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# Simulating the Permeation of Hazardous Chemicals through Barrier Materials

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## Extended Abstract

When a hazardous chemical is released, it often requires people to access the area and put themselves at risk of exposure to the hazard to rescue injured people, investigate the release and its impact, or conduct clean-up of the hazardous release. Chemical Weapons are a class of extremely hazardous chemicals that have been deliberately released several times over the last decade in public spaces where toxic releases can, and have, posed hazards to the public long after the initial release. Chemical weapons with low vapour pressures pose a liquid contact hazard to anyone who comes into contact with them and, in order to safely work around them, the use of personal protective equipment (PPE) is required. This PPE must be carefully selected and tested to ensure that anyone using it can balance their ability to work with their safety. A commonly used method to test permeation of Chemical Weapons through protective equipment is to apply droplets of the liquid agent to the surface a sample of the material and quantitatively evaluate for the presence of agent on the other side of the material until breakthrough is detected and use the data to characterize the membrane. Rivin et al. [1] completed work that suggested this method would produce errors in permeability values derived through such testing. In this paper, we used a finite difference method to numerically solve the three-dimensional cylindrical Fick's second law of diffusion for a liquid permeating through a non-porous rubbery membrane to determine the time the permeating species will emerge on the other side of the polymer membrane, such as protective gloves. We simulated various application patterns of the permeating species on the membrane area: droplets, rings, and complete coverage. Simulation of different surface area coverages and geometries of permeate on the membrane indicated that incomplete surface area coverage of the membrane led to errors in the estimation of the transport properties. The magnitude of the estimation error is inversely proportional to the amount of membrane surface covered by the permeate and proportional to the thickness of the membrane. These results suggest that incomplete coverage of membranes in permeation testing leads to error which will underestimate the permeability of the system and make the experimentally determined transport properties unsuitable for predictive use, as a lower permeability would lead to an overestimation of the amount of time it would take contaminants to permeate through the material. We simulated different permeation values to determine if the error was consistent over different permeate-membrane combinations and suggest a method to correct the experimentally determined permeability.