Illustrating Molecular-Level Phenomena and Molecular Simulation Techniques with Commonly Used Software

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Motivation

- Many grand challenges facing chemical engineers today involve molecular-level chemistry
- Having an appreciation for molecular-level phenomena will better prepare chemical engineers to handle problems in energy, water, food, catalysis, advanced materials, and other fields
- A major impediment to teaching and learning about molecular-level phenomena is the learning curve associated with molecular simulation software
- The goal of this work is to demonstrate molecular phenomena and simulation techniques using straightforward graphical user interfaces and familiar software
- Specifically, we focus on conceptual aspects of molecular-level chemical engineering, including students’ abilities to connect molecular-level phenomena with observable properties

Example Assignment #1: WebMO/Quantum Chemical Calculations/Intermolecular Forces

Objectives:
- Improve students’ understanding of how pairs of molecules interact during intermolecular interactions
- Improve students’ perceptions of quantum chemistry software

Students use WebMO, which uses an online graphical user interface, to set up and submit molecular simulations. WebMO was created by William F. Polk and Jordan R. Schmidt at Hope College. Anyone in the world can run WebMO with just an Internet connection.

Example Assignment #2: Excel/Monte Carlo/Safety and Risk

Objectives:
- Illustrate how process variables influence process outcomes
- Introduce or re-enforce reaction runaway and chemical reactor safety
- Practice chemical engineering design, particularly the balance between safety and maximizing production rates
- Introduce the method of Monte Carlo using familiar software

Example Assignment #3: MATLAB/Monte Carlo/Temperature Swing Adsorption

Objectives:
- Practice using Monte Carlo for molecular applications, including practicing operating the most important simulation parameters (intermolecular potential, temperature, number of moves, ratio of translate to replace moves)
- Demonstrate how the simulation parameters influence the number of moves required to achieve equilibrium
- Introduce the concepts of temperature swing adsorption and adsorptive separations. Learn how to tune operating conditions to achieve optimal performance for these two applications
- Demonstrate how molecules with different interaction strengths exhibit different adsorptive properties
- Develop an appreciation for how results obtained in a molecular simulation can be transposed to experimental or real world operation (e.g., trends rather than exact values)
- Improve students’ perceptions of and confidence in installing and using MATLAB

Other Available Assignments

- Improve how intermolecular interactions are quantum in nature
- Illustrate physical bonding and the use of the Lennard-Jones potential for modeling physical bonding
- Determine correlations between physical bond strength, Lennard-Jones parameters, and physical properties

All assignments (and more!) are available for public use on Canvas Commons. Search for “chemical engineering”.

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DIAGRAMS CREATED BY RACHEL B. GETMAN, UNIVERSITY OF MINNESOTA

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