

ASEE (WPI) Faculty Session, March 18<sup>th</sup>, 2006

**Using Software to Bridge the Gap between Fundamental Science and Engineering Applications**

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The methodology for the use of computational software in a graduate-level molecular modelling class is outlined. In many engineering curricula it is difficult to cover all of the fundamental concepts that are required to provide all students with an optimum base for the solution development of new problems and applications. However, by replacing the learning and understanding of fundamental concepts with starting parameters and a list of equations to use as tools, you are limiting the capabilities and potential accomplishments of the students. This trap is easy to fall into since it is nearly impossible to cover all the fundamentals in addition to the applications. Because of this, a chemist or physicist may be able to develop new ideas more readily since their training through education has taught them to derive the equations they are using. Engineers are typically admired for their ingenuity and their creativity, but with a curriculum that does not require them to derive and to consistently ask 'why' and 'from where,' engineers will soon lose these merits of which they are so well known.

Within a graduate-level molecular modelling class, computational software was used as a tool to bridge the gap that exists between fundamental concepts in chemistry to an application in the field of chemical engineering. In the case of reactor design problems in which rate expressions must be known, activation energies and rate constants are given as input parameters for a particular design equation. Since the methods for approximating rate constants are not taught in traditional chemical engineering courses, the development of a rate expression was chosen as one of the main objectives of the modelling course. Developing a rate expression involves many tasks, some of which include the development of a quantum mechanical-based potential energy surface (PES), and the understanding of kinetic tools such as Transition State Theory. Students cannot begin the development of a PES on the first day of class, so the basics of quantum mechanics had to be covered to understand the complicated aspects involved in carrying out this task, with the Gaussian software package serving as the computational tool. After completion of the course, a student can identify a reaction and know exactly the steps required for the development of a high-level theoretical rate prediction.