On the mechanism of benzene and toluene adsorption in single-compound and binary systems: energetic interactions and competitive effects

A. Erto\textsuperscript{a,}\textsuperscript{*}, S. Chianese\textsuperscript{b}, A. Lancia\textsuperscript{a}, D. Musmarra\textsuperscript{b}

\textsuperscript{a}Università degli Studi di Napoli Federico II, Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, P.le Tecchio 80, 80125, Napoli, Italy, Tel. +39 081 7682236; Fax: +39 081 5936936; emails: aleserto@unina.it (A. Erto), lancia@unina.it (A. Lancia)

\textsuperscript{b}Università degli Studi della Campania Luigi Vanvitelli, Dipartimento di Ingegneria Civile, Design, Edilizia e Ambiente, Via Roma 29, 81031, Aversa (CE), Italy, email: simeone.chianese@unicampania.it (S. Chianese), dino.musmarra@unicampania.it (D. Musmarra)

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\textbf{ABSTRACT}

This work reports an experimental and modelling analysis of benzene/toluene adsorption from model groundwater on a commercial activated carbon in single-compound and binary systems. Single-compound results show that toluene is more adsorbed than benzene and an increase in its adsorption capacity gives rise to lateral interactions between the adsorbed molecules. This is likely to be due to the presence of electron-donor methyl groups in the toluene molecule, which determines an increase in the electronegativity of the aromatic ring and, consequently, stronger attractions with the nucleophilic basal plane of activated carbon. Binary results indicate that toluene has the highest adsorption capacity, but some competitive effects arise for both the analytes. A modelling analysis of the binary system shows that the ideal adsorbed solution theory model can provide a very good prediction of adsorption data for both compounds, over the whole range of concentration investigated.

\textit{Keywords:} Groundwater; Benzene; Toluene; Competitive adsorption; Ideal adsorbed solution theory