367g Integration of Molecular Modeling Concepts in Thermodynamics and Kinetics Courses

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Recent workshops on the "revitalization of chemical engineering" have identified molecular-level modeling and molecular transformations as key focus areas for curriculum development. New materials must be developed over the next several years to bring about this implementation. The integration of molecular modeling in the core curriculum provides students with methods to visualize chemical reactions as they occur at the molecular scale, and introduces them to computational tools that will be important to the future of chemical engineering. We have made extensive use of computational chemistry software in undergraduate thermodynamics and kinetics courses to help connect thermodynamic and rate quantities to molecular-level phenomena. Classroom examples (including visual models and animations of reactants, products, and transition states), homework assignments, and web modules have been developed and used to emphasize molecular transformations concepts. In this presentation, we will provide examples of each of these three components that we have found useful in teaching molecular reaction engineering.