) and chloroform (TCM), which are associated to a number of industrial processes.

Nowadays, the main technique for the removal of these pollutants is incineration, but it may lead to more hazardous byproducts than the original contaminants, such as phosgene, dioxins and furans [5,6]. On the other hand, at low Cl-VOCs concentration the use of catalysts is required for reducing the thermal needs [7,8]. Thus,

<sup>\*</sup> Corresponding author. Tel.: +34 91 4976938; fax: +34 91 4973516.

E-mail address: [pepe.palomar@uam.es](mailto:pepe.palomar@uam.es) (J. Palomar).