

THERMODYNAMICS OF FLUIDS UNDER CONFINEMENT

Molecular models, structure
and physical property predictions

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Abstract: The structure and physical properties of fluids under confinement are significantly different compared to the structure and properties in bulk. Confined fluids are found in applications in chemical engineering and petroleum engineering (i.e., hydrocarbon fluids in geological formations). Molecular simulation using realistic force fields to account for fluid – fluid and fluid – confinement interactions provide valuable information regarding thermodynamic and transport properties over a broad range of temperature, pressure and composition, without any parameter adjustment to experimental data. Examples of direct industrial relevance are discussed.

Dr. Ioannis G. Economou is the Associate Dean for Academic Affairs and Professor of Chemical Engineering at Texas A&M University at Qatar. He worked as a post-doctoral researcher in Delft University of Technology - Netherlands (1993–94); in Exxon Research and Engineering Company - New Jersey, USA (1994–95); research fellow in University College London (1994–96) and Princeton University (2004–15); visiting Professor in the Technical University of Denmark (2001, 2007) and the American College of Greece (2007–09). He consulted extensively for major oil and chemical companies in North America, Europe and Middle East. He published more than 170 peer-reviewed research papers in leading journals in Chemical Engineering, Physical Chemistry and Polymer Science.