

THEORETICAL AND PRACTICAL COMPARATIVE STUDY ON THE USE OF CLAYS FOR THE TREATMENT OF WASTEWATER CONTAMINATED WITH PESTICIDES

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ABSTRACT

The purpose of this study is to compare the theoretical results which are calculated according to the DFT model, DFT calculations were performed using the code DMol3. To optimize the geometry, the triple numerical set plus the polarization base (TNP) was used. It was also used in combination with the M11L function within the generalized meta gradient (GGA) approximation. The solvent effect (H₂O) was incorporated through the conductor-like display model (COSMO). To visualize the adsorption geometry of the two selected adsorbents, namely: benalaxyl and atrazine on the surface of the clay material components, Monte Carlo (MC) simulation was performed, which was performed through the Adsorption Locator module as implemented in the Materials Studio software. 2017. Three types of clay minerals were selected for the simulation: Halloysite (a = 14,220 Å, b = 26,700 Å, c = 19,557 Å, AMCSD: 0018093), Kaolinite (a = 25,958 Å, b = 12,950 Å, c = 17,034 Å, AMCSD: 0002868) and Montmorillonite (a = 25,454 Å, b = 13,022, c = 40,427, AMCSD: 0002868). The selected separation plane is based on morphological calculations using the Bravais-Friedel-Donnay-Harker (BFDH) methodology. Achieved results in the experimental aspect realized with the methods: SEM -EDX VEGA3 LMU; Fluorescence Spectrometer X-Ray (XRF), ARL 9900 and GCMS-QP2010S, in relation to the adsorption of Atrazine and Benalaxyl on natural and activated Bray and Pear clays are in full agreement with the theoretical calculations.

Keywords: benalaxyl, atrazine, clay, brari, dardha, monte carlo.