Modeling of Alkane Oxidation Using Constituents and Species

This methodology is of interest to automobile manufacturers and other gas-turbine engine manufacturers.

NASA's Jet Propulsion Laboratory, Pasadena, California

It is currently not possible to perform simulations of turbulent reactive flows due in particular to complex chemistry, which may contain thousands of reactions and hundreds of species. This complex chemistry results in additional differential equations, making the numerical solution of the equation set computationally prohibitive. Reducing the chemical kinetics mathematical description is one of several important goals in turbulent reactive flow modeling. A chemical kinetics reduction model is proposed for alkane oxidation in air that is based on a parallel methodology to that used in turbulence modeling in the context of the Large Eddy Simulation. The objective of kinetic modeling is to predict the heat release and temperature evolution. This kinetic mechanism is valid over a pressure range from atmospheric to 60 bar, temperatures from 600 K to 2,500 K, and equivalence ratios from 0.125 to 8. This range encompasses diesel, HCCI, and gas-turbine engines, including cold ignition.

A computationally efficient kinetic reduction has been proposed for alkanes that has been illustrated for n-heptane using the LLNL heptane mechanism. This model is consistent with turbulence modeling in that scales were first categorized into either those modeled or those computed as progress variables. Species were identified as being either light or heavy. The heavy species were decomposed into defined 13 constituents, and their total molar density was shown to evolve in a quasi-steady manner. The light species behave either in a quasi-steady or unsteady manner. The modeled scales are the total constituent molar density, N_c, and the molar density of the quasi-steady light species.

The progress variables are the total constituent molar density rate evolution and the molar densities of the unsteady light species. The unsteady equations for the light species contain contributions of the type gain/loss rates from the heavy species that are modeled consistent with the developed mathematical forms for the total constituent molar density rate evolution; indeed, examination of these gain/loss rates shows that they also have a good quasi-steady behavior with a functional form resembling that of the constituent rate. This finding highlights the fact that the fitting technique provides a methodology that can be repeatedly used to obtain an accurate representation of full or skeletal kinetic models.

Assuming success with the modified reduced model, the advantage of the modeling approach is clear. Because this model is based on the N_c rate rather than on that of individual heavy species, even if the number of species increases with increased carbon number in the alkane group, providing that the quasi-steady rate aspect persists, then extension of this model to higher alkanes should be conceptually straightforward, although it remains to be seen if the functional fits would remain valid or would require reconstruction.

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Fabrication of Lanthanum Telluride 14-1-11 Zintl High-Temperature Thermoelectric Couple

This methodology will aid device fabrication for waste energy recovery applications in cars, power plants, and industrial processes and machinery.

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The development of more efficient thermoelectric couple technology capable of operating with high-grade heat sources up to 1,275 K is key to improving the performance of radioisotope thermoelectric generators. Lanthanum telluride $La_{3-x}Te_4$ and 14-1-11 Zintls ($Yb_{14}MnSb_{11}$) have been identified as very promising materials.

The fabrication of advanced high-temperature thermoelectric couples requires the joining of several dissimilar materials, typically including a number of diffusion bonding and brazing steps, to achieve a device capable of operating at elevated temperatures across a large temperature differential (up to 900 K). A thermoelectric couple typically comprises a heat collector/exchanger, metallic interconnects on both hot and cold sides, n-type and p-type conductivity thermoelectric elements, and cold-side hardware to connect to the cold-side heat rejection and provide electrical connections.

Differences in the physical, mechanical, and chemical properties of the materials that make up the thermoelectric couple, especially differences in the coefficients of thermal expansion (CTE), result in undesirable interfacial stresses that can lead to mechanical failure of the device. The problem is further complicated by the fact that the thermoelectric materials under consideration have large CTE values, are brittle, and cracks can propagate through them with minimal resistance.

The inherent challenge of bonding brittle, high-thermal-expansion thermoelectric materials to a hot shoe material