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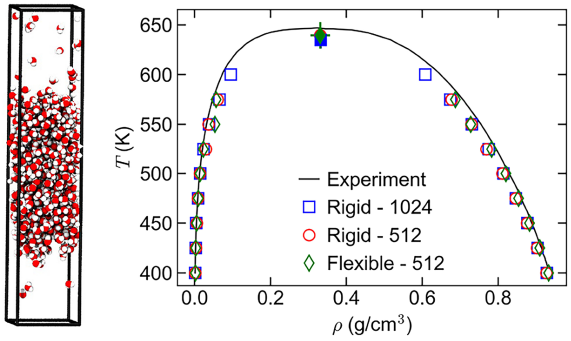
Combining the advanced MB-pol water model with a widely used molecular simulation software allows researchers to better understand how liquid transforms into water vapor and vice versa.



While water has been modeled by computer simulations for over five decades, most models focus on the dense liquid and ice phases and fall short in reproducing vapor-liquid coexistence properties. Muniz et al. use computer simulations to model the vapor-liquid equilibrium (VLE) of water and better understand how liquid transforms into water vapor and vice versa.

The researchers used the advanced MB-pol water model to accurately reproduce water's VLE, even though this model was not directly created for this purpose. This work focused on bulk properties of water, such as density and surface tension, but the simulations provided a picture of molecular-level details of the vapor-liquid interface.

VLE phenomena are present in many applications including domestic ones, such as cooking, and industrial ones, such as distillation and steam turbines used to produce electricity.

The researchers show how an implementation of MB-pol, interfaced with LAMMPS, a widely used molecular simulation software, allowed them to increase the time and length scales accessible using MB-pol and to perform the types of simulations needed to study VLE phenomena.

"The most surprising finding was the quality of the predictions at high temperatures, all the way to the liquid-vapor critical point, for a model that was not optimized to reproduce these properties," said author Athanassios Panagiotopoulos.

While the researchers evaluated MB-pol's VLE for pure water, for industrial applications, predicting the VLE of mixtures is important.

"It may be valuable to evaluate how the MP-pol water model performs in simulations of mixtures or to extend a similar approach to other important substances such as CO2 or methane," said Panagiotopoulos.

Source: "Vapor-liquid equilibrium of water with the MB-pol many-body potential," by Maria Carolina Muniz, Thomas Edward Gartner, Marc Riera, Christopher Knight, Shuwen Yue, Francesco Paesani, and Athanassios Z. Panagiotopoulos, *Journal of Chemical Physics* (2021). The article can be accessed at https://doi.org/10.1063/5.0050068.