

## Chemical Warfare Agent Simulant by Photocatalytic Filtering Reactor: Effect of Operating Parameters

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**Abstract :** Throughout history, the use of chemical weapons is not exclusive to combats between army corps; some of these weapons are also found in very targeted intelligence operations (political assassinations), organized crime, and terrorist organizations. To improve the speed of action, important technological devices have been developed in recent years, in particular in the field of protection and decontamination techniques to better protect and neutralize a chemical threat. In order to assess certain protective, decontaminating technologies or to improve medical countermeasures, tests must be conducted. In view of the great toxicity of toxic chemical agents from (real) wars, simulants can be used, chosen according to the desired application. Here, we present an investigation about using a photocatalytic filtering reactor (PFR) for highly contaminated environments containing diethyl sulfide (DES). This target pollutant is used as a simulant of CWA, namely of Yperite (Mustard Gas). The influence of the inlet concentration (until high concentrations of DES (1200 ppmv, i.e., 5 g/m<sup>3</sup> of air) has been studied. Also, the conversion rate was monitored under different relative humidity and different flow rates (respiratory flow - standards: ISO / DIS 8996 and NF EN 14387 + A1). In order to understand the efficacy of pollutant neutralization by PFR, a kinetic model based on the Langmuir-Hinshelwood (L-H) approach and taking into account the mass transfer step was developed. This allows us to determine the adsorption and kinetic degradation constants with no influence of mass transfer. The obtained results confirm that this small configuration of reactor presents an extremely promising way for the use of photocatalysis for treatment to deal with highly contaminated environments containing real chemical warfare agents. Also, they can give birth to an individual protection device (an autonomous cartridge for a gas mask).

**Keywords :** photocatalysis, photocatalytic filtering reactor, diethylsulfide, chemical warfare agents

**Conference Title :** ICCWCW 2021 : International Conference on Chemical Warfare and Chemical Weapons

**Conference Location :** Helsinki, Finland

**Conference Dates :** July 19-20, 2021