



Improving Combustion Systems through Modeling

With the rising costs of foreign oil, we need to continually move toward more efficient use of our fuel resources. Understanding the complex chemical reactions involved in combustion can lead to the design of more efficient combustion systems. Researchers at the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) and the University of Alabama, Tuscaloosa (UA) are carrying out quantum chemical calculations using a state-of-the-art parallel computing system to accurately predict thermodynamic information that is vital to understanding complex combustion reactions.

In one of the largest simulations ever brought to bear on this problem, EMSL and UA researchers performed pioneering first-principles calculations needed to predict the heat of formation of octane, a fairly simple molecule that is a key component of gasoline.

This study would not have been possible without the combination of the NWChem software developed by EMSL researchers and the multiple-processor computing resource available in EMSL's Molecular Science Computing Facility (MSCF). For comparison, running the calculation using the best one-processor desktop computer would have required a whopping 3 1/2 years and 2.5 Terabytes of memory.

Instead, the calculation—performed using 1400 parallel processors—took 23 hours to complete and achieved a sustained efficiency of 75%, an astonishing feat when compared to the 5-10% efficiency of most codes. NWChem achieves high efficiency in this computation by taking advantage of efficient algorithms and communication schemas and is ideally suited for massively parallel computers.

This initial benchmark study served two primary purposes—it validated the approach and helped define its limitations. These initial calculations also helped identify the level of theory needed for subsequent efforts to reliably predict the heats of formation of larger alkanes (e.g., the components of diesel fuel) for which there is very little experimental data, and for the heats of formation of key reactive intermediates, such as alkyl and alkoxy radicals, for which no experimental data is available.

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