Design and Implementation of the Chemical Warfare Agent Force Field

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In recent months there have been continuing reports of chemical warfare agents (CWAs) being used in conflict situations in Syria.[1] How these chemicals react with the body is well understood, however it is less clear how they interact with porous materials they can encounter in the field, such as sand, brick, soil, etc. Molecular simulations are an ideal way to investigate these highly toxic chemicals at an atomistic level. To this end we present the Chemical Warfare Agent Force Field (CWAFF), which has been parameterised to describe the nerve agents GB, VX, and VM, as well as the vesicant HD.

CWAFF has been used to model agent behaviour in a variety of substrates chosen to mimic chemical functionalities of materials with which the agents could come into contact. In order to obtain a more comprehensive understanding of the sorption and diffusion of CWAs, both organic and inorganic host materials were chosen, with a variety of chemical moieties and pore sizes. CWAFF has been implemented with DL_POLY[2] for molecular dynamics simulations and RASPA[3] for Grand Canonical Monte Carlo simulations.

[1] Associated Press, *The Guardian* https://www.theguardian.com/world/2016/aug/25/assad-regime-isis-chemical-attacks-syria-un-investigators (2016).

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