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Advances in Fundamental Materials Research

Approximate Analytical Treatment of Time-evolution of Sessile Droplets to Estimate Diffusivities into Barrier Materials

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Any practical technique to measure diffusivities of toxic industrial chemicals and chemical warfare agents in permeable solids should require handling only miniscule volume of chemicals. This was shown possible in a recent study using sessile drops of about 1 μL volume, wherein the diffusivities were estimated by fitting the contact angle vs time data to finite element numerical simulations of liquid evaporation into air and absorption into the solid. However, these simulations are computationally intensive and prevent the practical use of the sessile drop technique from day to day studies. To overcome this limitation, we develop an approximate analytical approach requiring negligible computational time. The approach is applicable irrespective of whether the basal radius of the sessile drop remains constant or changes during the evaporation/absorption process. The analytical approach is validated by comparing its diffusivity estimates against those from the finite element simulations, for the same experimental contact angle data, for both water and mustard gas (HD) as well as our own experimental data of water on aluminum to validate both the experimental procedure and analytical model. The analytical approach is then applied to three toxic chemicals, tetrachloroethylene, trichloroethylene and acetonitrile, to determine their diffusivities in air and in butyl rubber from captured time evolution of sessile drop profiles. The diffusivities of these chemicals were previously studied using the immersion testing method requiring large volumes of liquid chemicals and detection of small changes in mass of the substrate which leads to greater experimental error. This analytical approach thus makes possible the use of sessile drop technique for measuring diffusivity of toxic substances and aids in the development of new barrier materials (for clothing, face masks, gloves, etc.) to protect against chemical and biological threats.