Heriot-Watt Distinguished Lecture

Molecular Modeling and Simulation: Their Role in Applied Sciences & Engineering

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Theory and modeling methods can be classified according to the length and time scales for which they are appropriate: (a) the electronic scale (matter made up of fundamental particles), where the behavior is described by quantum mechanics; (b) the atomistic scale (matter composed of atoms), obeying the laws of statistical mechanics; (c) the meso-scale level (matter composed of 'blobs of matter'); and (d) the continuum level (matter is a continuum), with behavior obeying the well known macroscopic laws of experience. These different approaches will be discussed briefly, outlining their basis, areas of application, and limitations. The atomistic methods of Monte Carlo and Molecular Dynamics simulation will then be discussed in more detail. These solve the equations of statistical mechanics numerically, and can be applied to complex systems of industrial interest. Following this introduction, I will discuss several examples of application of these methods to problems that are relevant to the oil & gas, chemical, and pharmaceutical industries, including:

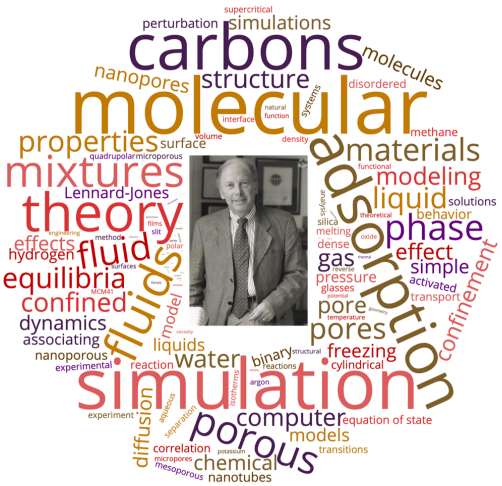
(1) the prediction of phase equilibria for complex mixtures, needed for oil & gas field operations, refining and chemical separations, and
(2) effects of confinement in a porous material on diffusion, phase separation and selective separations, needed for materials characterization, adsorption equipment operation, energy storage, discovery of new porous materials.

Finally, the current and future prospects for these methods will be discussed in the light of rapid advances in computational power and improved algorithms.

11 AM on Friday, May 19th, 2023

James Watt Centre 2 Hall**, Heriot-Watt University Edinburgh Campus

Tea, coffee, refreshments preceding lecture at 10:15 AM



About the speaker: Through his prolific research career (with over 600 publications cited 50,000 times with h-index 102) and seminal contributions in molecular theory (in particular, the statistical associating fluid theory, SAFT, now used throughout the world and in several leading process simulators) and molecular simulation applied to molecular fluids, interfaces, nano- and micro-porous materials, Keith Gubbins has pioneered the use of such techniques to solve outstanding problems of enduring chemical engineering interest (in particular phase equilibria and adsorption). His books have been field-altering, from the early, ahead-of-its-time "Applied Statistical Mechanics" co-written with his Florida colleague, the late Tim Reed, to the two-volume 1400-page encyclopedic treatise with collaborator Chris Gray on "Theory of Molecular Fluids" that is literally the bible on molecular theory and its applications. He has influenced, and provided intellectual leadership to, generations of chemical engineers working on applying molecular simulation and theory.

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