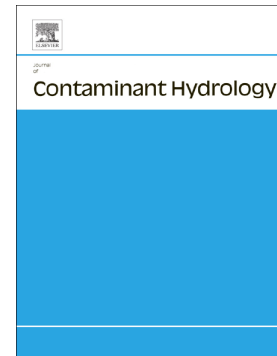


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# Dissolution kinetics of volatile organic compound vapors in water: an integrated experimental and computational study

Mojtaba G. Mahmoodlu<sup>a,b,\*</sup>, Elizabeth. M. Pontedeiro<sup>a,c</sup>, Jesús S. Pérez Guerrero<sup>d</sup>, Amir Raouf<sup>a</sup>,  
S. Majid Hassanizadeh<sup>a</sup>, and Martinus Th. van Genuchten<sup>a,f</sup>

<sup>a</sup>Department of Earth Sciences, Utrecht University, Utrecht, The Netherlands

<sup>b</sup>Department of Watershed and Rangeland Management, Gonbad Kavous University, Iran

<sup>c</sup>Department of Nuclear Engineering, Federal University of Rio de Janeiro, UFRJ, Rio de Janeiro, Brazil

<sup>d</sup>Radioactive Waste Division, Brazilian Nuclear Energy Commission, CNEN, Rio de Janeiro, Brazil

<sup>f</sup>NIDES Interdisciplinary Centre for Social Development, Federal University of Rio de Janeiro, UFRJ, Rio de Janeiro, Brazil

## Abstract

In this study we performed batch experiments to investigate the dissolution kinetics of trichloroethylene (TCE) and toluene vapors in water at room temperature and atmospheric pressure. The batch systems consisted of a water reservoir and a connected headspace, the latter containing a small glass cylinder filled with pure volatile organic compound (VOC). Results showed that air phase concentrations of both TCE and toluene increased relatively quickly to their maximum values and then became constant. We considered subsequent dissolution into both stirred and unstirred water reservoirs. Results of the stirred experiments showed a quick increase in the VOC concentrations with time up to their solubility limit in water. VOC vapor dissolution was found to be independent of pH. In contrast, salinity had a significant effect on the solubility of TCE and toluene vapors. VOC evaporation and vapor dissolution in the stirred water reservoirs followed first-order rate processes. Observed data could be described well using both simplified analytical solutions, which decoupled the VOC dynamics in the air and water phases, as well as using completely coupled solutions. However, the estimated evaporation ( $k^e$ )

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\* Corresponding author. Tel: +31302535024; Fax: +3130 2534900. E-mail address: m.gharehmahmoodlu@uu.nl / m.g.mahmoodlu@gmail.com

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